Full wwPDB X-ray Structure Validation Report (i)

Apr 24, 2024 – 01:59 pm BST

PDB ID	:	2VGI
Title	:	HUMAN ERYTHROCYTE PYRUVATE KINASE: R486W MUTANT
Authors	:	Valentini, G.; Chiarelli, L.; Fortin, R.; Dolzan, M.; Galizzi, A.; Abraham, D.J.; Wang, C.; Bianchi, P.; Zanella, A.; Mattevi, A.
Deposited on	:	2007-11-13
Resolution	:	2.87 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

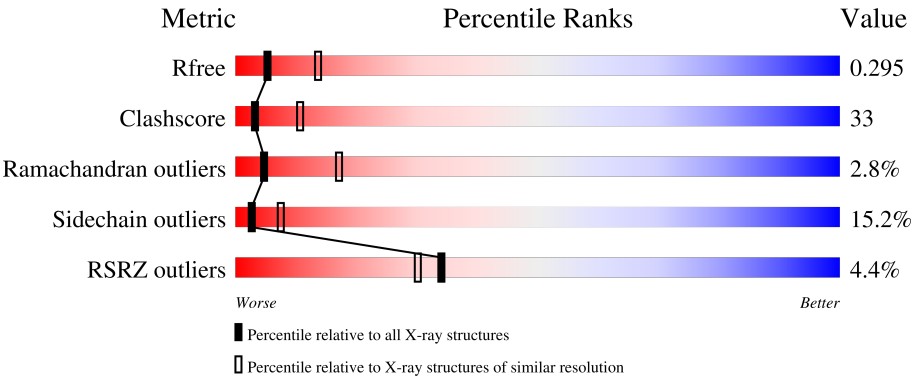
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.87 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	528	3% 41% 42% 13%
1	B	528	6% 42% 36% 9% 12%
1	C	528	4% 41% 46% 9%
1	D	528	3% 48% 39% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PGA	B	1575	-	-	X	-
3	PGA	C	1575	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15342 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

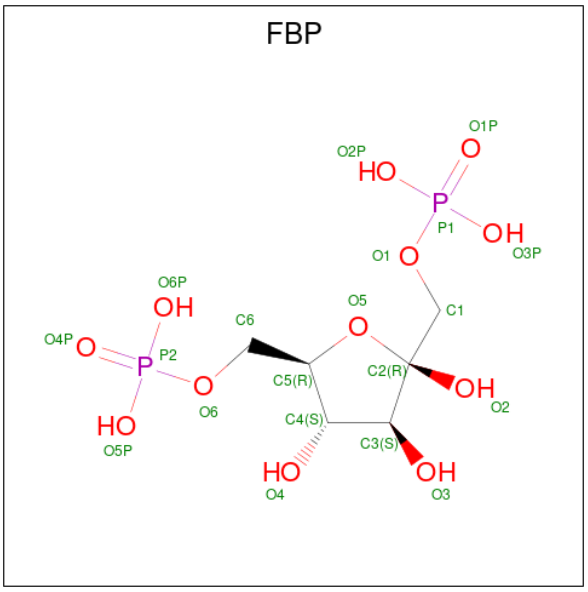
- Molecule 1 is a protein called PYRUVATE KINASE ISOZYMES R/L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	517	Total	C	N	O	S	0	0	0
			3915	2462	707	728	18			
1	B	463	Total	C	N	O	S	0	0	0
			3513	2214	629	652	18			
1	C	515	Total	C	N	O	S	0	0	0
			3899	2452	704	725	18			
1	D	513	Total	C	N	O	S	0	0	0
			3891	2448	702	723	18			

There are 4 discrepancies between the modelled and reference sequences:

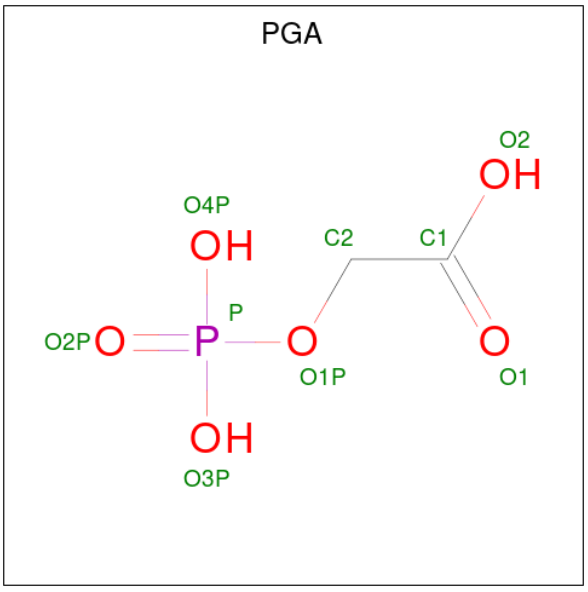
Chain	Residue	Modelled	Actual	Comment	Reference
A	486	TRP	ARG	engineered mutation	UNP P30613
B	486	TRP	ARG	engineered mutation	UNP P30613
C	486	TRP	ARG	engineered mutation	UNP P30613
D	486	TRP	ARG	engineered mutation	UNP P30613

- Molecule 2 is 1,6-di-O-phosphono-beta-D-fructofuranose (three-letter code: FBP) (formula: $C_6H_{14}O_{12}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			20	6	12	2		
2	B	1	Total	C	O	P	0	0
			20	6	12	2		
2	C	1	Total	C	O	P	0	0
			20	6	12	2		
2	D	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 3 is 2-PHOSPHOGLYCOLIC ACID (three-letter code: PGA) (formula: $C_2H_5O_6P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O P 9 2 6 1	0	0
3	B	1	Total C O P 9 2 6 1	0	0
3	C	1	Total C O P 9 2 6 1	0	0
3	D	1	Total C O P 9 2 6 1	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total K 1 1	0	0
4	B	1	Total K 1 1	0	0
4	C	1	Total K 1 1	0	0
4	D	1	Total K 1 1	0	0

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

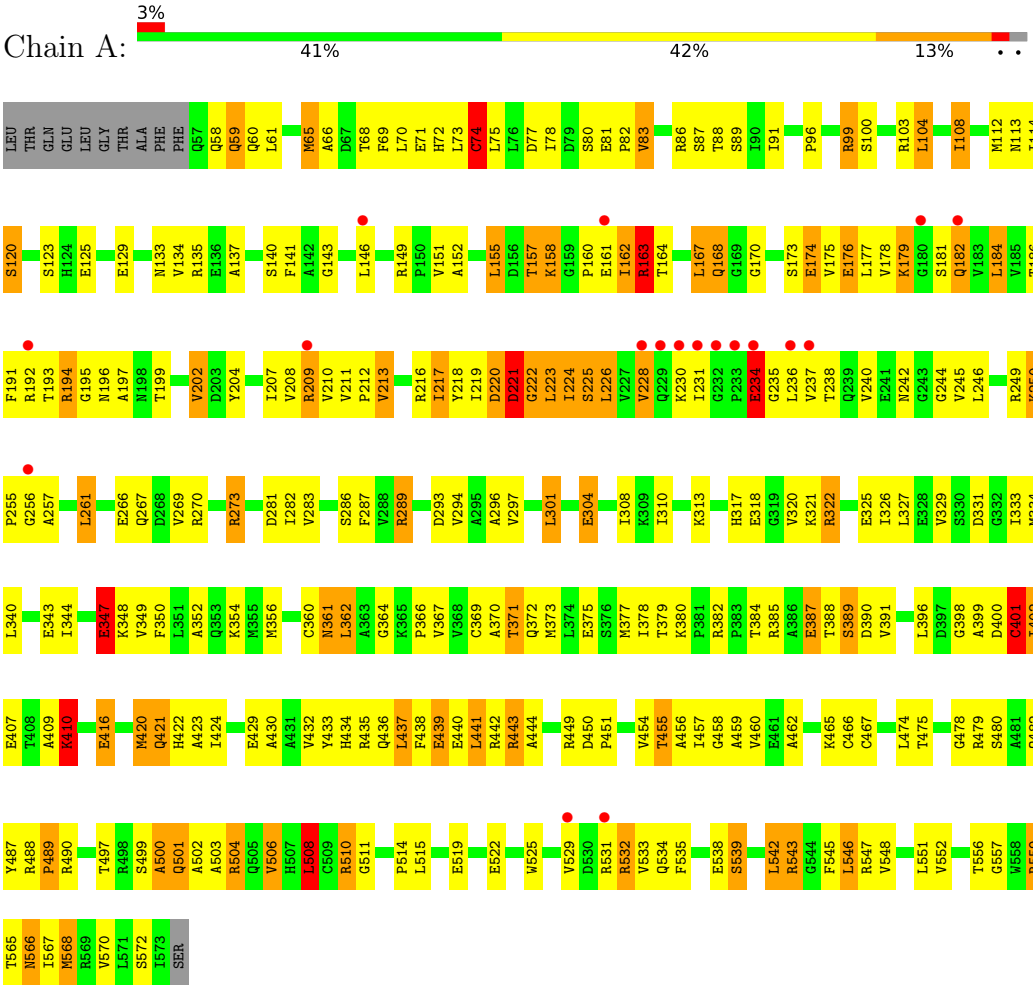
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mn 1 1	0	0
5	B	1	Total Mn 1 1	0	0
5	C	1	Total Mn 1 1	0	0
5	D	1	Total Mn 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

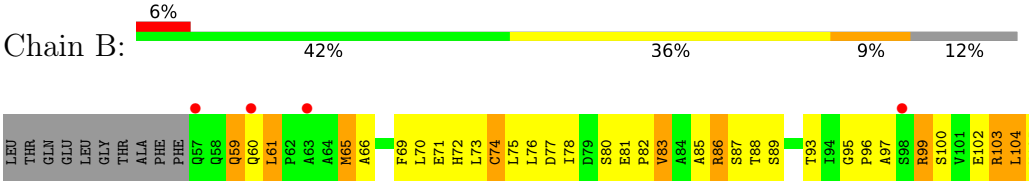
• Molecule 1: PYRUVATE KINASE ISOZYMES R/L

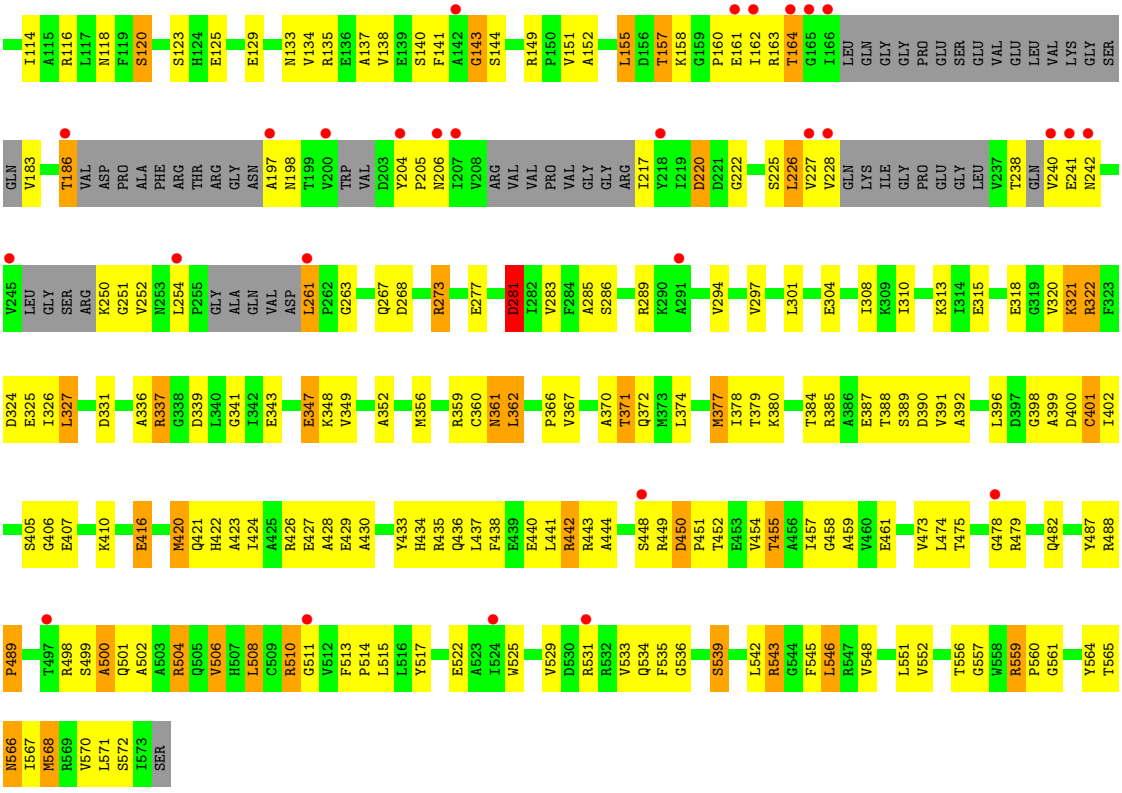
Chain A:



• Molecule 1: PYRUVATE KINASE ISOZYMES R/L

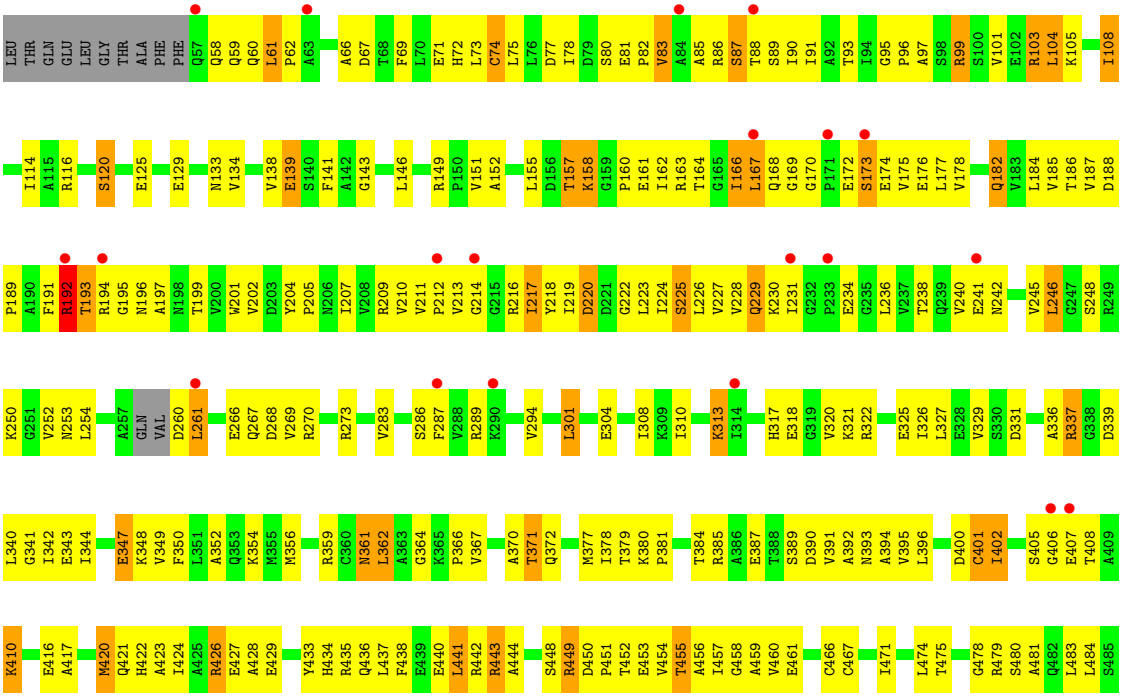
Chain B:

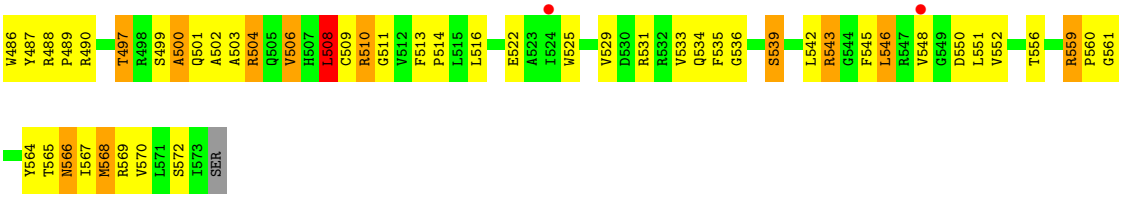




• Molecule 1: PYRUVATE KINASE ISOZYMES R/L

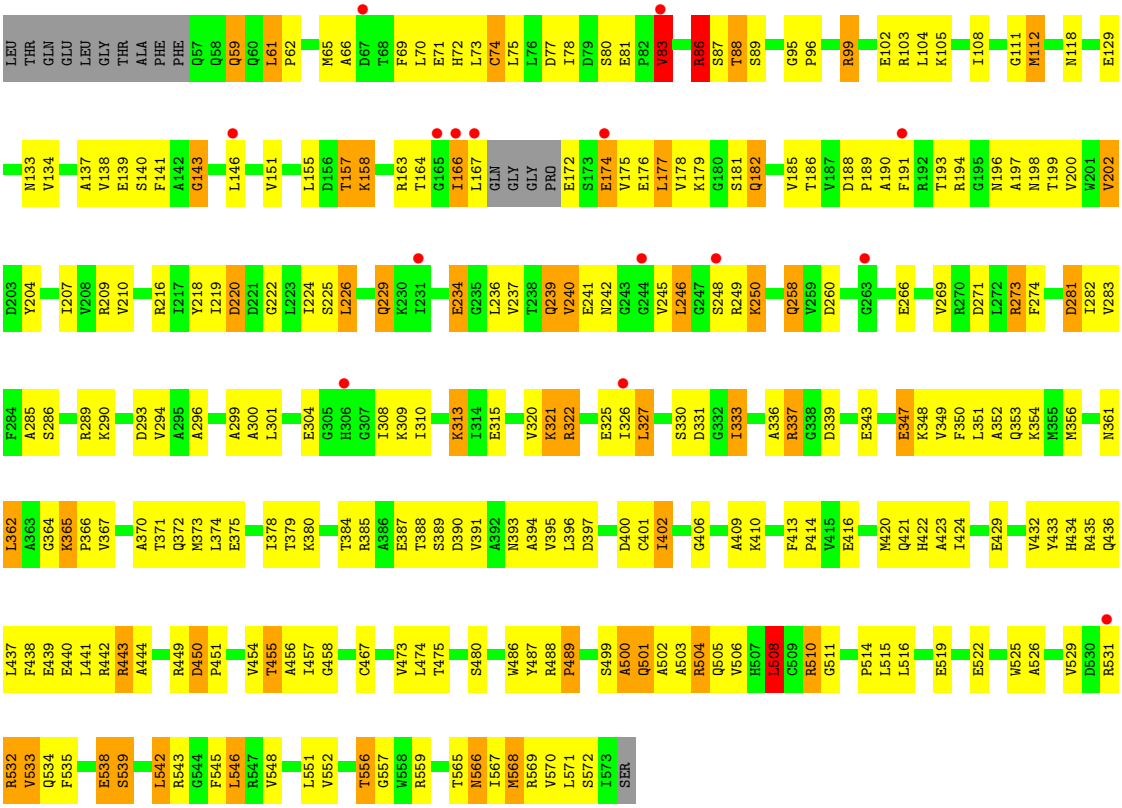
Chain C:





