Full wwPDB X-ray Structure Validation Report (i)

Nov 13, 2023 – 10:47 AM JST

PDB ID	:	5WYD
Title	:	Structural of Pseudomonas aeruginosa DspI
Authors	:	Liu, L.; Peng, C.; Li, T.; Li, C.; He, L.; Song, Y.; Zhu, Y.; Shen, Y.; Bao, R.
Deposited on	:	2017-01-12
Resolution	:	2.10 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 (1)) were used in the production of this report:

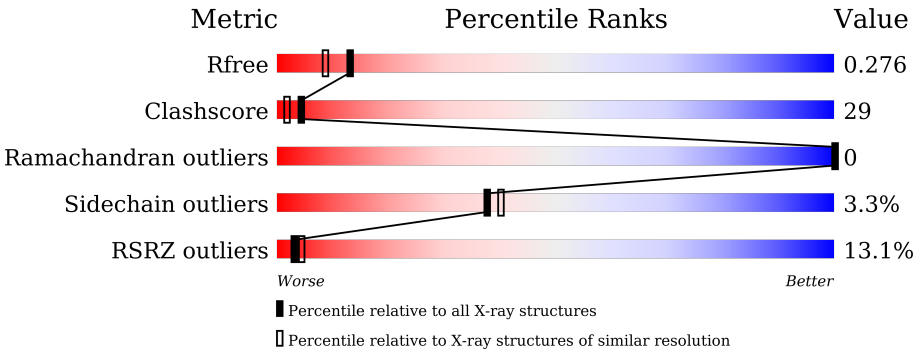
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	280	13% 49% 42% · 6%
1	B	280	11% 50% 42% · 6%
1	C	280	13% 44% 47% · 6%
1	D	280	9% 52% 39% · 6%
1	E	280	14% 48% 43% · 6%
1	F	280	13% 50% 41% · 6%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12387 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 Probable enoyl-CoA hydratase/isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	0	0
			2020	1263	375	373	9			
1	B	262	Total	C	N	O	S	0	1	0
			2030	1269	378	374	9			
1	C	262	Total	C	N	O	S	0	0	0
			2020	1263	375	373	9			
1	D	262	Total	C	N	O	S	0	0	0
			2020	1263	375	373	9			
1	E	262	Total	C	N	O	S	0	0	0
			2020	1263	375	373	9			
1	F	262	Total	C	N	O	S	0	0	0
			2020	1263	375	373	9			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	ASP	LEU	engineered mutation	UNP Q9I5I4
A	273	LEU	-	expression tag	UNP Q9I5I4
A	274	GLU	-	expression tag	UNP Q9I5I4
A	275	HIS	-	expression tag	UNP Q9I5I4
A	276	HIS	-	expression tag	UNP Q9I5I4
A	277	HIS	-	expression tag	UNP Q9I5I4
A	278	HIS	-	expression tag	UNP Q9I5I4
A	279	HIS	-	expression tag	UNP Q9I5I4
A	280	HIS	-	expression tag	UNP Q9I5I4
B	15	ASP	LEU	engineered mutation	UNP Q9I5I4
B	273	LEU	-	expression tag	UNP Q9I5I4
B	274	GLU	-	expression tag	UNP Q9I5I4
B	275	HIS	-	expression tag	UNP Q9I5I4
B	276	HIS	-	expression tag	UNP Q9I5I4
B	277	HIS	-	expression tag	UNP Q9I5I4
B	278	HIS	-	expression tag	UNP Q9I5I4
B	279	HIS	-	expression tag	UNP Q9I5I4