• Molecule 1: PYRUVATE KINASE ISOZYMES R/L

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.70Å 171.16Å 85.05Å 90.00° 91.61° 90.00°	Depositor
Resolution (Å)	20.00 – 2.87 53.63 – 2.87	Depositor EDS
% Data completeness (in resolution range)	88.7 (20.00-2.87) 88.6 (53.63-2.87)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.08 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.257 , 0.311 0.253 , 0.295	Depositor DCC
R_{free} test set	858 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å^2)	67.8	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 38.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.066 for h,-k,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	15342	wwPDB-VP
Average B, all atoms (Å^2)	2.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.42% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FBP, MN, PGA, K

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.19	14/3981 (0.4%)	1.17	19/5399 (0.4%)
1	B	1.02	5/3564 (0.1%)	0.99	10/4822 (0.2%)
1	C	1.07	3/3964 (0.1%)	1.05	8/5374 (0.1%)
1	D	1.08	2/3955 (0.1%)	1.14	17/5362 (0.3%)
All	All	1.10	24/15464 (0.2%)	1.09	54/20957 (0.3%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	186	THR	C-O	17.89	1.57	1.23
1	A	179	LYS	CE-NZ	15.06	1.86	1.49
1	A	401	CYS	CB-SG	-10.85	1.63	1.82
1	A	179	LYS	CD-CE	9.82	1.75	1.51
1	B	197	ALA	N-CA	9.28	1.65	1.46
1	B	197	ALA	CA-CB	8.91	1.71	1.52
1	A	439	GLU	CG-CD	7.85	1.63	1.51
1	A	369	CYS	CB-SG	-7.43	1.69	1.82
1	A	347	GLU	CG-CD	6.36	1.61	1.51
1	A	115	ALA	CA-CB	-6.27	1.39	1.52
1	A	74	CYS	CB-SG	-6.22	1.71	1.82
1	A	387	GLU	CD-OE2	5.96	1.32	1.25
1	A	416	GLU	CG-CD	5.91	1.60	1.51
1	A	187	VAL	CB-CG2	5.88	1.65	1.52
1	B	416	GLU	CG-CD	5.84	1.60	1.51
1	C	410	LYS	CB-CG	-5.69	1.37	1.52
1	B	410	LYS	CB-CG	-5.69	1.37	1.52
1	A	337	ARG	CZ-NH2	-5.51	1.25	1.33
1	C	401	CYS	CB-SG	-5.51	1.72	1.81
1	D	410	LYS	CB-CG	-5.33	1.38	1.52
1	A	179	LYS	CG-CD	5.32	1.70	1.52
1	D	86	ARG	CG-CD	-5.24	1.38	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	287	PHE	CE1-CZ	5.15	1.47	1.37
1	C	402	ILE	CA-CB	-5.01	1.43	1.54

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	504	ARG	NE-CZ-NH1	15.84	128.22	120.30
1	A	410	LYS	CD-CE-NZ	-15.29	76.55	111.70
1	A	510	ARG	NE-CZ-NH1	-15.03	112.79	120.30
1	A	510	ARG	NE-CZ-NH2	14.96	127.78	120.30
1	D	504	ARG	NE-CZ-NH2	-14.54	113.03	120.30
1	B	504	ARG	NE-CZ-NH1	13.42	127.01	120.30
1	B	504	ARG	NE-CZ-NH2	-12.42	114.09	120.30
1	C	504	ARG	NE-CZ-NH1	-11.22	114.69	120.30
1	C	504	ARG	NE-CZ-NH2	8.13	124.37	120.30
1	A	504	ARG	NE-CZ-NH2	7.87	124.24	120.30
1	A	221	ASP	CB-CG-OD1	-7.66	111.41	118.30
1	D	410	LYS	CB-CA-C	-7.37	95.66	110.40
1	A	510	ARG	CD-NE-CZ	7.28	133.80	123.60
1	A	74	CYS	CA-CB-SG	-7.28	100.89	114.00
1	B	410	LYS	CB-CA-C	-7.28	95.84	110.40
1	D	508	LEU	CA-CB-CG	6.54	130.34	115.30
1	D	281	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	D	112	MET	CG-SD-CE	-6.46	89.87	100.20
1	C	508	LEU	CB-CG-CD1	6.45	121.96	111.00
1	A	65	MET	CB-CG-SD	6.45	131.74	112.40
1	A	337	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	B	473	VAL	CB-CA-C	-6.33	99.38	111.40
1	C	426	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	D	467	CYS	CA-CB-SG	-6.14	102.95	114.00
1	C	510	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	A	504	ARG	NE-CZ-NH1	-6.06	117.27	120.30
1	A	404	LEU	CB-CG-CD2	-6.03	100.76	111.00
1	B	510	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	B	410	LYS	CD-CE-NZ	-5.92	98.07	111.70
1	D	504	ARG	CD-NE-CZ	5.87	131.82	123.60
1	A	532	ARG	NE-CZ-NH1	-5.85	117.38	120.30
1	D	450	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	D	450	ASP	CB-CG-OD1	5.78	123.50	118.30
1	A	226	LEU	CA-CB-CG	5.73	128.49	115.30
1	B	504	ARG	CD-NE-CZ	5.73	131.62	123.60
1	C	550	ASP	CB-CG-OD1	-5.51	113.34	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	510	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	B	442	ARG	NE-CZ-NH1	-5.47	117.57	120.30
1	C	508	LEU	CA-CB-CG	5.45	127.82	115.30
1	A	221	ASP	CB-CG-OD2	5.42	123.17	118.30
1	B	510	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	179	LYS	CD-CE-NZ	-5.41	99.25	111.70
1	A	508	LEU	CA-CB-CG	5.33	127.57	115.30
1	A	179	LYS	CG-CD-CE	-5.29	96.04	111.90
1	D	510	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	C	510	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	A	504	ARG	CD-NE-CZ	5.16	130.82	123.60
1	D	226	LEU	CA-CB-CG	5.13	127.09	115.30
1	A	163	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	D	532	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	D	281	ASP	CB-CG-OD1	5.08	122.87	118.30
1	D	473	VAL	CB-CA-C	-5.08	101.76	111.40
1	B	281	ASP	CB-CG-OD1	5.06	122.86	118.30
1	D	365	LYS	CD-CE-NZ	-5.03	100.13	111.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3915	0	3989	321	2
1	B	3513	0	3576	232	0
1	C	3899	0	3970	293	3
1	D	3891	0	3966	231	1
2	A	20	0	10	3	0
2	B	20	0	10	3	0
2	C	20	0	10	2	0
2	D	20	0	10	5	0
3	A	9	0	2	1	0
3	B	9	0	2	5	0
3	C	9	0	3	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	9	0	2	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	1	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	15342	0	15550	1027	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

All (1027) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:LYS:CD	1:A:179:LYS:CE	1.75	1.59
1:A:179:LYS:CE	1:A:179:LYS:NZ	1.86	1.39
3:C:1575:PGA:C1	3:C:1575:PGA:O2	1.76	1.33
1:A:225:SER:CB	1:A:242:ASN:HB2	1.77	1.13
1:A:167:LEU:HD12	1:A:168:GLN:H	1.10	1.13
1:A:225:SER:HB3	1:A:242:ASN:CB	1.81	1.11
1:A:184:LEU:HD11	1:A:235:GLY:HA3	1.12	1.06
1:D:225:SER:HB3	1:D:242:ASN:HB2	1.39	1.02
1:A:442:ARG:HH21	1:B:442:ARG:HH21	1.02	1.01
1:A:442:ARG:HH21	1:B:442:ARG:NH2	1.58	1.00
1:A:162:ILE:HG23	1:A:204:TYR:HB2	1.44	0.99
1:A:322:ARG:O	1:A:326:ILE:HD12	1.62	0.99
1:A:347:GLU:HG2	1:C:423:ALA:HB1	1.47	0.97
1:C:384:THR:OG1	1:C:387:GLU:HG3	1.64	0.96
1:D:177:LEU:N	1:D:177:LEU:HD23	1.83	0.93
1:C:436:GLN:O	1:C:440:GLU:HG3	1.68	0.93
1:A:184:LEU:CD1	1:A:235:GLY:HA3	1.99	0.92
1:C:87:SER:HB3	1:C:511:GLY:HA2	1.49	0.92
1:C:170:GLY:HA2	1:C:173:SER:OG	1.70	0.92
1:D:157:THR:HG22	1:D:286:SER:H	1.34	0.91
1:B:157:THR:HG22	1:B:286:SER:H	1.34	0.91
1:A:234:GLU:OE1	1:A:235:GLY:N	2.04	0.90
1:A:209:ARG:HH11	1:A:210:VAL:CG2	1.84	0.90
1:A:442:ARG:NH2	1:B:442:ARG:HH21	1.70	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:PRO:HB3	1:B:508:LEU:O	1.72	0.89
1:D:352:ALA:HB1	1:D:356:MET:CE	2.03	0.88
1:C:442:ARG:NH2	1:D:442:ARG:HH21	1.72	0.88
1:D:146:LEU:CB	1:D:542:LEU:HD12	2.04	0.88
1:A:216:ARG:HG2	1:A:218:TYR:CE1	2.08	0.87
1:D:366:PRO:HA	1:D:400:ASP:OD2	1.74	0.87
1:A:436:GLN:O	1:A:440:GLU:HG3	1.74	0.87
1:D:166:ILE:HA	1:D:248:SER:OG	1.74	0.87
1:A:204:TYR:O	1:A:204:TYR:CD2	2.28	0.87
1:B:99:ARG:NH2	1:B:129:GLU:OE1	2.07	0.87
1:A:208:VAL:HA	1:A:236:LEU:HD11	1.54	0.86
1:C:488:ARG:NH1	1:C:510:ARG:HD3	1.91	0.86
1:B:436:GLN:O	1:B:440:GLU:HG3	1.76	0.86
1:A:157:THR:HG22	1:A:286:SER:H	1.41	0.85
1:B:228:VAL:HG12	1:B:228:VAL:O	1.74	0.85
1:D:371:THR:HG22	1:D:372:GLN:HG3	1.58	0.85
1:A:170:GLY:HA3	1:A:173:SER:HB2	1.59	0.85
1:B:225:SER:HB3	1:B:242:ASN:HB2	1.59	0.85
1:C:184:LEU:HD22	1:C:236:LEU:O	1.76	0.84
1:D:99:ARG:NH2	1:D:129:GLU:OE1	2.10	0.83
1:A:228:VAL:HG12	1:A:228:VAL:O	1.78	0.83
1:C:69:PHE:O	1:C:72:HIS:HB3	1.78	0.83
1:C:166:ILE:HD12	1:C:166:ILE:H	1.43	0.83
1:C:487:TYR:O	1:C:488:ARG:HB2	1.77	0.83
1:C:313:LYS:HE3	3:C:1575:PGA:H22	1.61	0.83
1:D:146:LEU:HB3	1:D:542:LEU:HD12	1.60	0.83
1:A:337:ARG:HD3	1:A:370:ALA:O	1.77	0.83
1:C:87:SER:CB	1:C:511:GLY:HA2	2.08	0.82
1:A:167:LEU:HD12	1:A:168:GLN:N	1.93	0.82
1:A:191:PHE:HA	1:A:194:ARG:HB2	1.60	0.82
1:A:371:THR:HG22	1:A:372:GLN:HG3	1.59	0.82
1:A:179:LYS:CE	1:A:179:LYS:CG	2.57	0.82
1:D:86:ARG:NH1	1:D:422:HIS:ND1	2.28	0.82
1:A:402:ILE:HG13	1:A:421:GLN:NE2	1.95	0.81
1:C:225:SER:HB3	1:C:242:ASN:HB2	1.60	0.81
1:C:488:ARG:NH1	1:C:510:ARG:CB	2.44	0.81
1:B:423:ALA:HB1	1:D:347:GLU:HG2	1.63	0.81
1:C:441:LEU:O	1:C:442:ARG:C	2.19	0.81
1:D:174:GLU:OE2	1:D:245:VAL:HG11	1.80	0.81
1:C:182:GLN:HE21	1:C:182:GLN:HA	1.46	0.81
1:D:362:LEU:O	1:D:486:TRP:HZ2	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:ARG:NH1	1:A:510:ARG:HB3	1.96	0.79
1:C:434:HIS:O	1:C:437:LEU:N	2.15	0.79
1:B:228:VAL:HA	1:B:238:THR:HG22	1.64	0.79
1:A:155:LEU:HD23	1:A:155:LEU:C	2.02	0.79
1:C:120:SER:HA	1:C:158:LYS:HG3	1.63	0.79
1:C:162:ILE:O	1:C:252:VAL:N	2.14	0.79
1:C:313:LYS:HE3	3:C:1575:PGA:C2	2.12	0.79
1:A:209:ARG:HH11	1:A:210:VAL:HG23	1.48	0.79
1:A:158:LYS:O	1:A:158:LYS:HG2	1.81	0.79
1:A:347:GLU:HG2	1:C:423:ALA:CB	2.12	0.78
1:B:164:THR:HG23	1:B:252:VAL:HG21	1.64	0.78
1:A:175:VAL:CG1	1:A:176:GLU:N	2.46	0.78
1:A:385:ARG:HG3	1:C:337:ARG:HB3	1.66	0.78
1:A:407:GLU:OE1	1:A:407:GLU:N	2.15	0.78
1:C:407:GLU:OE1	1:C:407:GLU:N	2.15	0.78
1:D:204:TYR:OH	1:D:260:ASP:OD1	2.01	0.77
1:B:336:ALA:HB1	3:B:1575:PGA:C1	2.14	0.77
1:C:82:PRO:O	1:C:83:VAL:HG23	1.84	0.77
1:D:436:GLN:O	1:D:440:GLU:HG3	1.84	0.77
1:D:441:LEU:O	1:D:442:ARG:C	2.23	0.76
1:C:366:PRO:HB3	1:C:508:LEU:O	1.85	0.76
1:C:73:LEU:O	1:C:75:LEU:N	2.17	0.76
1:A:487:TYR:O	1:A:488:ARG:HB2	1.83	0.76
1:C:442:ARG:HH21	1:D:442:ARG:HH21	1.32	0.76
1:B:322:ARG:O	1:B:326:ILE:HD12	1.86	0.76
1:B:457:ILE:HG23	1:B:458:GLY:N	2.00	0.76
1:D:366:PRO:HB3	1:D:508:LEU:O	1.87	0.75
1:B:89:SER:HB2	1:B:401:CYS:HB3	1.68	0.75
1:C:188:ASP:HB3	1:C:191:PHE:HD1	1.52	0.75
1:C:81:GLU:OE1	1:C:81:GLU:HA	1.86	0.75
1:C:442:ARG:HH21	1:D:442:ARG:NH2	1.84	0.74
1:C:488:ARG:HH12	1:C:510:ARG:HB2	1.51	0.74
1:A:474:LEU:HD22	1:A:556:THR:HG22	1.67	0.74
1:C:322:ARG:O	1:C:326:ILE:HD12	1.87	0.74
1:C:87:SER:CB	1:C:511:GLY:CA	2.65	0.74
1:A:175:VAL:HG12	1:A:176:GLU:N	2.01	0.74
1:C:322:ARG:NH2	1:C:325:GLU:OE2	2.21	0.73
1:A:204:TYR:O	1:A:204:TYR:HD2	1.68	0.73
1:A:162:ILE:HG23	1:A:204:TYR:CB	2.18	0.73
1:B:437:LEU:HD12	1:B:437:LEU:O	1.88	0.73
1:A:366:PRO:HB3	1:A:508:LEU:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:402:ILE:HG13	1:D:421:GLN:NE2	2.03	0.73
1:D:362:LEU:O	1:D:486:TRP:CZ2	2.41	0.73
1:C:535:PHE:O	1:C:539:SER:OG	2.07	0.72
1:A:193:THR:HG23	1:A:194:ARG:HG3	1.70	0.72
1:A:162:ILE:CG2	1:A:204:TYR:CB	2.68	0.72
1:C:506:VAL:O	1:C:506:VAL:HG13	1.89	0.72
1:D:210:VAL:HG12	1:D:210:VAL:O	1.87	0.72
1:A:221:ASP:HB3	1:A:223:LEU:HG	1.72	0.72
1:B:281:ASP:OD2	1:B:504:ARG:HD2	1.90	0.72
1:C:488:ARG:NH1	1:C:510:ARG:HB3	2.05	0.72
1:B:441:LEU:O	1:B:442:ARG:C	2.25	0.72
1:C:561:GLY:O	2:C:1574:FBP:O4	2.06	0.72
1:D:155:LEU:C	1:D:155:LEU:HD23	2.10	0.72
1:A:146:LEU:HB2	1:A:542:LEU:HD12	1.72	0.72
1:B:488:ARG:NH1	1:B:510:ARG:HD3	2.05	0.72
1:A:441:LEU:O	1:A:442:ARG:C	2.25	0.72
1:C:85:ALA:HB2	1:C:545:PHE:CE2	2.25	0.72
1:C:151:VAL:O	1:C:504:ARG:HD2	1.88	0.72
1:C:367:VAL:H	1:C:400:ASP:HB2	1.54	0.72
1:A:202:VAL:HG13	1:A:204:TYR:H	1.55	0.71
1:A:437:LEU:HD12	1:A:437:LEU:O	1.90	0.71
1:C:175:VAL:CG1	1:C:197:ALA:HA	2.19	0.71
1:A:162:ILE:CG2	1:A:204:TYR:HB2	2.20	0.71
1:C:551:LEU:HD23	1:C:572:SER:HA	1.72	0.71
1:D:185:VAL:HB	1:D:236:LEU:HB2	1.72	0.71
1:D:73:LEU:O	1:D:75:LEU:N	2.24	0.71
1:C:175:VAL:HG11	1:C:197:ALA:HA	1.72	0.71
1:D:83:VAL:O	1:D:83:VAL:CG1	2.38	0.71
1:A:146:LEU:CB	1:A:542:LEU:HD12	2.21	0.70
1:A:182:GLN:HA	1:A:182:GLN:HE21	1.56	0.70
1:A:286:SER:HA	1:A:313:LYS:HE2	1.73	0.70
1:A:533:VAL:HG12	1:A:534:GLN:N	2.06	0.70
1:A:216:ARG:HG2	1:A:218:TYR:HE1	1.54	0.70
1:B:451:PRO:O	1:B:455:THR:OG1	2.09	0.70
1:A:170:GLY:HA3	1:A:173:SER:CB	2.22	0.70
1:C:87:SER:HB2	1:C:511:GLY:CA	2.21	0.70
1:D:337:ARG:HD3	1:D:370:ALA:O	1.91	0.70
1:A:96:PRO:HD2	1:A:409:ALA:O	1.92	0.70
1:A:175:VAL:HG13	1:A:197:ALA:HB2	1.74	0.70
1:A:209:ARG:NH1	1:A:210:VAL:CG2	2.54	0.70
1:A:331:ASP:O	1:A:366:PRO:HD2	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:LEU:HB2	1:D:542:LEU:HD12	1.73	0.69
1:D:258:GLN:O	1:D:258:GLN:HG2	1.90	0.69
1:A:373:MET:O	1:A:387:GLU:HB3	1.92	0.69
1:D:499:SER:O	1:D:501:GLN:N	2.25	0.69
1:B:339:ASP:OD2	5:B:1577:MN:MN	1.51	0.69
1:C:170:GLY:CA	1:C:173:SER:OG	2.40	0.69
1:C:442:ARG:NH2	1:D:442:ARG:NH2	2.39	0.69
1:C:488:ARG:HH12	1:C:510:ARG:CB	2.06	0.68
1:B:155:LEU:C	1:B:155:LEU:HD23	2.13	0.68
1:B:157:THR:CG2	1:B:286:SER:H	2.06	0.68
1:C:87:SER:HB3	1:C:511:GLY:CA	2.23	0.68
1:D:158:LYS:O	1:D:158:LYS:HG2	1.88	0.68
1:C:216:ARG:HD2	1:C:241:GLU:OE1	1.93	0.68
1:D:352:ALA:HB1	1:D:356:MET:HE3	1.75	0.68
1:A:219:ILE:HB	1:A:224:ILE:CG2	2.24	0.68
1:B:283:VAL:HG23	1:B:308:ILE:HG21	1.75	0.68
1:B:434:HIS:O	1:B:437:LEU:N	2.26	0.68
1:C:87:SER:HB2	1:C:511:GLY:N	2.09	0.68
1:D:533:VAL:HG12	1:D:534:GLN:N	2.08	0.68
1:A:488:ARG:NH1	1:A:510:ARG:CB	2.57	0.67
1:C:161:GLU:OE1	1:C:163:ARG:NE	2.18	0.67
1:D:81:GLU:HA	1:D:81:GLU:OE1	1.93	0.67
1:A:207:ILE:HD11	1:A:254:LEU:HD21	1.76	0.67
1:B:125:GLU:CD	1:B:125:GLU:H	1.97	0.67
1:B:228:VAL:O	1:B:228:VAL:CG1	2.41	0.67
1:B:533:VAL:HG12	1:B:534:GLN:N	2.08	0.67
1:C:488:ARG:CZ	1:C:510:ARG:HD3	2.25	0.67
1:D:137:ALA:O	1:D:140:SER:OG	2.11	0.67
1:D:229:GLN:HG3	1:D:237:VAL:O	1.95	0.67
1:D:166:ILE:HA	1:D:248:SER:HG	1.59	0.67
1:A:338:GLY:O	1:C:385:ARG:NH2	2.26	0.67
1:A:83:VAL:HG12	1:A:83:VAL:O	1.92	0.67
1:D:283:VAL:HG23	1:D:308:ILE:HG21	1.76	0.67
1:D:434:HIS:O	1:D:437:LEU:N	2.28	0.67
1:C:85:ALA:HB1	1:C:513:PHE:CE2	2.29	0.66
1:C:185:VAL:HB	1:C:236:LEU:HB2	1.77	0.66
1:A:402:ILE:HG13	1:A:421:GLN:HE22	1.60	0.66
1:D:66:ALA:HB1	1:D:71:GLU:HG2	1.76	0.66
1:B:487:TYR:O	1:B:488:ARG:HB2	1.95	0.66
1:D:457:ILE:HG23	1:D:458:GLY:N	2.10	0.66
1:A:228:VAL:HA	1:A:238:THR:HG22	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:ARG:HD3	1:C:227:VAL:HG22	1.76	0.66
1:C:336:ALA:HB1	3:C:1575:PGA:C1	2.26	0.66
1:C:267:GLN:O	1:C:270:ARG:N	2.29	0.66
1:B:371:THR:HG22	1:B:372:GLN:HG3	1.77	0.66
1:D:157:THR:CG2	1:D:286:SER:H	2.09	0.65
1:A:184:LEU:HD11	1:A:235:GLY:CA	2.08	0.65
1:A:178:VAL:O	1:A:181:SER:OG	2.07	0.65
1:B:120:SER:HA	1:B:158:LYS:HG3	1.78	0.65
1:D:258:GLN:H	1:D:258:GLN:HE21	1.45	0.65
1:A:155:LEU:HD23	1:A:155:LEU:O	1.96	0.65
1:A:196:ASN:OD1	1:A:199:THR:N	2.29	0.65
1:A:441:LEU:O	1:A:443:ARG:N	2.30	0.65
1:B:347:GLU:HG2	1:D:423:ALA:HB1	1.77	0.65
1:C:283:VAL:HG23	1:C:308:ILE:HG21	1.78	0.64
1:B:78:ILE:HD13	1:D:320:VAL:HG11	1.78	0.64
1:B:337:ARG:HB3	1:D:385:ARG:HG3	1.77	0.64
1:D:364:GLY:HA2	1:D:486:TRP:CD1	2.32	0.64
1:C:193:THR:HG23	1:C:193:THR:O	1.98	0.64
1:D:378:ILE:HD11	1:D:406:GLY:HA3	1.79	0.64
1:B:535:PHE:O	1:B:539:SER:OG	2.16	0.64
1:A:194:ARG:HH11	1:A:194:ARG:HB3	1.61	0.64
1:A:225:SER:HB3	1:A:242:ASN:HB2	0.85	0.64
1:D:285:ALA:O	1:D:313:LYS:HB2	1.98	0.64
1:D:475:THR:HA	2:D:1574:FBP:H61	1.79	0.64
1:D:545:PHE:HB2	1:D:546:LEU:HD23	1.79	0.64
1:A:219:ILE:HG21	1:A:246:LEU:HD13	1.80	0.63
1:C:318:GLU:O	1:C:322:ARG:HG3	1.98	0.63
1:A:86:ARG:NH1	1:A:422:HIS:ND1	2.45	0.63
1:B:227:VAL:O	1:B:238:THR:HB	1.97	0.63
1:A:317:HIS:O	1:A:320:VAL:N	2.32	0.63
1:C:99:ARG:NH2	1:C:129:GLU:OE1	2.31	0.63
1:A:188:ASP:O	1:A:190:ALA:N	2.32	0.63
1:C:157:THR:HG22	1:C:286:SER:H	1.63	0.63
1:C:384:THR:OG1	1:C:387:GLU:CG	2.43	0.63
1:A:255:PRO:O	1:A:257:ALA:N	2.32	0.63
1:A:125:GLU:CD	1:A:125:GLU:H	2.02	0.62
1:A:217:ILE:N	1:A:226:LEU:O	2.28	0.62
1:B:315:GLU:OE2	1:B:339:ASP:OD2	2.16	0.62
1:C:245:VAL:HG12	1:C:245:VAL:O	1.98	0.62
1:C:349:VAL:O	1:C:352:ALA:N	2.31	0.62
1:D:219:ILE:HB	1:D:224:ILE:HB	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:532:ARG:HH22	2:D:1574:FBP:P1	2.23	0.62
1:A:162:ILE:CG2	1:A:204:TYR:HB3	2.28	0.62
1:A:402:ILE:HG12	1:A:402:ILE:O	2.00	0.62
1:B:337:ARG:HD3	1:B:370:ALA:O	1.99	0.62
1:C:433:TYR:O	1:C:434:HIS:C	2.37	0.62
1:D:322:ARG:NH2	1:D:325:GLU:OE2	2.31	0.62
1:B:488:ARG:NH1	1:B:510:ARG:CB	2.63	0.62
1:A:442:ARG:NH2	1:B:442:ARG:NH2	2.36	0.62
1:C:451:PRO:O	1:C:455:THR:OG1	2.18	0.62
1:C:317:HIS:O	1:C:320:VAL:N	2.33	0.62
1:D:133:ASN:O	1:D:134:VAL:C	2.37	0.62
1:D:551:LEU:HD23	1:D:572:SER:HA	1.81	0.62
1:A:218:TYR:HD2	1:A:222:GLY:HA2	1.64	0.61
1:A:207:ILE:HD11	1:A:254:LEU:CD2	2.30	0.61
1:D:327:LEU:HD22	1:D:327:LEU:O	2.00	0.61
1:A:240:VAL:HG13	1:A:242:ASN:O	2.00	0.61
1:A:360:CYS:O	1:A:361:ASN:C	2.36	0.61
1:D:350:PHE:O	1:D:354:LYS:HG3	2.00	0.61
1:A:164:THR:O	1:A:249:ARG:HA	2.00	0.61
1:A:283:VAL:HG23	1:A:308:ILE:HG21	1.82	0.61
1:C:568:MET:HE1	1:C:570:VAL:HG23	1.82	0.61
1:A:347:GLU:HB3	1:C:424:ILE:HA	1.83	0.61
1:A:367:VAL:H	1:A:400:ASP:HB2	1.66	0.61
1:A:441:LEU:O	1:A:444:ALA:N	2.33	0.61
1:C:66:ALA:HB1	1:C:71:GLU:HG2	1.83	0.61
1:D:177:LEU:N	1:D:177:LEU:CD2	2.57	0.61
1:C:188:ASP:HB3	1:C:191:PHE:CD1	2.36	0.60
1:C:218:TYR:HB3	1:C:222:GLY:HA2	1.83	0.60
1:A:194:ARG:HH11	1:A:194:ARG:CG	2.14	0.60
1:C:125:GLU:CD	1:C:125:GLU:H	2.03	0.60
1:D:474:LEU:HD22	1:D:556:THR:HG22	1.81	0.60
1:B:420:MET:O	1:B:421:GLN:C	2.36	0.60
1:B:423:ALA:CB	1:D:347:GLU:HG2	2.31	0.60
1:D:433:TYR:O	1:D:434:HIS:C	2.39	0.60
1:D:514:PRO:O	1:D:515:LEU:HD23	2.02	0.60
1:C:83:VAL:HG12	1:C:83:VAL:O	2.01	0.60
1:D:210:VAL:O	1:D:210:VAL:CG1	2.50	0.60
1:A:255:PRO:C	1:A:257:ALA:H	2.05	0.60
1:B:331:ASP:O	1:B:366:PRO:HD2	2.01	0.60
1:D:456:ALA:O	1:D:457:ILE:C	2.38	0.60
1:A:87:SER:N	1:A:429:GLU:OE1	2.25	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ASP:HB3	1:A:223:LEU:CG	2.30	0.59
1:B:457:ILE:CG2	1:B:458:GLY:N	2.65	0.59
1:A:488:ARG:HH11	1:A:510:ARG:HB3	1.62	0.59
1:D:155:LEU:HD23	1:D:155:LEU:O	2.01	0.59
1:C:567:ILE:HG12	1:D:569:ARG:HG2	1.84	0.59
1:A:551:LEU:HD23	1:A:572:SER:HA	1.84	0.59
1:B:86:ARG:HH11	1:B:86:ARG:HG2	1.68	0.59
1:A:99:ARG:NH2	1:A:129:GLU:OE1	2.35	0.59
1:A:466:CYS:O	1:A:467:CYS:HB2	2.01	0.59
1:C:202:VAL:HG12	1:C:204:TYR:H	1.68	0.59
1:C:568:MET:CE	1:C:570:VAL:HG23	2.33	0.59
1:A:160:PRO:HB3	1:A:261:LEU:HB3	1.85	0.59
1:A:81:GLU:OE1	1:A:81:GLU:HA	2.03	0.59
1:D:532:ARG:NH2	2:D:1574:FBP:O1P	2.33	0.59
1:B:551:LEU:HD23	1:B:572:SER:HA	1.85	0.58
1:C:93:THR:HA	1:C:116:ARG:HB3	1.84	0.58
1:D:83:VAL:O	1:D:83:VAL:HG12	2.01	0.58
1:B:488:ARG:NH1	1:B:510:ARG:HB3	2.18	0.58
1:D:349:VAL:O	1:D:352:ALA:N	2.37	0.58
1:A:175:VAL:O	1:A:245:VAL:HG13	2.02	0.58
1:A:340:LEU:O	1:A:344:ILE:HG12	2.03	0.58
1:B:318:GLU:O	1:B:322:ARG:HG3	2.03	0.58
1:C:167:LEU:HD12	1:C:195:GLY:HA3	1.83	0.58
1:A:162:ILE:HG21	1:A:204:TYR:HB3	1.84	0.58
1:A:322:ARG:C	1:A:326:ILE:HD12	2.24	0.58
1:B:315:GLU:HG2	1:B:339:ASP:HB2	1.85	0.58
1:D:322:ARG:O	1:D:326:ILE:HD12	2.03	0.58
1:A:83:VAL:O	1:A:83:VAL:CG1	2.51	0.58
1:B:163:ARG:NH1	1:B:250:LYS:HA	2.18	0.58
1:B:352:ALA:HB1	1:B:356:MET:CE	2.33	0.58
1:D:487:TYR:O	1:D:488:ARG:HB2	2.02	0.58
1:A:137:ALA:O	1:A:140:SER:OG	2.18	0.58
1:A:175:VAL:HG11	1:A:197:ALA:HA	1.86	0.58
1:B:286:SER:HA	1:B:313:LYS:HE2	1.86	0.58
1:A:69:PHE:O	1:A:72:HIS:HB3	2.03	0.58
1:A:188:ASP:O	1:A:189:PRO:C	2.40	0.58
1:B:183:VAL:HG22	1:B:198:ASN:HA	1.84	0.58
1:B:226:LEU:HD22	1:B:240:VAL:HG22	1.85	0.58
1:C:339:ASP:O	1:C:343:GLU:HG2	2.04	0.58
1:D:532:ARG:NH1	2:D:1574:FBP:O2P	2.34	0.58
1:A:475:THR:HA	2:A:1574:FBP:H61	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:354:LYS:NZ	1:D:397:ASP:OD1	2.35	0.58
1:A:175:VAL:CG1	1:A:197:ALA:HB2	2.34	0.58
1:A:488:ARG:O	1:A:489:PRO:O	2.21	0.58
1:D:488:ARG:NH1	1:D:510:ARG:HD3	2.18	0.58
1:C:214:GLY:N	1:C:228:VAL:O	2.35	0.57
1:C:506:VAL:O	1:C:506:VAL:CG1	2.52	0.57
1:D:347:GLU:CD	1:D:347:GLU:H	2.07	0.57
1:A:545:PHE:C	1:A:546:LEU:HD23	2.24	0.57
1:B:86:ARG:HG2	1:B:86:ARG:NH1	2.17	0.57
1:D:225:SER:CB	1:D:242:ASN:HB2	2.23	0.57
1:C:488:ARG:NH1	1:C:510:ARG:HB2	2.13	0.57
1:C:499:SER:O	1:C:501:GLN:N	2.37	0.57
1:D:88:THR:HG22	1:D:401:CYS:HA	1.87	0.57
1:B:450:ASP:O	1:B:454:VAL:HG23	2.05	0.57
1:D:188:ASP:O	1:D:189:PRO:C	2.43	0.57
1:B:339:ASP:O	1:B:343:GLU:HG2	2.04	0.57
1:A:322:ARG:NH2	1:A:325:GLU:OE2	2.33	0.57
1:C:151:VAL:O	1:C:504:ARG:CD	2.51	0.57
1:A:87:SER:HB2	1:A:511:GLY:N	2.20	0.57
1:C:73:LEU:C	1:C:75:LEU:H	2.08	0.57
1:A:388:THR:HG22	1:A:389:SER:N	2.19	0.57
1:A:479:ARG:O	1:A:482:GLN:HB3	2.05	0.57
1:B:204:TYR:CE1	1:B:261:LEU:HD13	2.40	0.57
1:B:161:GLU:C	1:B:162:ILE:HG13	2.24	0.57
1:B:85:ALA:HB2	1:B:545:PHE:CE2	2.40	0.56
1:D:565:THR:O	1:D:566:ASN:HB3	2.04	0.56
1:B:81:GLU:HA	1:B:81:GLU:OE1	2.03	0.56
1:B:475:THR:HA	2:B:1574:FBP:H61	1.86	0.56
1:C:210:VAL:O	1:C:212:PRO:HD3	2.06	0.56
1:C:337:ARG:HD3	1:C:370:ALA:O	2.06	0.56