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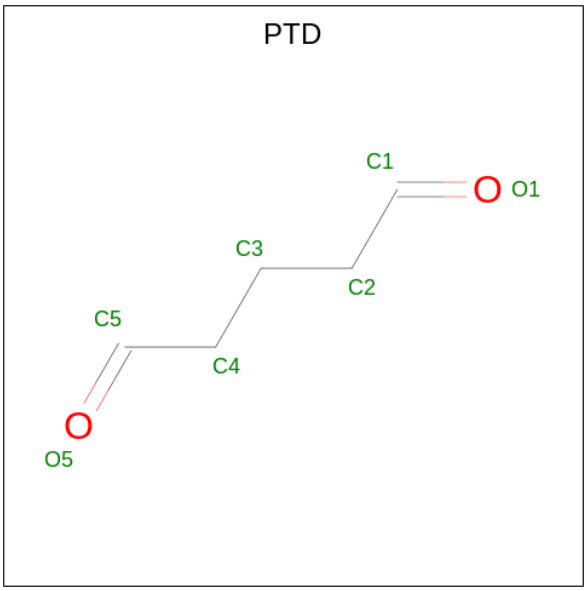
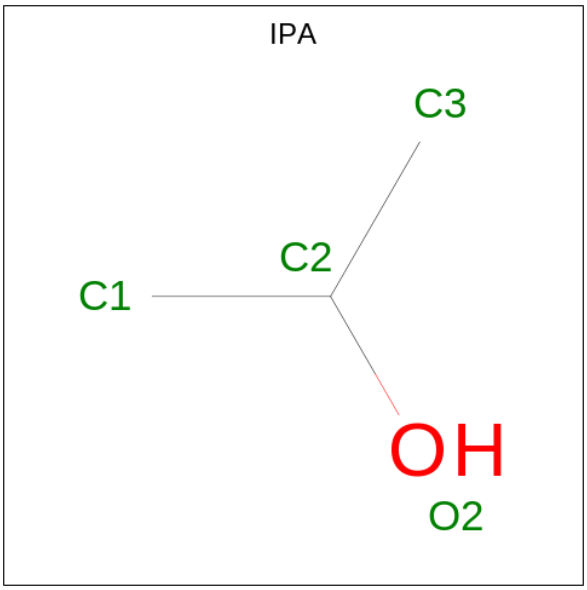
Chain	Residue	Modelled	Actual	Comment	Reference
B	280	HIS	-	expression tag	UNP Q9I5I4
C	15	ASP	LEU	engineered mutation	UNP Q9I5I4
C	273	LEU	-	expression tag	UNP Q9I5I4
C	274	GLU	-	expression tag	UNP Q9I5I4
C	275	HIS	-	expression tag	UNP Q9I5I4
C	276	HIS	-	expression tag	UNP Q9I5I4
C	277	HIS	-	expression tag	UNP Q9I5I4
C	278	HIS	-	expression tag	UNP Q9I5I4
C	279	HIS	-	expression tag	UNP Q9I5I4
C	280	HIS	-	expression tag	UNP Q9I5I4
D	15	ASP	LEU	engineered mutation	UNP Q9I5I4
D	273	LEU	-	expression tag	UNP Q9I5I4
D	274	GLU	-	expression tag	UNP Q9I5I4
D	275	HIS	-	expression tag	UNP Q9I5I4
D	276	HIS	-	expression tag	UNP Q9I5I4
D	277	HIS	-	expression tag	UNP Q9I5I4
D	278	HIS	-	expression tag	UNP Q9I5I4
D	279	HIS	-	expression tag	UNP Q9I5I4
D	280	HIS	-	expression tag	UNP Q9I5I4
E	15	ASP	LEU	engineered mutation	UNP Q9I5I4
E	273	LEU	-	expression tag	UNP Q9I5I4
E	274	GLU	-	expression tag	UNP Q9I5I4
E	275	HIS	-	expression tag	UNP Q9I5I4
E	276	HIS	-	expression tag	UNP Q9I5I4
E	277	HIS	-	expression tag	UNP Q9I5I4
E	278	HIS	-	expression tag	UNP Q9I5I4
E	279	HIS	-	expression tag	UNP Q9I5I4
E	280	HIS	-	expression tag	UNP Q9I5I4
F	15	ASP	LEU	engineered mutation	UNP Q9I5I4
F	273	LEU	-	expression tag	UNP Q9I5I4
F	274	GLU	-	expression tag	UNP Q9I5I4
F	275	HIS	-	expression tag	UNP Q9I5I4
F	276	HIS	-	expression tag	UNP Q9I5I4
F	277	HIS	-	expression tag	UNP Q9I5I4
F	278	HIS	-	expression tag	UNP Q9I5I4
F	279	HIS	-	expression tag	UNP Q9I5I4
F	280	HIS	-	expression tag	UNP Q9I5I4

- Molecule 2 is PENTANEDIAL (three-letter code: PTD) (formula: $C_5H_8O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 7 5 2	0	0
2	D	1	Total C O 6 5 1	0	0
2	E	1	Total C O 7 5 2	0	0