1:C:458:GLY:O	1:C:459:ALA:C	2.41	0.56
1:D:393:ASN:O	1:D:394:ALA:C	2.39	0.56
1:D:535:PHE:O	1:D:539:SER:OG	2.22	0.56
1:A:168:GLN:HB2	1:A:195:GLY:O	2.05	0.56
1:A:349:VAL:O	1:A:352:ALA:N	2.38	0.56
1:A:194:ARG:HH11	1:A:194:ARG:CB	2.18	0.56
1:A:437:LEU:HD12	1:A:437:LEU:C	2.24	0.56
1:C:337:ARG:HH22	1:C:390:ASP:CG	2.08	0.56
1:C:502:ALA:O	1:C:504:ARG:N	2.39	0.56
1:A:210:VAL:HG12	1:A:210:VAL:O	2.05	0.56
1:B:61:LEU:O	1:B:65:MET:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:GLU:OE1	1:C:245:VAL:CG1	2.54	0.56
1:D:134:VAL:O	1:D:138:VAL:HG23	2.06	0.56
1:A:74:CYS:SG	1:C:359:ARG:HG3	2.45	0.56
1:D:488:ARG:NH1	1:D:510:ARG:HB3	2.20	0.56
1:B:66:ALA:HB1	1:B:71:GLU:HG2	1.86	0.56
1:C:89:SER:HB2	1:C:401:CYS:SG	2.46	0.56
1:D:339:ASP:O	1:D:343:GLU:HG2	2.05	0.56
1:A:190:ALA:HB3	1:A:191:PHE:CD1	2.41	0.56
1:A:478:GLY:O	1:A:479:ARG:C	2.44	0.55
1:C:322:ARG:HH21	1:C:325:GLU:CD	2.09	0.55
1:A:228:VAL:O	1:A:228:VAL:CG1	2.50	0.55
1:A:429:GLU:HA	1:A:432:VAL:HG23	1.88	0.55
1:B:367:VAL:H	1:B:400:ASP:HB2	1.70	0.55
1:D:176:GLU:C	1:D:177:LEU:HD23	2.27	0.55
1:D:499:SER:O	1:D:500:ALA:C	2.45	0.55
1:A:337:ARG:HB3	1:C:385:ARG:HG3	1.87	0.55
1:A:434:HIS:O	1:A:437:LEU:N	2.40	0.55
1:D:196:ASN:N	1:D:199:THR:O	2.37	0.55
1:D:545:PHE:CB	1:D:546:LEU:HD23	2.37	0.55
1:A:347:GLU:CD	1:A:347:GLU:H	2.10	0.55
1:B:87:SER:HB2	1:B:511:GLY:N	2.21	0.55
1:A:223:LEU:HD22	1:C:380:LYS:NZ	2.22	0.55
1:C:192:ARG:HG3	1:C:201:TRP:CZ2	2.41	0.55
1:B:420:MET:O	1:B:422:HIS:N	2.40	0.55
1:A:267:GLN:O	1:A:270:ARG:N	2.40	0.55
1:A:499:SER:O	1:A:501:GLN:N	2.40	0.55
1:B:452:THR:HG23	1:B:565:THR:HB	1.89	0.55
1:B:488:ARG:C	1:B:489:PRO:O	2.44	0.55
1:B:545:PHE:HB2	1:B:546:LEU:HD23	1.89	0.55
1:D:108:ILE:HD13	1:D:151:VAL:HG21	1.88	0.55
1:A:459:ALA:O	1:A:462:ALA:HB3	2.07	0.54
1:B:225:SER:OG	1:B:241:GLU:HB3	2.07	0.54
1:D:451:PRO:O	1:D:455:THR:OG1	2.25	0.54
1:D:457:ILE:CG2	1:D:458:GLY:N	2.70	0.54
1:D:488:ARG:C	1:D:489:PRO:O	2.43	0.54
1:C:371:THR:HG22	1:C:372:GLN:HG3	1.88	0.54
1:D:402:ILE:HG13	1:D:421:GLN:HE22	1.68	0.54
1:A:420:MET:O	1:A:421:GLN:C	2.43	0.54
1:A:451:PRO:O	1:A:455:THR:OG1	2.24	0.54
1:A:385:ARG:HE	1:C:341:GLY:HA3	1.72	0.54
1:B:69:PHE:O	1:B:72:HIS:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:LEU:HD22	1:B:556:THR:HG22	1.90	0.54
1:C:539:SER:O	1:C:543:ARG:HG3	2.08	0.54
1:A:514:PRO:O	1:A:515:LEU:HD23	2.08	0.54
1:B:545:PHE:CB	1:B:546:LEU:HD23	2.38	0.54
1:D:172:GLU:CD	1:D:172:GLU:N	2.61	0.54
1:A:157:THR:HG22	1:A:286:SER:N	2.17	0.54
1:A:378:ILE:HD11	1:A:406:GLY:HA3	1.90	0.54
1:A:488:ARG:C	1:A:489:PRO:O	2.43	0.54
1:B:479:ARG:O	1:B:482:GLN:HB3	2.08	0.54
1:C:499:SER:O	1:C:500:ALA:C	2.46	0.54
1:D:349:VAL:O	1:D:351:LEU:N	2.41	0.54
1:D:352:ALA:HB1	1:D:356:MET:HE2	1.88	0.54
1:A:219:ILE:CG2	1:A:246:LEU:CD1	2.86	0.54
1:D:73:LEU:O	1:D:74:CYS:C	2.46	0.54
1:A:438:PHE:O	1:A:439:GLU:C	2.47	0.54
1:B:320:VAL:HG11	1:D:78:ILE:HD13	1.88	0.54
1:B:545:PHE:C	1:B:546:LEU:HD23	2.28	0.54
1:C:204:TYR:CE1	1:C:261:LEU:HD13	2.43	0.54
1:A:367:VAL:O	1:A:367:VAL:HG13	2.08	0.53
1:C:204:TYR:OH	1:C:260:ASP:OD1	2.19	0.53
1:C:402:ILE:HG13	1:C:402:ILE:O	2.07	0.53
1:D:216:ARG:HG2	1:D:218:TYR:CE1	2.43	0.53
1:A:458:GLY:O	1:A:459:ALA:C	2.44	0.53
1:D:429:GLU:HA	1:D:432:VAL:HG23	1.89	0.53
1:B:420:MET:O	1:B:423:ALA:N	2.41	0.53
1:B:488:ARG:HH12	1:B:510:ARG:HB2	1.74	0.53
1:D:96:PRO:HD2	1:D:409:ALA:O	2.09	0.53
1:A:525:TRP:NE1	1:A:560:PRO:HG3	2.23	0.53
1:C:522:GLU:CD	1:C:531:ARG:HE	2.12	0.53
1:A:339:ASP:O	1:A:343:GLU:HG2	2.08	0.53
1:A:547:ARG:HH11	1:A:547:ARG:HB3	1.73	0.53
1:C:174:GLU:OE1	1:C:245:VAL:HG11	2.09	0.53
1:C:405:SER:O	1:C:406:GLY:C	2.47	0.53
1:D:175:VAL:HG12	1:D:177:LEU:CD2	2.38	0.53
1:A:89:SER:O	1:A:401:CYS:HB3	2.09	0.53
1:A:535:PHE:O	1:A:539:SER:OG	2.26	0.53
1:B:405:SER:O	1:B:406:GLY:C	2.46	0.53
1:A:112:MET:HG2	1:A:113:ASN:N	2.24	0.53
1:B:87:SER:HB2	1:B:511:GLY:CA	2.39	0.53
1:B:162:ILE:HG23	1:B:204:TYR:HB2	1.91	0.53
1:C:73:LEU:C	1:C:75:LEU:N	2.60	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ASN:OD1	1:A:120:SER:HB2	2.09	0.53
1:B:88:THR:OG1	1:B:429:GLU:OE2	2.16	0.53
1:D:283:VAL:HG23	1:D:308:ILE:CG2	2.38	0.53
1:D:441:LEU:O	1:D:444:ALA:N	2.41	0.53
1:A:450:ASP:O	1:A:454:VAL:HG23	2.09	0.53
1:C:146:LEU:HD23	1:C:535:PHE:CE1	2.43	0.53
1:C:204:TYR:O	1:C:207:ILE:HG22	2.09	0.53
1:D:164:THR:O	1:D:249:ARG:HA	2.10	0.53
1:D:258:GLN:HE21	1:D:258:GLN:N	2.07	0.53
1:A:151:VAL:O	1:A:504:ARG:HD2	2.10	0.52
1:B:336:ALA:HB1	3:B:1575:PGA:C2	2.39	0.52
1:A:438:PHE:CZ	1:A:442:ARG:HD3	2.44	0.52
1:C:352:ALA:HB1	1:C:356:MET:HE2	1.89	0.52
1:C:488:ARG:HH11	1:C:510:ARG:HB3	1.71	0.52
1:C:513:PHE:N	1:C:513:PHE:CD1	2.75	0.52
1:A:123:SER:HB2	1:A:125:GLU:OE1	2.09	0.52
1:B:513:PHE:N	1:B:513:PHE:CD1	2.77	0.52
1:A:525:TRP:CE2	1:A:560:PRO:HG3	2.45	0.52
1:B:283:VAL:HG23	1:B:308:ILE:CG2	2.38	0.52
1:A:487:TYR:O	1:A:488:ARG:CB	2.51	0.52
1:C:384:THR:HG1	1:C:387:GLU:HG3	1.73	0.52
1:C:488:ARG:NH1	1:C:510:ARG:CD	2.70	0.52
1:A:423:ALA:HB1	1:C:347:GLU:HG2	1.90	0.52
1:A:525:TRP:CD1	1:A:560:PRO:HG3	2.44	0.52
1:B:488:ARG:CZ	1:B:510:ARG:HD3	2.39	0.52
1:C:449:ARG:HG3	1:D:551:LEU:HD12	1.92	0.52
1:A:320:VAL:HG11	1:C:78:ILE:HD13	1.92	0.52
1:B:347:GLU:CD	1:B:347:GLU:H	2.11	0.52
1:B:384:THR:OG1	1:B:387:GLU:HG3	2.09	0.52
1:C:77:ASP:HB3	1:C:80:SER:HB2	1.92	0.52
1:C:313:LYS:HE3	3:C:1575:PGA:O1P	2.09	0.52
1:D:402:ILE:HG12	1:D:402:ILE:O	2.08	0.52
1:C:155:LEU:HD23	1:C:155:LEU:C	2.30	0.52
1:D:69:PHE:O	1:D:72:HIS:HB3	2.08	0.52
1:A:162:ILE:O	1:A:252:VAL:HB	2.10	0.52
1:C:379:THR:O	1:C:379:THR:HG22	2.10	0.52
1:B:77:ASP:HB3	1:B:80:SER:HB2	1.92	0.51
1:C:86:ARG:HB3	1:C:426:ARG:HG2	1.91	0.51
1:A:211:VAL:HG21	1:A:217:ILE:HD11	1.91	0.51
1:A:364:GLY:HA2	1:A:486:TRP:CD1	2.45	0.51
1:B:336:ALA:HB1	3:B:1575:PGA:H22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:VAL:HG12	1:C:139:GLU:OE2	2.10	0.51
1:C:391:VAL:CG1	1:C:424:ILE:HG21	2.39	0.51
1:D:370:ALA:O	1:D:371:THR:HB	2.10	0.51
1:D:384:THR:OG1	1:D:387:GLU:HG3	2.10	0.51
1:B:87:SER:CB	1:B:511:GLY:HA2	2.40	0.51
1:B:163:ARG:HH11	1:B:250:LYS:HA	1.72	0.51
1:A:219:ILE:HB	1:A:224:ILE:HG22	1.92	0.51
1:A:219:ILE:HG21	1:A:246:LEU:CD1	2.39	0.51
1:C:163:ARG:HA	1:C:250:LYS:O	2.09	0.51
1:B:86:ARG:NH1	1:B:422:HIS:ND1	2.59	0.51
1:C:441:LEU:O	1:C:443:ARG:N	2.42	0.51
1:C:450:ASP:O	1:C:454:VAL:HG23	2.11	0.51
1:C:457:ILE:HG23	1:C:458:GLY:N	2.25	0.51
1:D:225:SER:HB3	1:D:242:ASN:CB	2.27	0.51
1:A:141:PHE:C	1:A:143:GLY:H	2.12	0.51
1:A:565:THR:O	1:A:566:ASN:HB3	2.11	0.51
1:B:427:GLU:O	1:B:428:ALA:C	2.46	0.51
1:B:433:TYR:O	1:B:434:HIS:C	2.47	0.51
1:D:322:ARG:HH21	1:D:325:GLU:CD	2.13	0.51
1:A:100:SER:O	1:A:104:LEU:HD22	2.10	0.51
1:A:167:LEU:CD1	1:A:168:GLN:H	2.01	0.51
1:B:327:LEU:HD22	1:B:327:LEU:O	2.11	0.51
1:C:133:ASN:O	1:C:134:VAL:C	2.47	0.51
1:C:391:VAL:HG12	1:C:424:ILE:CG2	2.40	0.51
1:C:406:GLY:O	1:C:407:GLU:C	2.45	0.51
1:A:202:VAL:O	1:A:202:VAL:CG1	2.58	0.51
1:C:158:LYS:HG2	1:C:161:GLU:HG3	1.93	0.51
1:D:151:VAL:O	1:D:504:ARG:HD3	2.10	0.51
1:D:269:VAL:O	1:D:273:ARG:HG2	2.11	0.51
1:A:175:VAL:HG13	1:A:176:GLU:H	1.76	0.51
1:B:83:VAL:O	1:B:83:VAL:HG12	2.11	0.51
1:B:155:LEU:HD23	1:B:155:LEU:O	2.10	0.51
1:C:73:LEU:O	1:C:74:CYS:C	2.50	0.51
1:A:404:LEU:HD11	1:A:421:GLN:HG3	1.92	0.50
1:B:458:GLY:O	1:B:459:ALA:C	2.48	0.50
1:A:379:THR:HG22	1:A:380:LYS:HG3	1.94	0.50
1:A:532:ARG:O	1:A:535:PHE:HB3	2.11	0.50
1:B:499:SER:O	1:B:501:GLN:N	2.44	0.50
1:B:557:GLY:HA3	2:B:1574:FBP:O3	2.11	0.50
1:D:367:VAL:O	1:D:400:ASP:N	2.44	0.50
1:D:522:GLU:CD	1:D:531:ARG:HE	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:538:GLU:O	1:D:539:SER:C	2.50	0.50
1:A:318:GLU:O	1:A:322:ARG:HG3	2.11	0.50
1:C:108:ILE:HD13	1:C:151:VAL:HG21	1.94	0.50
1:C:347:GLU:CD	1:C:347:GLU:H	2.15	0.50
1:D:77:ASP:HB3	1:D:80:SER:HB2	1.93	0.50
1:A:240:VAL:HG12	1:A:240:VAL:O	2.11	0.50
1:B:217:ILE:N	1:B:226:LEU:O	2.44	0.50
1:C:83:VAL:O	1:C:83:VAL:CG1	2.60	0.50
1:C:438:PHE:CZ	1:C:442:ARG:HD3	2.47	0.50
1:A:350:PHE:CZ	1:C:428:ALA:HA	2.47	0.50
1:B:108:ILE:HD13	1:B:151:VAL:HG21	1.94	0.50
1:A:557:GLY:HA3	2:A:1574:FBP:O3	2.11	0.50
1:B:349:VAL:O	1:B:352:ALA:N	2.45	0.50
1:C:177:LEU:HD11	1:C:246:LEU:HD22	1.94	0.50
1:D:66:ALA:CB	1:D:71:GLU:HG2	2.42	0.50
1:D:441:LEU:O	1:D:443:ARG:N	2.45	0.50
1:A:561:GLY:O	2:A:1574:FBP:O4	2.23	0.50
1:C:471:ILE:HD13	1:C:484:LEU:HD22	1.93	0.50
1:B:141:PHE:C	1:B:143:GLY:N	2.64	0.50
1:C:226:LEU:CD2	1:C:240:VAL:HG22	2.41	0.50
1:A:146:LEU:HB3	1:A:542:LEU:HD12	1.93	0.50
1:A:387:GLU:O	1:A:388:THR:C	2.47	0.50
1:B:407:GLU:OE1	1:B:407:GLU:N	2.27	0.50
1:C:423:ALA:O	1:C:424:ILE:C	2.50	0.50
1:C:474:LEU:HD22	1:C:556:THR:HG22	1.94	0.50
1:D:373:MET:O	1:D:374:LEU:HD12	2.12	0.50
1:A:522:GLU:CD	1:A:531:ARG:HE	2.16	0.49
1:B:86:ARG:O	1:B:86:ARG:HG3	2.05	0.49
1:B:437:LEU:HD12	1:B:437:LEU:C	2.32	0.49
1:C:433:TYR:O	1:C:435:ARG:N	2.45	0.49
1:D:174:GLU:OE2	1:D:245:VAL:CG1	2.54	0.49
1:C:58:GLN:O	1:C:60:GLN:N	2.45	0.49
1:C:219:ILE:HB	1:C:224:ILE:CG2	2.43	0.49
1:C:227:VAL:O	1:C:238:THR:HB	2.13	0.49
1:B:398:GLY:O	1:B:399:ALA:C	2.50	0.49
1:C:395:VAL:HG11	1:C:429:GLU:HG3	1.94	0.49
1:D:229:GLN:CG	1:D:237:VAL:O	2.58	0.49
1:C:196:ASN:OD1	1:C:199:THR:HB	2.12	0.49
1:A:88:THR:HG22	1:A:401:CYS:HA	1.93	0.49
1:A:179:LYS:CD	1:A:179:LYS:NZ	2.76	0.49
1:C:193:THR:O	1:C:193:THR:CG2	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:434:HIS:HA	1:C:437:LEU:HB3	1.93	0.49
1:C:474:LEU:CD2	1:C:529:VAL:HG13	2.42	0.49
1:D:185:VAL:HG22	1:D:200:VAL:HG23	1.93	0.49
1:B:134:VAL:O	1:B:138:VAL:HG23	2.12	0.49
1:A:266:GLU:O	1:A:269:VAL:HB	2.12	0.49
1:C:525:TRP:NE1	1:C:560:PRO:HG3	2.27	0.49
1:D:196:ASN:C	1:D:198:ASN:N	2.63	0.49
1:A:82:PRO:O	1:A:83:VAL:HG23	2.12	0.49
1:A:402:ILE:O	1:A:402:ILE:CG1	2.60	0.49
1:B:434:HIS:HA	1:B:437:LEU:HB3	1.95	0.49
1:B:561:GLY:O	2:B:1574:FBP:O4	2.15	0.49
1:D:474:LEU:HD21	1:D:529:VAL:HG13	1.94	0.49
1:B:391:VAL:O	1:B:392:ALA:C	2.49	0.49
1:C:337:ARG:NH2	1:C:390:ASP:OD2	2.38	0.49
1:B:434:HIS:O	1:B:435:ARG:C	2.51	0.49
1:C:533:VAL:HG12	1:C:534:GLN:N	2.28	0.49
1:B:87:SER:HB3	1:B:511:GLY:HA2	1.95	0.48
1:C:85:ALA:CB	1:C:513:PHE:CE2	2.95	0.48
1:A:219:ILE:O	1:A:220:ASP:O	2.31	0.48
1:A:352:ALA:HB1	1:A:356:MET:CE	2.42	0.48
1:C:141:PHE:C	1:C:143:GLY:N	2.66	0.48
1:C:174:GLU:CD	1:C:245:VAL:CG1	2.81	0.48
1:C:175:VAL:HG12	1:C:176:GLU:N	2.28	0.48
1:C:217:ILE:HD13	1:C:254:LEU:CD2	2.43	0.48
1:D:66:ALA:HB1	1:D:71:GLU:CG	2.43	0.48
1:A:348:LYS:HZ3	1:C:427:GLU:CD	2.16	0.48
1:B:104:LEU:O	1:B:105:LYS:C	2.51	0.48
1:C:416:GLU:CD	1:C:416:GLU:H	2.16	0.48
1:A:255:PRO:C	1:A:257:ALA:N	2.67	0.48
1:C:91:ILE:HG12	1:C:114:ILE:HB	1.94	0.48
1:C:182:GLN:HA	1:C:182:GLN:NE2	2.24	0.48
1:A:283:VAL:HG23	1:A:308:ILE:CG2	2.43	0.48
1:A:559:ARG:HD2	1:A:564:TYR:CD1	2.48	0.48
1:B:391:VAL:HB	1:B:424:ILE:HG21	1.96	0.48
1:C:217:ILE:N	1:C:226:LEU:O	2.45	0.48
1:C:545:PHE:HB2	1:C:546:LEU:HD23	1.96	0.48
1:D:73:LEU:C	1:D:75:LEU:H	2.16	0.48
1:A:367:VAL:O	1:A:367:VAL:CG1	2.61	0.48
1:C:225:SER:CB	1:C:242:ASN:HB2	2.36	0.48
1:C:361:ASN:HD21	1:C:488:ARG:HH21	1.62	0.48
1:C:441:LEU:O	1:C:444:ALA:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:438:PHE:CZ	1:D:442:ARG:HD3	2.48	0.48
1:A:175:VAL:CG1	1:A:176:GLU:H	2.23	0.48
1:D:196:ASN:C	1:D:198:ASN:H	2.17	0.48
1:D:330:SER:O	1:D:365:LYS:NZ	2.30	0.48
1:A:174:GLU:CB	1:A:245:VAL:CG1	2.92	0.48
1:A:434:HIS:O	1:A:437:LEU:HB3	2.13	0.48
1:C:81:GLU:OE1	1:C:81:GLU:CA	2.60	0.48
1:C:104:LEU:O	1:C:105:LYS:C	2.52	0.48
1:D:226:LEU:HD23	1:D:240:VAL:HA	1.96	0.48
1:A:281:ASP:C	1:A:282:ILE:HG13	2.35	0.48
1:C:456:ALA:O	1:C:457:ILE:C	2.52	0.48
1:D:73:LEU:C	1:D:75:LEU:N	2.64	0.48
1:A:133:ASN:O	1:A:134:VAL:C	2.53	0.47
1:A:420:MET:CE	1:C:347:GLU:HG3	2.44	0.47
1:B:133:ASN:O	1:B:134:VAL:C	2.49	0.47
1:B:158:LYS:O	1:B:158:LYS:HG2	2.13	0.47
1:B:565:THR:O	1:B:566:ASN:HB3	2.14	0.47
1:C:475:THR:O	1:C:497:THR:HB	2.14	0.47
1:D:434:HIS:O	1:D:435:ARG:C	2.53	0.47
1:A:58:GLN:O	1:A:60:GLN:N	2.47	0.47
1:A:194:ARG:HH11	1:A:194:ARG:HG2	1.79	0.47
1:A:474:LEU:CD2	1:A:529:VAL:HG13	2.44	0.47
1:B:102:GLU:O	1:B:105:LYS:HB2	2.14	0.47
1:B:378:ILE:HD11	1:B:406:GLY:HA3	1.96	0.47
1:C:267:GLN:O	1:C:268:ASP:C	2.51	0.47
1:C:433:TYR:O	1:C:433:TYR:CG	2.67	0.47
1:A:405:SER:O	1:A:406:GLY:C	2.53	0.47
1:C:474:LEU:HD21	1:C:529:VAL:HG13	1.95	0.47
1:D:271:ASP:O	1:D:274:PHE:HB3	2.15	0.47
1:A:141:PHE:C	1:A:143:GLY:N	2.67	0.47
1:A:385:ARG:NE	1:C:341:GLY:HA3	2.29	0.47
1:A:456:ALA:O	1:A:457:ILE:C	2.51	0.47
1:D:310:ILE:N	1:D:331:ASP:OD2	2.35	0.47
1:D:570:VAL:C	1:D:571:LEU:HD23	2.34	0.47
1:A:545:PHE:CB	1:A:546:LEU:HD23	2.44	0.47
1:D:474:LEU:N	1:D:474:LEU:CD1	2.78	0.47
1:A:322:ARG:HH21	1:A:325:GLU:CD	2.18	0.47
1:A:350:PHE:O	1:A:354:LYS:HG3	2.15	0.47
1:A:404:LEU:HD23	1:A:404:LEU:HA	1.59	0.47
1:A:499:SER:O	1:A:500:ALA:C	2.53	0.47
1:B:315:GLU:HG3	1:B:336:ALA:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:THR:HG23	1:C:400:ASP:O	2.14	0.47
1:C:525:TRP:CD1	1:C:560:PRO:HG3	2.48	0.47
1:D:434:HIS:O	1:D:437:LEU:HB3	2.14	0.47
1:B:551:LEU:HD23	1:B:551:LEU:HA	1.72	0.47
1:C:166:ILE:HA	1:C:248:SER:HB3	1.96	0.47
1:C:188:ASP:OD1	1:C:188:ASP:C	2.52	0.47
1:C:331:ASP:O	1:C:366:PRO:HD2	2.14	0.47
1:C:416:GLU:O	1:C:417:ALA:C	2.50	0.47
1:C:434:HIS:O	1:C:437:LEU:HB3	2.15	0.47
1:D:557:GLY:HA3	2:D:1574:FBP:O3	2.14	0.47
1:A:182:GLN:HA	1:A:182:GLN:NE2	2.27	0.47
1:A:551:LEU:HD23	1:A:551:LEU:HA	1.66	0.47
1:C:85:ALA:HB1	1:C:513:PHE:HE2	1.78	0.47
1:D:218:TYR:HB3	1:D:222:GLY:HA2	1.97	0.47
1:C:166:ILE:HD12	1:C:166:ILE:N	2.22	0.47
1:C:228:VAL:HA	1:C:238:THR:HG22	1.97	0.47
1:D:327:LEU:HD22	1:D:365:LYS:HD2	1.96	0.47
1:A:501:GLN:O	1:A:502:ALA:C	2.50	0.47
1:B:134:VAL:HG12	1:B:135:ARG:N	2.28	0.47
1:B:322:ARG:NH2	1:B:325:GLU:OE2	2.45	0.47
1:B:506:VAL:O	1:B:506:VAL:HG13	2.15	0.47
1:B:420:MET:C	1:B:422:HIS:N	2.64	0.46
1:A:313:LYS:HD2	1:A:334:MET:SD	2.56	0.46
1:A:371:THR:OG1	3:A:1575:PGA:O1	2.25	0.46
1:B:70:LEU:CD2	1:D:362:LEU:HD12	2.45	0.46
1:C:86:ARG:CB	1:C:426:ARG:HG2	2.46	0.46
1:D:500:ALA:HA	1:D:516:LEU:HD13	1.96	0.46
1:A:146:LEU:HD22	1:A:539:SER:HA	1.97	0.46
1:A:416:GLU:H	1:A:416:GLU:CD	2.15	0.46
1:A:474:LEU:HD21	1:A:529:VAL:HG13	1.96	0.46
1:B:155:LEU:C	1:B:155:LEU:CD2	2.82	0.46
1:B:267:GLN:O	1:B:268:ASP:C	2.53	0.46
1:B:297:VAL:CG1	1:B:310:ILE:HD13	2.46	0.46
1:A:66:ALA:O	1:A:433:TYR:OH	2.25	0.46
1:A:87:SER:HB2	1:A:511:GLY:CA	2.46	0.46
1:B:478:GLY:O	1:B:479:ARG:C	2.53	0.46
1:C:141:PHE:C	1:C:143:GLY:H	2.19	0.46
1:D:551:LEU:HD23	1:D:551:LEU:HA	1.64	0.46
1:A:350:PHE:HZ	1:C:428:ALA:HA	1.81	0.46
1:B:102:GLU:OE1	1:B:105:LYS:HD2	2.16	0.46
1:C:67:ASP:HA	1:C:435:ARG:NH1	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LEU:HD21	1:C:362:LEU:HD12	1.98	0.46
1:B:297:VAL:HG11	1:B:310:ILE:HD13	1.96	0.46
1:B:566:ASN:OD1	1:B:567:ILE:HG13	2.16	0.46
1:C:545:PHE:CB	1:C:546:LEU:HD23	2.45	0.46
1:A:120:SER:HA	1:A:158:LYS:HG3	1.97	0.46
1:A:433:TYR:O	1:A:434:HIS:C	2.54	0.46
1:A:488:ARG:HH12	1:A:510:ARG:CB	2.29	0.46
1:B:321:LYS:HA	1:B:321:LYS:HD3	1.56	0.46
1:C:377:MET:HA	1:C:380:LYS:O	2.16	0.46
1:D:258:GLN:O	1:D:258:GLN:CG	2.59	0.46
1:A:209:ARG:NH1	1:A:210:VAL:HG21	2.31	0.46
1:A:457:ILE:HG23	1:A:458:GLY:N	2.31	0.46
1:A:499:SER:O	1:A:502:ALA:N	2.48	0.46
1:B:60:GLN:HB2	1:B:430:ALA:O	2.16	0.46
1:B:66:ALA:HB1	1:B:71:GLU:CG	2.45	0.46
1:C:569:ARG:HG2	1:D:567:ILE:HG12	1.97	0.46
1:B:502:ALA:O	1:B:504:ARG:N	2.49	0.46
1:C:420:MET:O	1:C:421:GLN:C	2.51	0.46
1:D:175:VAL:CG1	1:D:197:ALA:HA	2.44	0.46
1:D:191:PHE:HA	1:D:194:ARG:HB2	1.98	0.46
1:D:387:GLU:O	1:D:388:THR:C	2.54	0.46
1:A:179:LYS:CG	1:A:179:LYS:HE2	2.45	0.45
1:B:250:LYS:O	1:B:251:GLY:C	2.52	0.45
1:B:438:PHE:CZ	1:B:442:ARG:HD3	2.52	0.45
1:A:202:VAL:O	1:A:202:VAL:HG12	2.16	0.45
1:A:73:LEU:O	1:A:75:LEU:N	2.49	0.45
1:A:391:VAL:CG1	1:A:424:ILE:HG21	2.46	0.45
1:C:322:ARG:C	1:C:326:ILE:HD12	2.37	0.45
1:C:340:LEU:O	1:C:344:ILE:HG12	2.16	0.45
1:D:83:VAL:O	1:D:83:VAL:HG13	2.16	0.45
1:A:174:GLU:HB3	1:A:245:VAL:CG1	2.46	0.45
1:A:465:LYS:HE3	1:B:448:SER:HB3	1.98	0.45
1:B:241:GLU:HG2	1:B:241:GLU:O	2.16	0.45
1:B:339:ASP:OD2	3:B:1575:PGA:O1	2.33	0.45
1:C:286:SER:HA	1:C:313:LYS:HE2	1.97	0.45
1:C:301:LEU:HD12	1:C:301:LEU:HA	1.86	0.45
1:D:438:PHE:O	1:D:439:GLU:C	2.54	0.45
1:A:337:ARG:HH22	1:A:390:ASP:CG	2.19	0.45
1:A:484:LEU:O	1:A:489:PRO:HD3	2.16	0.45
1:A:68:THR:HB	1:C:440:GLU:OE2	2.17	0.45
1:A:457:ILE:HG12	1:B:461:GLU:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ASN:OD1	1:B:120:SER:HB2	2.16	0.45
1:B:226:LEU:HD23	1:B:240:VAL:HA	1.98	0.45
1:C:160:PRO:HD2	1:C:287:PHE:CD1	2.52	0.45
1:A:209:ARG:O	1:A:209:ARG:HD3	2.17	0.45
1:A:479:ARG:HG3	1:A:479:ARG:NH1	2.32	0.45
1:B:362:LEU:HD12	1:D:70:LEU:CD2	2.46	0.45
1:C:434:HIS:O	1:C:435:ARG:C	2.54	0.45
1:D:202:VAL:HG12	1:D:204:TYR:H	1.81	0.45
1:A:163:ARG:HH11	1:A:163:ARG:HB3	1.82	0.45
1:B:66:ALA:CB	1:B:71:GLU:HG2	2.47	0.45
1:C:559:ARG:HD2	1:C:564:TYR:CD1	2.52	0.45
1:D:141:PHE:C	1:D:143:GLY:N	2.69	0.45
1:D:474:LEU:CD2	1:D:529:VAL:HG13	2.47	0.45
1:D:499:SER:O	1:D:502:ALA:N	2.50	0.45
1:B:367:VAL:HG13	1:B:399:ALA:HA	1.99	0.45
1:A:167:LEU:HD21	1:A:175:VAL:HB	1.99	0.45
1:B:160:PRO:HG3	1:B:263:GLY:HA2	1.99	0.45
1:B:498:ARG:HG2	1:B:517:TYR:O	2.16	0.45
1:B:568:MET:CE	1:B:570:VAL:HG23	2.47	0.45
1:C:86:ARG:NH2	1:C:90:ILE:HD12	2.31	0.45
1:D:95:GLY:O	1:D:96:PRO:C	2.55	0.45
1:D:188:ASP:O	1:D:190:ALA:N	2.49	0.45
1:A:377:MET:HA	1:A:380:LYS:O	2.17	0.44
1:B:95:GLY:O	1:B:96:PRO:C	2.53	0.44
1:B:97:ALA:O	1:B:103:ARG:HD3	2.17	0.44
1:B:273:ARG:O	1:B:277:GLU:HG3	2.17	0.44
1:C:152:ALA:HA	1:C:504:ARG:HD2	1.99	0.44
1:C:219:ILE:HB	1:C:224:ILE:HB	1.99	0.44
1:D:321:LYS:HA	1:D:321:LYS:HD3	1.36	0.44
1:A:119:PHE:O	1:A:158:LYS:HB2	2.16	0.44
1:B:78:ILE:CD1	1:D:320:VAL:HG11	2.46	0.44
1:B:474:LEU:HD21	1:B:529:VAL:HG13	1.99	0.44
1:C:261:LEU:HD12	1:C:261:LEU:HA	1.57	0.44
1:D:61:LEU:O	1:D:65:MET:HG2	2.18	0.44
1:D:488:ARG:NH1	1:D:510:ARG:CB	2.80	0.44
1:A:434:HIS:O	1:A:435:ARG:C	2.55	0.44
1:C:97:ALA:O	1:C:103:ARG:HD3	2.16	0.44
1:A:168:GLN:HE22	1:A:196:ASN:HB3	1.82	0.44
1:C:86:ARG:NH1	1:C:422:HIS:ND1	2.63	0.44
1:C:134:VAL:O	1:C:138:VAL:HG23	2.17	0.44
1:C:176:GLU:OE1	1:C:178:VAL:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:478:GLY:O	1:C:479:ARG:C	2.56	0.44
1:B:352:ALA:HB1	1:B:356:MET:HE2	1.99	0.44
1:B:362:LEU:HD12	1:D:70:LEU:HD21	1.99	0.44
1:C:391:VAL:CG1	1:C:424:ILE:CG2	2.95	0.44
1:A:77:ASP:HB3	1:A:80:SER:HB2	1.99	0.44
1:A:188:ASP:C	1:A:190:ALA:N	2.71	0.44
1:A:193:THR:C	1:A:195:GLY:H	2.21	0.44
1:A:204:TYR:CD2	1:A:204:TYR:C	2.91	0.44
1:A:566:ASN:OD1	1:A:567:ILE:HG13	2.18	0.44
1:C:566:ASN:OD1	1:C:567:ILE:HG13	2.17	0.44
1:A:242:ASN:ND2	1:C:381:PRO:HB2	2.33	0.44
1:B:75:LEU:HD23	1:B:75:LEU:HA	1.83	0.44
1:B:320:VAL:HG11	1:D:78:ILE:CD1	2.48	0.44
1:B:341:GLY:HA3	1:D:385:ARG:HE	1.83	0.44
1:C:191:PHE:O	1:C:194:ARG:N	2.46	0.44
1:D:181:SER:O	1:D:240:VAL:HG23	2.18	0.44
1:A:194:ARG:HG2	1:A:194:ARG:NH1	2.33	0.44
1:A:404:LEU:HD22	1:A:407:GLU:HB2	1.99	0.44
1:A:568:MET:HE1	1:A:570:VAL:HG23	1.98	0.44
1:B:123:SER:HB2	1:B:125:GLU:OE1	2.18	0.44
1:C:61:LEU:HD12	1:C:61:LEU:HA	1.75	0.44
1:C:191:PHE:O	1:C:193:THR:N	2.51	0.44
1:C:213:VAL:HA	1:C:228:VAL:HG12	1.99	0.44
1:D:155:LEU:C	1:D:155:LEU:CD2	2.83	0.44
1:A:174:GLU:HB2	1:A:245:VAL:CG1	2.48	0.44
1:B:83:VAL:O	1:B:83:VAL:CG1	2.66	0.44
1:B:488:ARG:NH1	1:B:510:ARG:HB2	2.29	0.44
1:D:337:ARG:HH22	1:D:390:ASP:CG	2.21	0.44
1:D:370:ALA:O	1:D:371:THR:CB	2.66	0.44
1:D:501:GLN:O	1:D:502:ALA:C	2.54	0.44
1:D:568:MET:HE1	1:D:570:VAL:HG23	2.00	0.44
1:A:108:ILE:HG12	1:A:112:MET:CE	2.48	0.43
1:A:191:PHE:CD1	1:A:191:PHE:N	2.86	0.43
1:A:191:PHE:O	1:A:193:THR:N	2.51	0.43
1:A:219:ILE:CG2	1:A:246:LEU:HD13	2.47	0.43
1:B:385:ARG:HG3	1:D:337:ARG:HB3	1.99	0.43
1:C:167:LEU:HD12	1:C:167:LEU:HA	1.76	0.43
1:C:475:THR:HA	2:C:1574:FBP:H61	2.00	0.43
1:D:87:SER:HB2	1:D:511:GLY:N	2.33	0.43
1:D:281:ASP:C	1:D:282:ILE:HG13	2.38	0.43
1:C:66:ALA:HB1	1:C:71:GLU:CG	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:500:ALA:HA	1:C:516:LEU:HD13	1.99	0.43
1:C:545:PHE:C	1:C:546:LEU:HD23	2.38	0.43
1:D:178:VAL:HG12	1:D:179:LYS:O	2.17	0.43
1:A:155:LEU:C	1:A:155:LEU:CD2	2.76	0.43
1:A:301:LEU:HD12	1:A:301:LEU:HA	1.87	0.43
1:B:86:ARG:HB3	1:B:426:ARG:HG2	1.99	0.43
1:B:149:ARG:HE	1:B:149:ARG:HB2	1.67	0.43
1:B:379:THR:O	1:B:379:THR:HG22	2.18	0.43
1:B:522:GLU:CD	1:B:531:ARG:HE	2.22	0.43
1:C:101:VAL:O	1:C:101:VAL:HG12	2.17	0.43
1:C:406:GLY:O	1:C:408:THR:N	2.50	0.43
1:D:220:ASP:OD1	1:D:220:ASP:C	2.57	0.43
1:A:78:ILE:HD13	1:C:320:VAL:HG11	2.00	0.43
1:A:391:VAL:HG12	1:A:424:ILE:CG2	2.48	0.43
1:A:503:ALA:O	1:A:514:PRO:HG3	2.18	0.43
1:B:273:ARG:HD2	1:B:273:ARG:HA	1.74	0.43
1:B:377:MET:HA	1:B:380:LYS:O	2.18	0.43
1:B:379:THR:O	1:B:379:THR:CG2	2.65	0.43
1:C:61:LEU:N	1:C:62:PRO:CD	2.82	0.43
1:D:488:ARG:CZ	1:D:510:ARG:HD3	2.49	0.43
1:A:125:GLU:CD	1:A:125:GLU:N	2.71	0.43
1:B:61:LEU:HD12	1:B:61:LEU:HA	1.78	0.43
1:B:125:GLU:CD	1:B:125:GLU:N	2.68	0.43
1:B:488:ARG:HH12	1:B:510:ARG:CB	2.29	0.43
1:C:480:SER:O	1:C:481:ALA:C	2.50	0.43
1:D:532:ARG:O	1:D:535:PHE:HB3	2.19	0.43
1:B:474:LEU:CD2	1:B:529:VAL:HG13	2.49	0.43
1:B:525:TRP:CE2	1:B:560:PRO:HG3	2.54	0.43
1:C:391:VAL:HG12	1:C:424:ILE:HG21	1.98	0.43
1:C:533:VAL:O	1:C:536:GLY:N	2.52	0.43
1:D:234:GLU:C	1:D:234:GLU:OE1	2.57	0.43
1:D:499:SER:C	1:D:501:GLN:N	2.72	0.43
1:B:73:LEU:O	1:B:75:LEU:N	2.51	0.43
1:B:87:SER:CB	1:B:511:GLY:CA	2.97	0.43
1:B:377:MET:O	1:B:378:ILE:C	2.54	0.43
1:C:317:HIS:O	1:C:318:GLU:C	2.55	0.43
1:D:450:ASP:O	1:D:454:VAL:HG23	2.19	0.43
1:A:60:GLN:HB2	1:A:430:ALA:O	2.19	0.43
1:A:384:THR:N	1:A:387:GLU:OE1	2.35	0.43
1:A:483:LEU:HD23	1:A:483:LEU:HA	1.78	0.43
1:B:85:ALA:HB1	1:B:513:PHE:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:PHE:C	1:B:143:GLY:H	2.22	0.43
1:C:452:THR:HG23	1:C:565:THR:HB	2.00	0.43
1:A:410:LYS:HE3	1:A:410:LYS:HB2	1.72	0.43
1:B:93:THR:OG1	1:B:116:ARG:NH1	2.44	0.43
1:B:151:VAL:O	1:B:504:ARG:HD3	2.18	0.43
1:C:434:HIS:NE2	1:C:490:ARG:HB2	2.33	0.43
1:D:89:SER:HB2	1:D:401:CYS:SG	2.58	0.43
1:B:89:SER:CB	1:B:401:CYS:HB3	2.45	0.43
1:B:457:ILE:CG2	1:B:458:GLY:H	2.31	0.43
1:B:514:PRO:O	1:B:515:LEU:HD23	2.19	0.43
1:B:533:VAL:O	1:B:536:GLY:N	2.51	0.43
1:C:167:LEU:O	1:C:169:GLY:N	2.52	0.43
1:C:457:ILE:CG2	1:C:458:GLY:N	2.81	0.43
1:D:413:PHE:N	1:D:414:PRO:HD3	2.34	0.43
1:A:296:ALA:O	1:A:297:VAL:C	2.58	0.42
1:A:545:PHE:HB2	1:A:546:LEU:HD23	1.99	0.42
1:D:163:ARG:HA	1:D:250:LYS:O	2.18	0.42
1:B:322:ARG:C	1:B:326:ILE:HD12	2.38	0.42
1:B:406:GLY:O	1:B:407:GLU:C	2.57	0.42
1:C:176:GLU:OE1	1:C:178:VAL:CG2	2.67	0.42
1:C:188:ASP:HA	1:C:189:PRO:HD3	1.93	0.42
1:A:210:VAL:O	1:A:210:VAL:CG1	2.67	0.42
1:A:220:ASP:HB2	1:A:250:LYS:HB3	2.02	0.42
1:A:223:LEU:O	1:C:381:PRO:HG2	2.19	0.42
1:A:329:VAL:HG12	1:A:329:VAL:O	2.19	0.42
1:B:93:THR:HA	1:B:116:ARG:HB3	2.00	0.42
1:B:100:SER:O	1:B:104:LEU:HD22	2.18	0.42
1:B:220:ASP:C	1:B:222:GLY:H	2.22	0.42
1:B:297:VAL:HG12	1:B:310:ILE:CD1	2.50	0.42
1:B:570:VAL:C	1:B:571:LEU:HD23	2.40	0.42
1:C:502:ALA:O	1:C:503:ALA:C	2.57	0.42
1:D:146:LEU:HD22	1:D:539:SER:HA	2.01	0.42
1:D:393:ASN:C	1:D:395:VAL:N	2.71	0.42
1:A:188:ASP:HB3	1:A:191:PHE:HD1	1.85	0.42
1:A:441:LEU:C	1:A:443:ARG:N	2.72	0.42
1:A:568:MET:CE	1:A:570:VAL:HG23	2.49	0.42
1:B:227:VAL:C	1:B:238:THR:HB	2.39	0.42
1:C:220:ASP:OD1	1:C:220:ASP:C	2.57	0.42
1:D:196:ASN:O	1:D:198:ASN:N	2.53	0.42
1:A:120:SER:OG	1:A:161:GLU:OE2	2.30	0.42
1:B:285:ALA:O	1:B:313:LYS:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:GLN:O	1:C:230:LYS:HG2	2.20	0.42
1:D:348:LYS:O	1:D:349:VAL:C	2.56	0.42
1:A:304:GLU:H	1:A:304:GLU:HG2	1.55	0.42
1:B:502:ALA:C	1:B:504:ARG:N	2.73	0.42
1:C:146:LEU:CD2	1:C:535:PHE:CE1	3.02	0.42
1:C:266:GLU:O	1:C:269:VAL:HB	2.19	0.42
1:C:329:VAL:HG12	1:C:329:VAL:O	2.19	0.42
1:D:333:ILE:HD13	1:D:333:ILE:HA	1.92	0.42
1:C:184:LEU:O	1:C:199:THR:HA	2.19	0.42
1:C:502:ALA:C	1:C:504:ARG:N	2.71	0.42
1:D:286:SER:HA	1:D:313:LYS:HE2	2.01	0.42
1:D:525:TRP:O	1:D:526:ALA:C	2.58	0.42
1:A:162:ILE:HB	1:A:252:VAL:HB	2.02	0.42
1:A:261:LEU:HD12	1:A:261:LEU:HA	1.67	0.42
1:B:336:ALA:CB	3:B:1575:PGA:H22	2.49	0.42
1:C:466:CYS:O	1:C:467:CYS:HB2	2.18	0.42
1:A:273:ARG:HD2	1:A:273:ARG:HA	1.74	0.42
1:A:460:VAL:HG22	1:A:489:PRO:HG3	2.02	0.42
1:B:423:ALA:O	1:B:424:ILE:C	2.58	0.42
1:C:66:ALA:CB	1:C:71:GLU:HG2	2.48	0.42
1:C:175:VAL:HG13	1:C:197:ALA:HA	1.99	0.42
1:C:377:MET:C	1:C:379:THR:N	2.71	0.42
1:D:402:ILE:O	1:D:402:ILE:CG1	2.68	0.42
1:D:503:ALA:O	1:D:514:PRO:CB	2.68	0.42
1:A:204:TYR:O	1:A:204:TYR:CG	2.68	0.42
1:C:393:ASN:O	1:C:394:ALA:C	2.56	0.42
1:D:157:THR:HG22	1:D:286:SER:HB2	2.02	0.42
1:D:416:GLU:H	1:D:416:GLU:CD	2.22	0.42
1:A:224:ILE:HD11	1:A:244:GLY:O	2.20	0.41
1:B:86:ARG:CB	1:B:426:ARG:HG2	2.50	0.41
1:C:95:GLY:O	1:C:96:PRO:C	2.58	0.41
1:C:253:ASN:ND2	1:C:342:ILE:HD12	2.34	0.41
1:C:475:THR:HG21	1:C:478:GLY:HA2	2.02	0.41
1:C:488:ARG:C	1:C:489:PRO:O	2.55	0.41
1:D:331:ASP:O	1:D:366:PRO:HD2	2.20	0.41
1:B:360:CYS:O	1:B:361:ASN:C	2.58	0.41
1:B:441:LEU:O	1:B:444:ALA:N	2.53	0.41
1:C:364:GLY:HA2	1:C:486:TRP:CD1	2.55	0.41
1:C:377:MET:O	1:C:378:ILE:C	2.58	0.41
1:C:448:SER:OG	1:C:449:ARG:N	2.52	0.41
1:D:138:VAL:HG12	1:D:139:GLU:OE2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ASP:HB3	1:A:80:SER:CB	2.50	0.41
1:A:223:LEU:HD22	1:C:380:LYS:HZ3	1.85	0.41
1:A:362:LEU:HD13	1:C:74:CYS:SG	2.61	0.41
1:B:76:LEU:HA	1:B:76:LEU:HD23	1.85	0.41
1:B:499:SER:O	1:B:500:ALA:C	2.58	0.41
1:C:350:PHE:O	1:C:354:LYS:HG3	2.19	0.41
1:C:483:LEU:HA	1:C:483:LEU:HD23	1.66	0.41
1:D:182:GLN:HE21	1:D:182:GLN:HA	1.85	0.41
1:D:266:GLU:O	1:D:269:VAL:HB	2.20	0.41
1:A:212:PRO:O	1:A:213:VAL:C	2.58	0.41
1:B:348:LYS:O	1:B:349:VAL:C	2.58	0.41
1:C:185:VAL:HG11	1:C:236:LEU:HD12	2.02	0.41
1:C:204:TYR:HE1	1:C:261:LEU:HD13	1.85	0.41
1:D:111:GLY:O	1:D:112:MET:C	2.56	0.41
1:D:434:HIS:HA	1:D:437:LEU:HB3	2.01	0.41
1:A:193:THR:O	1:A:195:GLY:N	2.49	0.41
1:A:216:ARG:CG	1:A:218:TYR:CE1	2.94	0.41
1:B:157:THR:HG22	1:B:286:SER:HB2	2.03	0.41
1:C:175:VAL:CG1	1:C:176:GLU:N	2.83	0.41
1:C:487:TYR:O	1:C:488:ARG:CB	2.46	0.41
1:C:509:CYS:O	1:C:510:ARG:C	2.58	0.41
1:D:61:LEU:N	1:D:62:PRO:CD	2.84	0.41
1:D:175:VAL:HG12	1:D:177:LEU:HD21	2.02	0.41
1:D:367:VAL:O	1:D:367:VAL:HG13	2.20	0.41
1:D:391:VAL:CG1	1:D:424:ILE:HG21	2.50	0.41
1:A:91:ILE:HG13	1:A:114:ILE:HB	2.03	0.41
1:A:114:ILE:HG12	1:A:152:ALA:HB3	2.03	0.41
1:A:134:VAL:O	1:A:135:ARG:C	2.59	0.41
1:B:88:THR:N	1:B:429:GLU:OE2	2.49	0.41
1:B:164:THR:HG23	1:B:252:VAL:CG2	2.42	0.41
1:C:82:PRO:O	1:C:83:VAL:CG2	2.63	0.41
1:D:175:VAL:HG13	1:D:197:ALA:HA	2.02	0.41
1:A:163:ARG:HA	1:A:250:LYS:O	2.20	0.41
1:A:289:ARG:HG3	1:A:293:ASP:OD2	2.21	0.41
1:A:322:ARG:HE	1:A:322:ARG:HB3	1.59	0.41
1:C:501:GLN:O	1:C:502:ALA:C	2.57	0.41
1:A:175:VAL:HG11	1:A:197:ALA:CA	2.50	0.41
1:A:380:LYS:CE	1:C:223:LEU:HD13	2.50	0.41
1:A:398:GLY:O	1:A:399:ALA:C	2.59	0.41
1:C:460:VAL:O	1:C:461:GLU:C	2.57	0.41
1:C:565:THR:O	1:C:566:ASN:HB3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:LEU:HB2	1:D:542:LEU:CD1	2.48	0.41
1:D:309:LYS:HG2	1:D:505:GLN:HG2	2.03	0.41
1:A:66:ALA:HB1	1:A:71:GLU:HB3	2.03	0.41
1:B:82:PRO:O	1:B:83:VAL:HG23	2.21	0.41
1:B:137:ALA:O	1:B:140:SER:OG	2.38	0.41
1:B:366:PRO:HA	1:B:400:ASP:OD2	2.21	0.41
1:B:545:PHE:HB2	1:B:546:LEU:CD2	2.50	0.41
1:C:348:LYS:O	1:C:349:VAL:C	2.59	0.41
1:C:379:THR:O	1:C:379:THR:CG2	2.68	0.41
1:C:391:VAL:O	1:C:392:ALA:C	2.56	0.41
1:C:433:TYR:CD2	1:C:436:GLN:HB3	2.56	0.41
1:D:118:ASN:C	1:D:118:ASN:OD1	2.57	0.41
1:D:219:ILE:HG21	1:D:246:LEU:CD1	2.51	0.41
1:D:239:GLN:O	1:D:241:GLU:N	2.54	0.41
1:D:293:ASP:O	1:D:296:ALA:HB3	2.21	0.41
1:D:322:ARG:C	1:D:326:ILE:HD12	2.41	0.41
1:D:379:THR:O	1:D:379:THR:HG22	2.20	0.41
1:A:506:VAL:O	1:A:506:VAL:HG13	2.21	0.41
1:B:416:GLU:OE1	1:B:416:GLU:N	2.39	0.41
1:A:209:ARG:CD	1:A:209:ARG:C	2.90	0.40
1:A:367:VAL:O	1:A:400:ASP:HB2	2.20	0.40
1:B:114:ILE:HG12	1:B:152:ALA:HB3	2.04	0.40
1:B:450:ASP:HA	1:B:451:PRO:HD3	1.83	0.40
1:C:138:VAL:CG1	1:C:139:GLU:OE2	2.70	0.40
1:D:174:GLU:HB2	1:D:245:VAL:HG13	2.02	0.40
1:D:315:GLU:HG3	1:D:336:ALA:HB3	2.02	0.40
1:D:367:VAL:H	1:D:400:ASP:HB2	1.86	0.40
1:D:433:TYR:O	1:D:435:ARG:N	2.54	0.40
1:D:450:ASP:HA	1:D:451:PRO:HD3	1.87	0.40
1:A:191:PHE:C	1:A:193:THR:H	2.24	0.40
1:A:497:THR:CG2	1:A:503:ALA:HB2	2.51	0.40
1:A:539:SER:O	1:A:543:ARG:HG3	2.21	0.40
1:B:220:ASP:O	1:B:222:GLY:N	2.54	0.40
1:B:324:ASP:CG	1:B:359:ARG:HH21	2.24	0.40
1:B:337:ARG:HH22	1:B:390:ASP:CG	2.25	0.40
1:B:457:ILE:HG23	1:B:458:GLY:H	1.81	0.40
1:B:539:SER:O	1:B:543:ARG:HG3	2.21	0.40
1:B:559:ARG:HD2	1:B:564:TYR:CD1	2.56	0.40
1:D:102:GLU:O	1:D:105:LYS:HB2	2.21	0.40
1:D:299:ALA:O	1:D:300:ALA:C	2.60	0.40
1:A:333:ILE:CG2	1:A:334:MET:N	2.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:ARG:HG3	1:A:479:ARG:HH11	1.85	0.40
1:A:538:GLU:O	1:A:539:SER:C	2.59	0.40
1:D:488:ARG:HH11	1:D:488:ARG:HD3	1.73	0.40
1:A:75:LEU:HD23	1:A:75:LEU:HA	1.90	0.40
1:B:162:ILE:O	1:B:252:VAL:HG23	2.21	0.40
1:B:420:MET:CE	1:D:347:GLU:HG3	2.51	0.40
1:C:149:ARG:HE	1:C:149:ARG:HB2	1.72	0.40
1:C:164:THR:HA	1:C:201:TRP:O	2.21	0.40
1:C:448:SER:CB	1:C:453:GLU:OE2	2.70	0.40
1:C:506:VAL:CG1	1:C:514:PRO:HD3	2.52	0.40
1:D:290:LYS:O	1:D:293:ASP:HB2	2.22	0.40
1:D:353:GLN:NE2	1:D:397:ASP:OD2	2.54	0.40
1:A:433:TYR:CD2	1:A:436:GLN:HB3	2.56	0.40
1:B:73:LEU:O	1:B:74:CYS:C	2.59	0.40
1:B:220:ASP:C	1:B:222:GLY:N	2.74	0.40
1:B:488:ARG:HH11	1:B:510:ARG:HB3	1.84	0.40
1:C:189:PRO:O	1:C:192:ARG:HB2	2.22	0.40
1:C:211:VAL:HA	1:C:212:PRO:HD3	1.75	0.40
1:C:352:ALA:HB1	1:C:356:MET:CE	2.51	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:ARG:NH1	1:D:273:ARG:NH2[1_556]	1.60	0.60
1:A:209:ARG:NE	1:C:449:ARG:CD[1_655]	2.01	0.19
1:A:209:ARG:NH2	1:C:449:ARG:CD[1_655]	2.06	0.14

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	515/528 (98%)	431 (84%)	65 (13%)	19 (4%)	3 12
1	B	445/528 (84%)	385 (86%)	49 (11%)	11 (2%)	5 19
1	C	511/528 (97%)	440 (86%)	60 (12%)	11 (2%)	6 22
1	D	509/528 (96%)	438 (86%)	57 (11%)	14 (3%)	5 17
All	All	1980/2112 (94%)	1694 (86%)	231 (12%)	55 (3%)	5 17

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	83	VAL
1	A	192	ARG
1	A	220	ASP
1	A	489	PRO
1	A	566	ASN
1	B	59	GLN
1	B	220	ASP
1	B	566	ASN
1	C	59	GLN
1	C	74	CYS
1	C	83	VAL
1	C	192	ARG
1	C	500	ALA
1	D	83	VAL
1	D	240	VAL
1	D	375	GLU
1	D	500	ALA
1	D	566	ASN
1	A	74	CYS
1	A	119	PHE
1	A	222	GLY
1	A	228	VAL
1	A	256	GLY
1	A	500	ALA
1	B	83	VAL
1	B	143	GLY
1	B	500	ALA
1	C	168	GLN
1	C	566	ASN
1	D	74	CYS
1	A	338	GLY
1	B	205	PRO

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Mol	Chain	Res	Type
1	B	206	ASN
1	B	489	PRO
1	C	220	ASP
1	D	59	GLN
1	D	220	ASP
1	A	189	PRO
1	A	441	LEU
1	D	143	GLY
1	D	207	ILE
1	A	213	VAL
1	A	234	GLU
1	A	371	THR
1	B	74	CYS
1	B	371	THR
1	C	371	THR
1	C	441	LEU
1	D	489	PRO
1	D	519	GLU
1	D	538	GLU
1	A	519	GLU
1	D	533	VAL
1	C	205	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	414/423 (98%)	339 (82%)	75 (18%)	1 4
1	B	372/423 (88%)	320 (86%)	52 (14%)	3 9
1	C	412/423 (97%)	354 (86%)	58 (14%)	3 9
1	D	412/423 (97%)	352 (85%)	60 (15%)	3 8
All	All	1610/1692 (95%)	1365 (85%)	245 (15%)	3 7

All (245) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	61	LEU
1	A	65	MET
1	A	99	ARG
1	A	103	ARG
1	A	104	LEU
1	A	108	ILE
1	A	120	SER
1	A	149	ARG
1	A	155	LEU
1	A	157	THR
1	A	158	LYS
1	A	162	ILE
1	A	163	ARG
1	A	167	LEU
1	A	168	GLN
1	A	174	GLU
1	A	176	GLU
1	A	177	LEU
1	A	182	GLN
1	A	184	LEU
1	A	186	THR
1	A	194	ARG
1	A	202	VAL
1	A	209	ARG
1	A	217	ILE
1	A	221	ASP
1	A	223	LEU
1	A	224	ILE
1	A	225	SER
1	A	230	LYS
1	A	231	ILE
1	A	234	GLU
1	A	237	VAL
1	A	250	LYS
1	A	261	LEU
1	A	273	ARG
1	A	289	ARG
1	A	294	VAL
1	A	301	LEU
1	A	304	GLU
1	A	310	ILE
1	A	321	LYS

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Mol	Chain	Res	Type
1	A	322	ARG
1	A	327	LEU
1	A	337	ARG
1	A	347	GLU
1	A	361	ASN
1	A	362	LEU
1	A	375	GLU
1	A	382	ARG
1	A	389	SER
1	A	396	LEU
1	A	401	CYS
1	A	402	ILE
1	A	410	LYS
1	A	420	MET
1	A	421	GLN
1	A	437	LEU
1	A	443	ARG
1	A	449	ARG
1	A	455	THR
1	A	480	SER
1	A	490	ARG
1	A	501	GLN
1	A	506	VAL
1	A	508	LEU
1	A	539	SER
1	A	542	LEU
1	A	543	ARG
1	A	546	LEU
1	A	548	VAL
1	A	552	VAL
1	A	559	ARG
1	A	568	MET
1	B	59	GLN
1	B	61	LEU
1	B	65	MET
1	B	86	ARG
1	B	99	ARG
1	B	103	ARG
1	B	104	LEU
1	B	108	ILE
1	B	120	SER
1	B	144	SER

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Mol	Chain	Res	Type
1	B	155	LEU
1	B	157	THR
1	B	164	THR
1	B	186	THR
1	B	226	LEU
1	B	254	LEU
1	B	261	LEU
1	B	273	ARG
1	B	281	ASP
1	B	289	ARG
1	B	294	VAL
1	B	301	LEU
1	B	304	GLU
1	B	321	LYS
1	B	322	ARG
1	B	327	LEU
1	B	337	ARG
1	B	347	GLU
1	B	361	ASN
1	B	362	LEU
1	B	374	LEU
1	B	377	MET
1	B	388	THR
1	B	389	SER
1	B	396	LEU
1	B	401	CYS
1	B	402	ILE
1	B	420	MET
1	B	443	ARG
1	B	449	ARG
1	B	450	ASP
1	B	455	THR
1	B	506	VAL
1	B	508	LEU
1	B	539	SER
1	B	542	LEU
1	B	543	ARG
1	B	546	LEU
1	B	548	VAL
1	B	552	VAL
1	B	559	ARG
1	B	568	MET

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Mol	Chain	Res	Type
1	C	61	LEU
1	C	87	SER
1	C	99	ARG
1	C	103	ARG
1	C	104	LEU
1	C	108	ILE
1	C	120	SER
1	C	139	GLU
1	C	157	THR
1	C	158	LYS
1	C	166	ILE
1	C	167	LEU
1	C	172	GLU
1	C	173	SER
1	C	182	GLN
1	C	186	THR
1	C	187	VAL
1	C	192	ARG
1	C	193	THR
1	C	209	ARG
1	C	217	ILE
1	C	225	SER
1	C	229	GLN
1	C	231	ILE
1	C	234	GLU
1	C	246	LEU
1	C	261	LEU
1	C	273	ARG
1	C	289	ARG
1	C	294	VAL
1	C	301	LEU
1	C	304	GLU
1	C	310	ILE
1	C	313	LYS
1	C	321	LYS
1	C	327	LEU
1	C	337	ARG
1	C	347	GLU
1	C	361	ASN
1	C	362	LEU
1	C	389	SER
1	C	396	LEU

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Mol	Chain	Res	Type
1	C	410	LYS
1	C	420	MET
1	C	443	ARG
1	C	449	ARG
1	C	455	THR
1	C	497	THR
1	C	506	VAL
1	C	508	LEU
1	C	539	SER
1	C	542	LEU
1	C	543	ARG
1	C	546	LEU
1	C	548	VAL
1	C	552	VAL
1	C	559	ARG
1	C	568	MET
1	D	59	GLN
1	D	61	LEU
1	D	83	VAL
1	D	86	ARG
1	D	88	THR
1	D	99	ARG
1	D	103	ARG
1	D	104	LEU
1	D	157	THR
1	D	158	LYS
1	D	166	ILE
1	D	167	LEU
1	D	174	GLU
1	D	177	LEU
1	D	182	GLN
1	D	186	THR
1	D	193	THR
1	D	202	VAL
1	D	209	ARG
1	D	229	GLN
1	D	234	GLU
1	D	239	GLN
1	D	246	LEU
1	D	250	LYS
1	D	258	GLN
1	D	273	ARG

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Mol	Chain	Res	Type
1	D	289	ARG
1	D	294	VAL
1	D	301	LEU
1	D	304	GLU
1	D	313	LYS
1	D	321	LYS
1	D	322	ARG
1	D	327	LEU
1	D	333	ILE
1	D	337	ARG
1	D	347	GLU
1	D	361	ASN
1	D	362	LEU
1	D	380	LYS
1	D	389	SER
1	D	396	LEU
1	D	402	ILE
1	D	420	MET
1	D	443	ARG
1	D	449	ARG
1	D	455	THR
1	D	480	SER
1	D	501	GLN
1	D	506	VAL
1	D	508	LEU
1	D	539	SER
1	D	542	LEU
1	D	543	ARG
1	D	546	LEU
1	D	548	VAL
1	D	552	VAL
1	D	556	THR
1	D	559	ARG
1	D	568	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	HIS
1	A	133	ASN
1	A	168	GLN
1	A	182	GLN

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Mol	Chain	Res	Type
1	A	229	GLN
1	A	239	GLN
1	A	253	ASN
1	A	361	ASN
1	A	393	ASN
1	A	421	GLN
1	B	124	HIS
1	B	133	ASN
1	B	253	ASN
1	B	361	ASN
1	B	393	ASN
1	B	436	GLN
1	C	121	HIS
1	C	133	ASN
1	C	168	GLN
1	C	182	GLN
1	C	198	ASN
1	C	253	ASN
1	C	361	ASN
1	C	393	ASN
1	C	421	GLN
1	C	436	GLN
1	D	133	ASN
1	D	182	GLN
1	D	253	ASN
1	D	258	GLN
1	D	361	ASN
1	D	393	ASN
1	D	421	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FBP	B	1574	-	18,20,20	0.88	0	23,32,32	1.24	3 (13%)
2	FBP	C	1574	-	18,20,20	1.23	1 (5%)	23,32,32	1.26	2 (8%)
2	FBP	D	1574	-	18,20,20	1.46	3 (16%)	23,32,32	1.29	3 (13%)
3	PGA	C	1575	4,5	8,8,8	4.88	1 (12%)	10,11,11	1.29	2 (20%)
3	PGA	D	1575	5	8,8,8	2.09	1 (12%)	10,11,11	1.48	2 (20%)
3	PGA	A	1575	4,5	8,8,8	1.52	1 (12%)	10,11,11	1.49	3 (30%)
2	FBP	A	1574	-	18,20,20	0.88	1 (5%)	23,32,32	1.12	1 (4%)
3	PGA	B	1575	4,5	8,8,8	1.81	1 (12%)	10,11,11	1.48	2 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FBP	B	1574	-	-	5/13/32/32	0/1/1/1
2	FBP	C	1574	-	-	5/13/32/32	0/1/1/1
2	FBP	D	1574	-	-	5/13/32/32	0/1/1/1
3	PGA	C	1575	4,5	-	6/6/6/6	-
3	PGA	D	1575	5	-	4/6/6/6	-
3	PGA	A	1575	4,5	-	5/6/6/6	-
2	FBP	A	1574	-	-	5/13/32/32	0/1/1/1
3	PGA	B	1575	4,5	-	5/6/6/6	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1575	PGA	O2-C1	13.46	1.76	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1575	PGA	O1P-C2	-5.43	1.39	1.43
3	B	1575	PGA	O1P-C2	-3.85	1.40	1.43
3	A	1575	PGA	O1P-C2	-3.70	1.40	1.43
2	D	1574	FBP	O2-C2	3.24	1.46	1.40
2	C	1574	FBP	O5-C2	-2.83	1.38	1.43
2	A	1574	FBP	O2-C2	2.66	1.45	1.40
2	D	1574	FBP	P1-O1P	2.35	1.58	1.50
2	D	1574	FBP	P2-O6	2.34	1.67	1.60

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1574	FBP	O3P-P1-O1P	3.25	123.41	110.68
3	C	1575	PGA	O1P-P-O2P	3.02	114.96	106.47
3	B	1575	PGA	O1P-C2-C1	-2.76	106.38	110.54
3	A	1575	PGA	O1P-C2-C1	-2.73	106.43	110.54
2	C	1574	FBP	O3P-P1-O1	-2.69	99.57	106.73
2	D	1574	FBP	P2-O6-C6	2.53	125.25	118.30
2	C	1574	FBP	O4-C4-C3	-2.51	104.63	112.15
2	B	1574	FBP	P1-O1-C1	2.51	125.21	118.30
3	D	1575	PGA	O4P-P-O1P	2.50	113.39	106.73
2	D	1574	FBP	O6-P2-O4P	2.48	113.44	106.47
3	D	1575	PGA	O1P-C2-C1	-2.42	106.89	110.54
3	A	1575	PGA	O2-C1-C2	2.37	124.33	113.34
3	B	1575	PGA	O1P-P-O2P	2.30	112.92	106.47
3	C	1575	PGA	O2-C1-O1	2.25	128.91	123.30
2	D	1574	FBP	P1-O1-C1	2.15	124.22	118.30
2	B	1574	FBP	O4-C4-C3	-2.06	106.00	112.15
3	A	1575	PGA	O2-C1-O1	-2.05	118.18	123.30
2	A	1574	FBP	O6-P2-O4P	2.04	112.21	106.47

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1574	FBP	C6-O6-P2-O4P
2	B	1574	FBP	O5-C5-C6-O6
2	B	1574	FBP	C6-O6-P2-O5P
2	B	1574	FBP	C6-O6-P2-O6P
2	C	1574	FBP	C6-O6-P2-O5P
2	C	1574	FBP	C6-O6-P2-O6P
2	D	1574	FBP	C6-O6-P2-O5P

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Mol	Chain	Res	Type	Atoms
2	D	1574	FBP	C6-O6-P2-O6P
3	A	1575	PGA	C2-O1P-P-O3P
3	A	1575	PGA	C2-O1P-P-O4P
3	B	1575	PGA	C2-O1P-P-O2P
3	B	1575	PGA	C2-O1P-P-O3P
3	B	1575	PGA	C2-O1P-P-O4P
3	C	1575	PGA	C2-O1P-P-O2P
3	C	1575	PGA	C2-O1P-P-O3P
3	C	1575	PGA	C2-O1P-P-O4P
3	D	1575	PGA	C2-O1P-P-O3P
3	D	1575	PGA	C2-O1P-P-O4P
2	B	1574	FBP	C4-C5-C6-O6
2	C	1574	FBP	O5-C5-C6-O6
2	D	1574	FBP	C4-C5-C6-O6
2	D	1574	FBP	O5-C5-C6-O6
3	A	1575	PGA	O1-C1-C2-O1P
3	A	1575	PGA	O2-C1-C2-O1P
3	B	1575	PGA	O2-C1-C2-O1P
3	C	1575	PGA	O2-C1-C2-O1P
3	C	1575	PGA	C1-C2-O1P-P
3	C	1575	PGA	O1-C1-C2-O1P
2	C	1574	FBP	C4-C5-C6-O6
2	B	1574	FBP	C6-O6-P2-O4P
2	C	1574	FBP	C6-O6-P2-O4P
2	D	1574	FBP	C6-O6-P2-O4P
3	A	1575	PGA	C2-O1P-P-O2P
3	D	1575	PGA	C2-O1P-P-O2P
2	A	1574	FBP	O5-C5-C6-O6
3	B	1575	PGA	O1-C1-C2-O1P
2	A	1574	FBP	C6-O6-P2-O5P
2	A	1574	FBP	C4-C5-C6-O6
2	A	1574	FBP	C6-O6-P2-O6P
3	D	1575	PGA	C1-C2-O1P-P

There are no ring outliers.

7 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1574	FBP	3	0
2	C	1574	FBP	2	0
2	D	1574	FBP	5	0
3	C	1575	PGA	5	0

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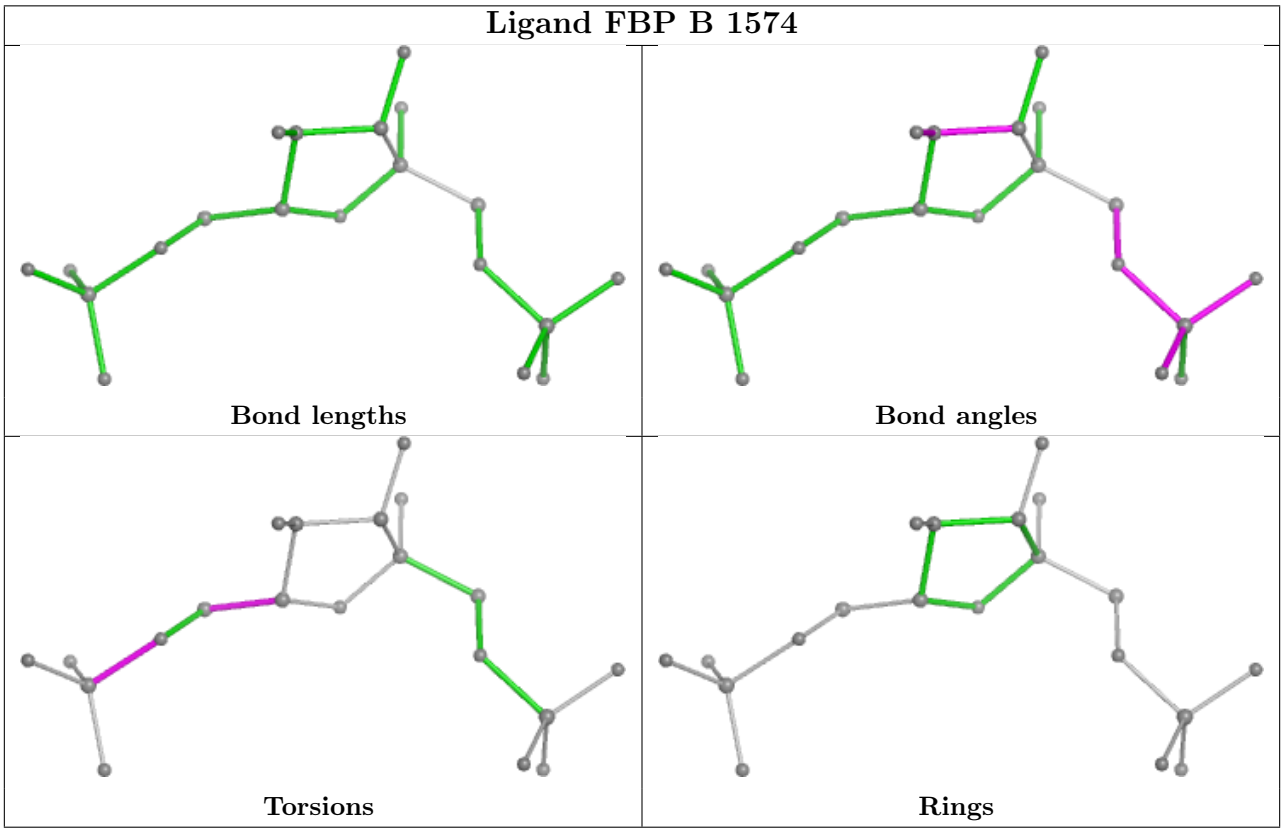
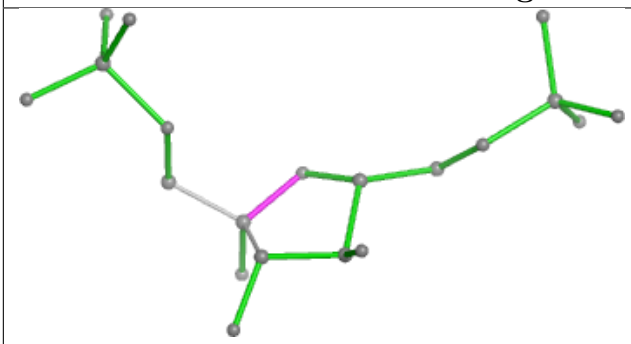
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1575	PGA	1	0
2	A	1574	FBP	3	0
3	B	1575	PGA	5	0

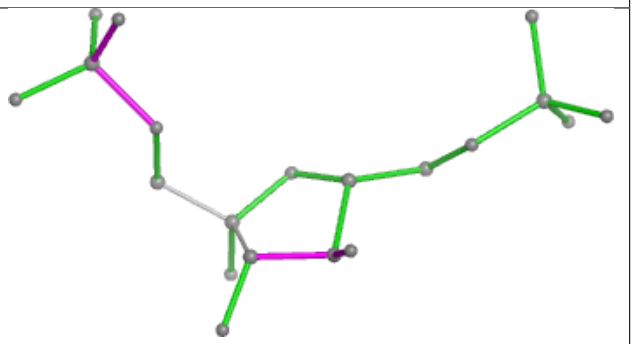
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



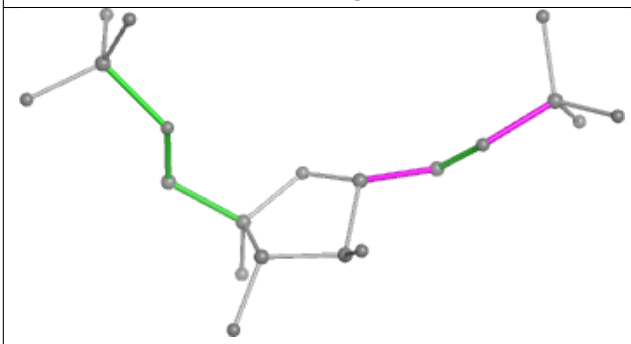
Ligand FBP C 1574



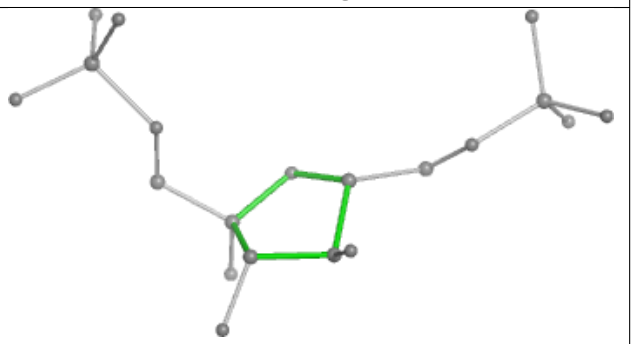
Bond lengths



Bond angles

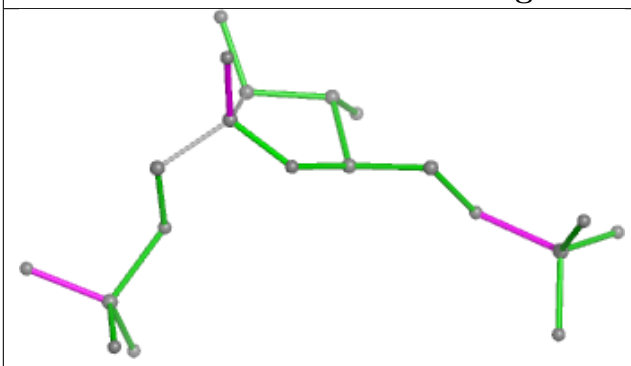


Torsions

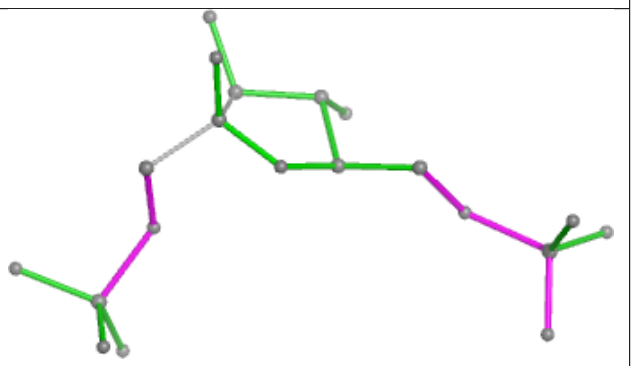


Rings

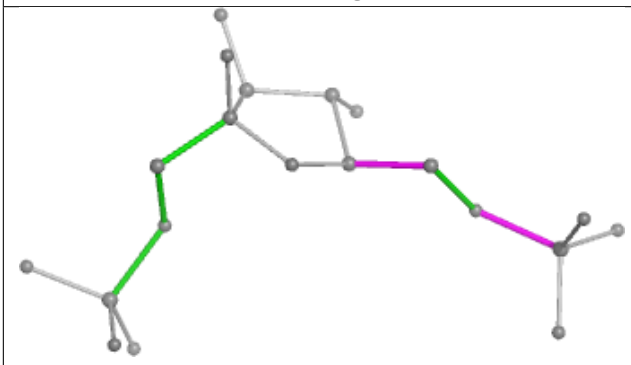
Ligand FBP D 1574



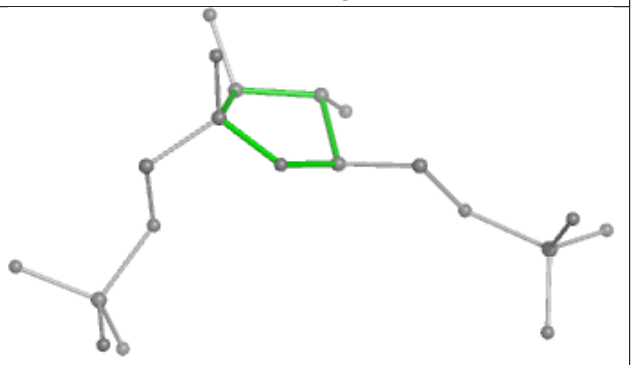
Bond lengths



Bond angles

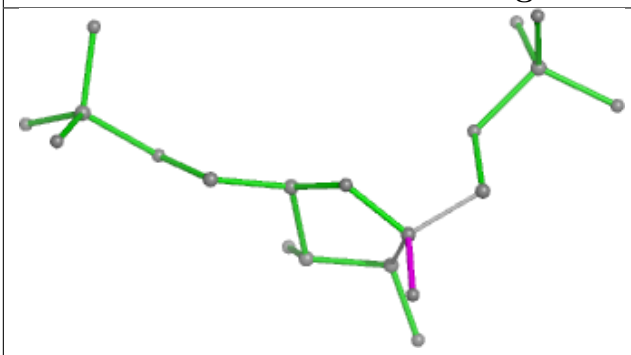


Torsions

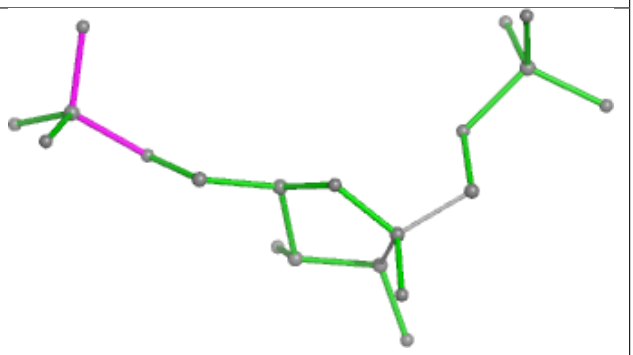


Rings

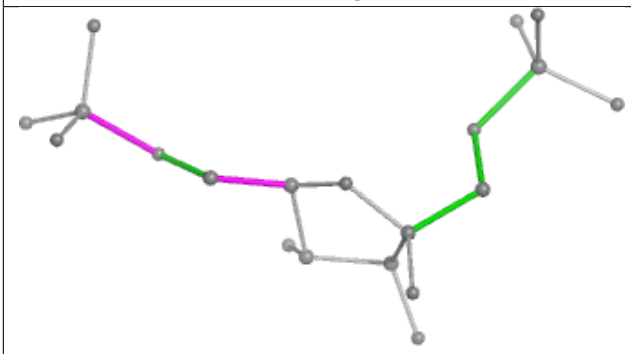
Ligand FBP A 1574



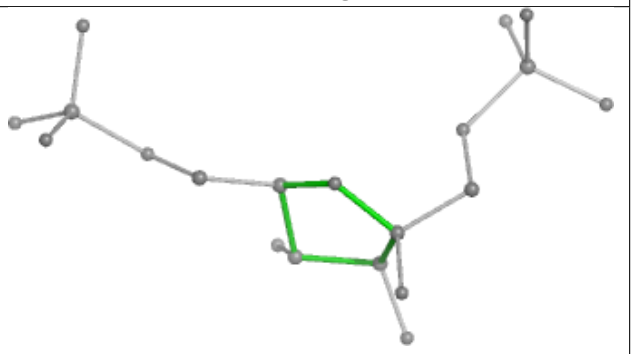
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	517/528 (97%)	0.29	18 (3%)	44	39	2, 2, 2, 2	0
1	B	463/528 (87%)	0.47	33 (7%)	16	12	2, 2, 2, 2	0
1	C	515/528 (97%)	0.25	22 (4%)	35	31	2, 2, 2, 2	0
1	D	513/528 (97%)	0.16	15 (2%)	51	48	2, 2, 2, 2	0
All	All	2008/2112 (95%)	0.29	88 (4%)	34	30	2, 2, 2, 2	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	166	ILE	8.9
1	D	146	LEU	6.9
1	A	231	ILE	6.7
1	B	204	TYR	6.1
1	B	164	THR	5.4
1	B	245	VAL	5.0
1	A	232	GLY	4.7
1	D	306	HIS	4.7
1	B	227	VAL	4.3
1	B	228	VAL	4.1
1	B	186	THR	4.1
1	B	448	SER	4.0
1	A	233	PRO	3.9
1	B	60	GLN	3.9
1	B	197	ALA	3.8
1	A	182	GLN	3.8
1	D	174	GLU	3.8
1	C	261	LEU	3.7
1	A	230	LYS	3.7
1	C	171	PRO	3.7
1	B	242	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	67	ASP	3.6
1	B	207	ILE	3.5
1	B	165	GLY	3.4
1	C	192	ARG	3.3
1	C	241	GLU	3.3
1	B	206	ASN	3.2
1	A	146	LEU	3.2
1	A	529	VAL	3.0
1	D	231	ILE	2.9
1	B	161	GLU	2.9
1	A	192	ARG	2.8
1	D	165	GLY	2.8
1	B	63	ALA	2.8
1	B	142	ALA	2.8
1	C	290	LYS	2.8
1	B	291	ALA	2.8
1	B	98	SER	2.8
1	B	531	ARG	2.8
1	B	200	VAL	2.7
1	C	287	PHE	2.7
1	D	83	VAL	2.7
1	B	162	ILE	2.6
1	A	236	LEU	2.6
1	C	173	SER	2.6
1	D	326	ILE	2.6
1	B	261	LEU	2.6
1	A	256	GLY	2.6
1	C	88	THR	2.5
1	B	524	ILE	2.5
1	A	209	ARG	2.5
1	B	240	VAL	2.5
1	C	214	GLY	2.4
1	C	524	ILE	2.4
1	C	194	ARG	2.4
1	C	314	ILE	2.4
1	C	233	PRO	2.4
1	D	191	PHE	2.4
1	A	161	GLU	2.4
1	B	57	GLN	2.4
1	B	254	LEU	2.4
1	B	511	GLY	2.3
1	C	548	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	406	GLY	2.3
1	C	407	GLU	2.3
1	D	167	LEU	2.3
1	A	228	VAL	2.3
1	B	241	GLU	2.2
1	D	248	SER	2.2
1	C	212	PRO	2.2
1	B	218	TYR	2.2
1	D	244	GLY	2.2
1	A	531	ARG	2.2
1	A	237	VAL	2.1
1	C	57	GLN	2.1
1	D	166	ILE	2.1
1	A	180	GLY	2.1
1	C	231	ILE	2.1
1	A	229	GLN	2.1
1	D	263	GLY	2.1
1	B	478	GLY	2.1
1	A	234	GLU	2.1
1	B	110	ALA	2.0
1	B	497	THR	2.0
1	C	167	LEU	2.0
1	D	531	ARG	2.0
1	C	63	ALA	2.0
1	C	84	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

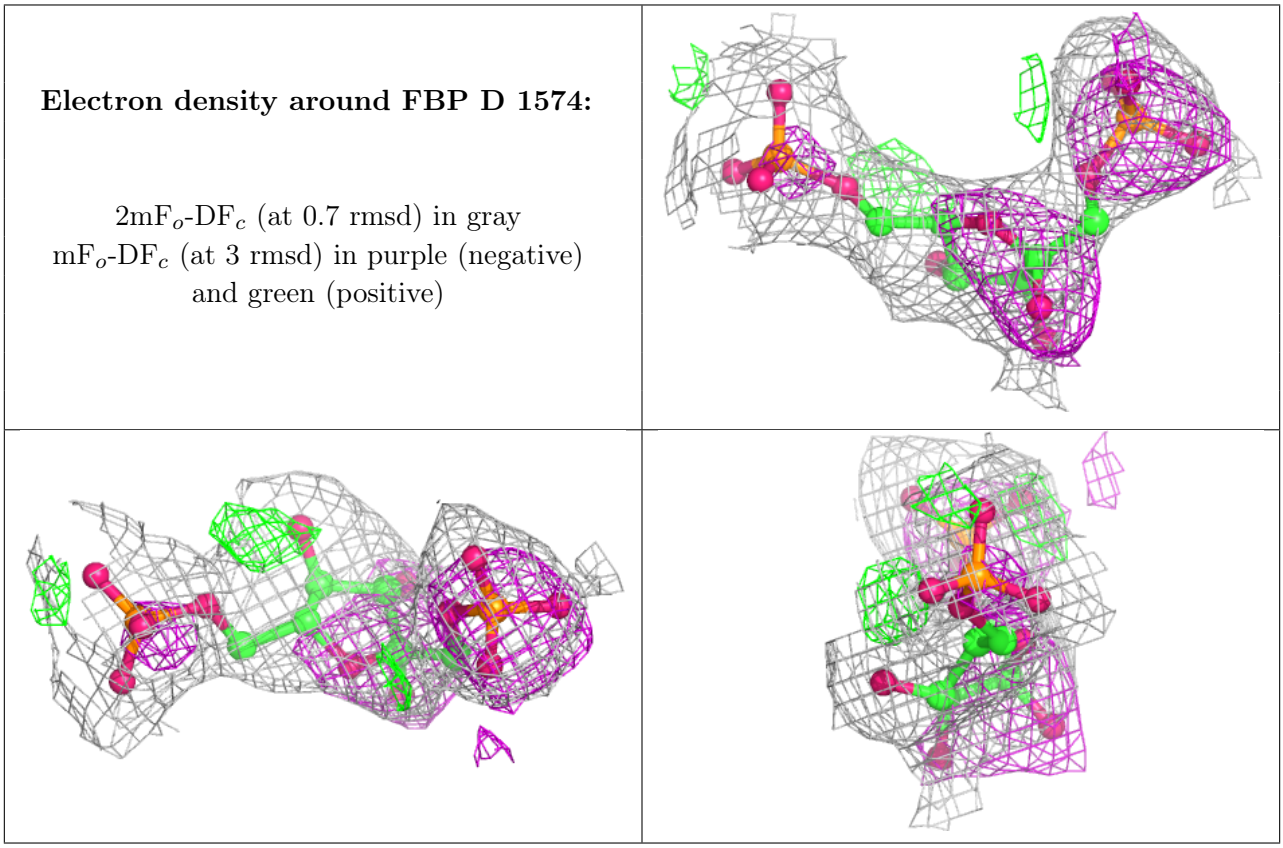
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FBP	D	1574	20/20	0.92	0.19	2,2,2,2	0
2	FBP	C	1574	20/20	0.95	0.15	2,2,2,2	0
2	FBP	B	1574	20/20	0.96	0.14	2,2,2,2	0
3	PGA	A	1575	9/9	0.96	0.18	2,2,2,2	0
3	PGA	D	1575	9/9	0.96	0.19	2,2,2,2	0
4	K	A	1576	1/1	0.96	0.08	2,2,2,2	0
4	K	B	1576	1/1	0.96	0.09	2,2,2,2	0
4	K	D	1576	1/1	0.96	0.14	2,2,2,2	0
3	PGA	B	1575	9/9	0.97	0.14	2,2,2,2	0
3	PGA	C	1575	9/9	0.97	0.14	2,2,2,2	0
4	K	C	1576	1/1	0.97	0.09	2,2,2,2	0
2	FBP	A	1574	20/20	0.97	0.17	2,2,2,2	0
5	MN	A	1577	1/1	0.97	0.05	2,2,2,2	0
5	MN	B	1577	1/1	0.97	0.07	2,2,2,2	0
5	MN	C	1577	1/1	0.99	0.04	2,2,2,2	0
5	MN	D	1577	1/1	0.99	0.06	2,2,2,2	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

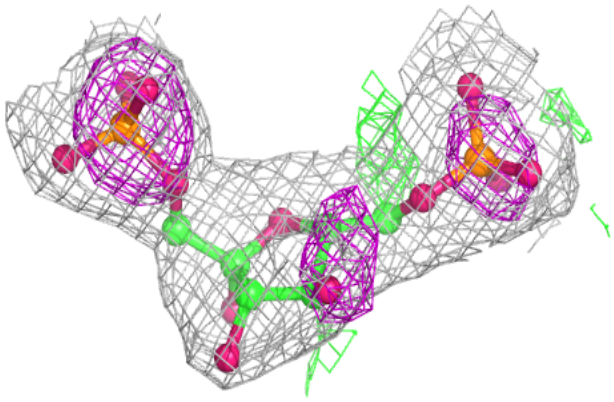
Electron density around FBP D 1574:

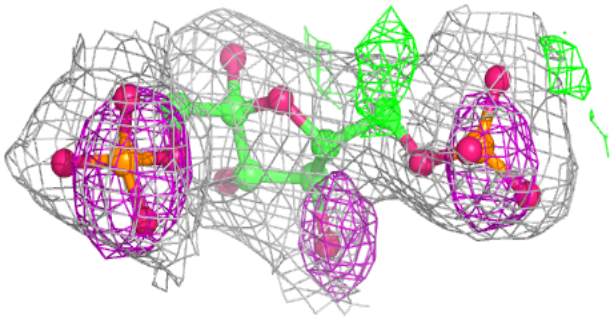
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

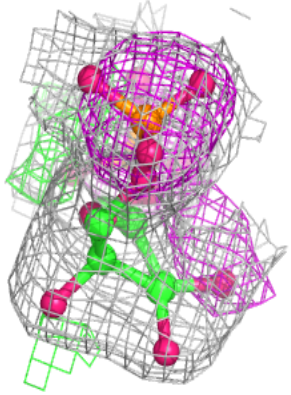


Electron density around FBP C 1574:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

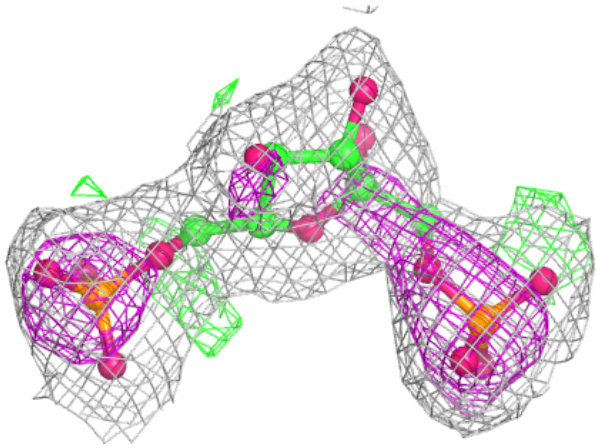


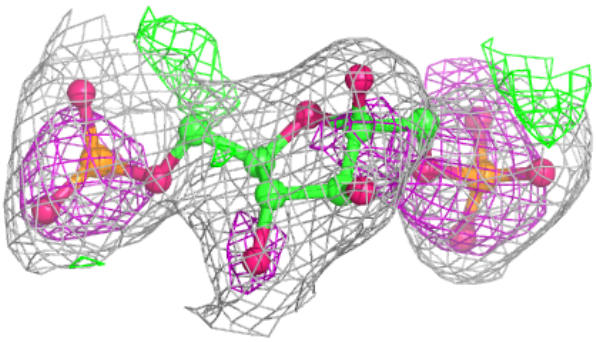


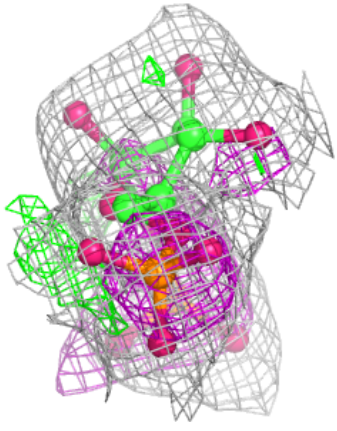


Electron density around FBP B 1574:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

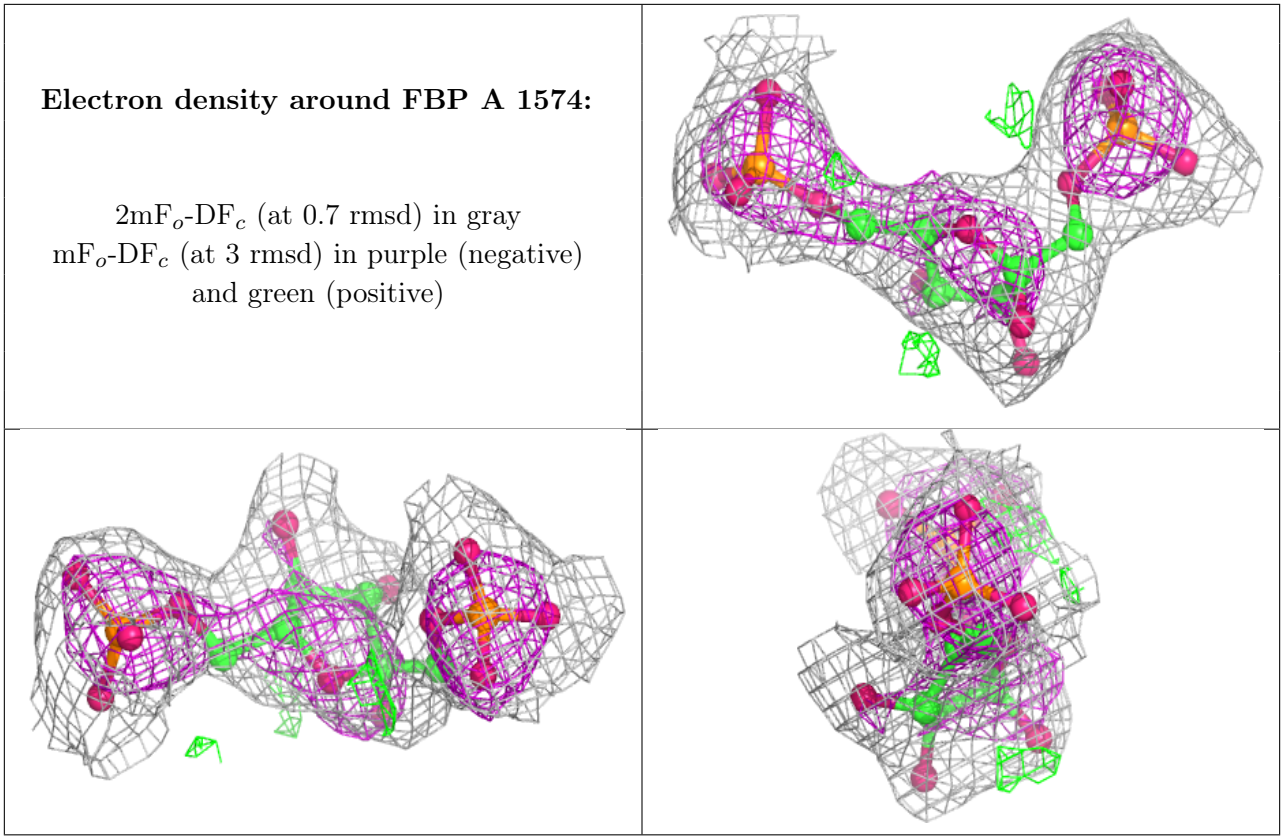






Electron density around FBP A 1574:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.