- Molecule 3 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 4 3 1	0	0

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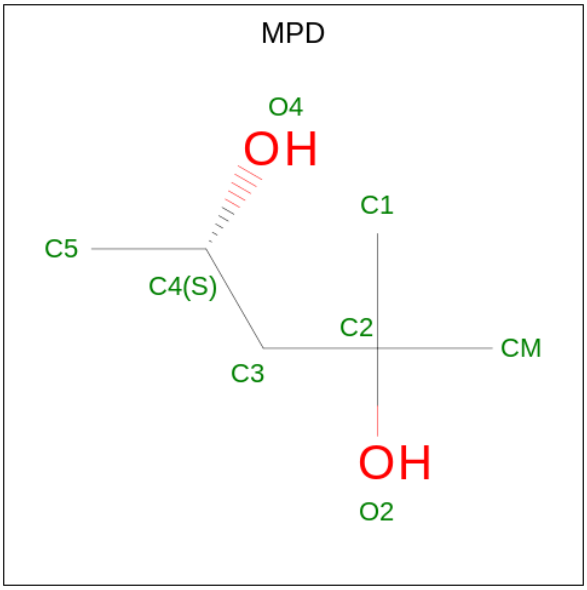
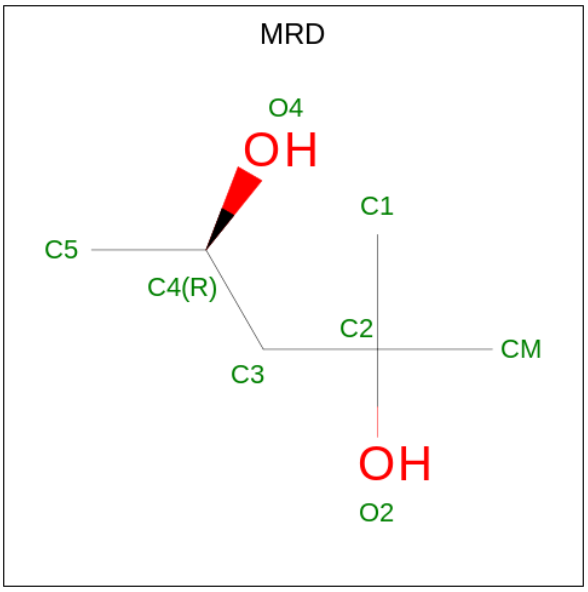
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 4 3 1	0	0
3	C	1	Total C O 4 3 1	0	0
3	E	1	Total C O 4 3 1	0	0
3	F	1	Total C O 4 3 1	0	0
3	F	1	Total C O 4 3 1	0	0
3	F	1	Total C O 4 3 1	0	0

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 8 6 2	0	0

- Molecule 5 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	1	Total C O 8 6 2	0	0

- Molecule 6 is water.

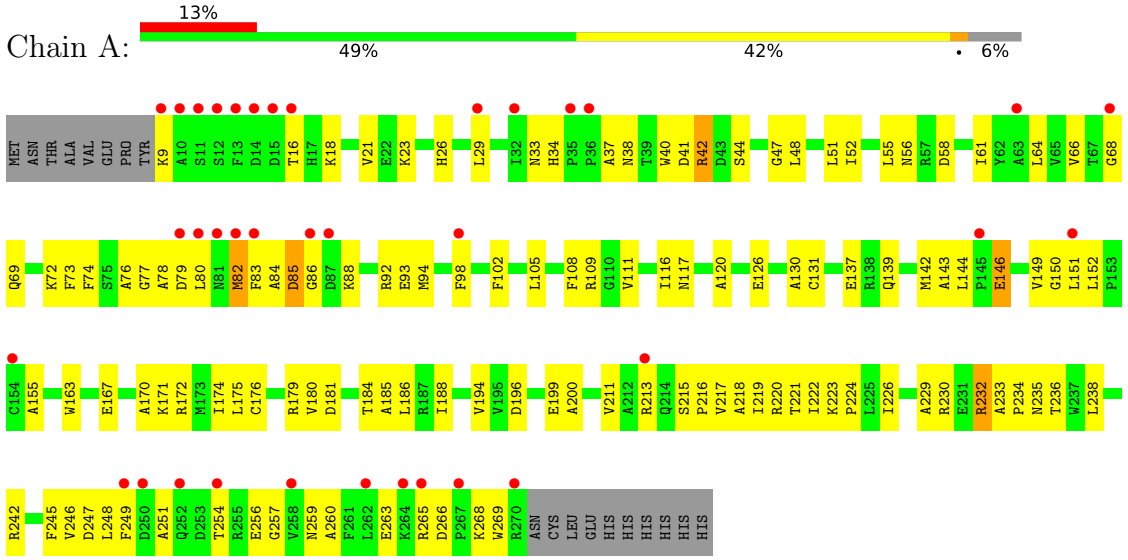
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	30	Total O 30 30	0	0
6	B	32	Total O 32 32	0	0
6	C	36	Total O 36 36	0	0
6	D	29	Total O 29 29	0	0
6	E	33	Total O 33 33	0	0
6	F	33	Total O 33 33	0	0

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.

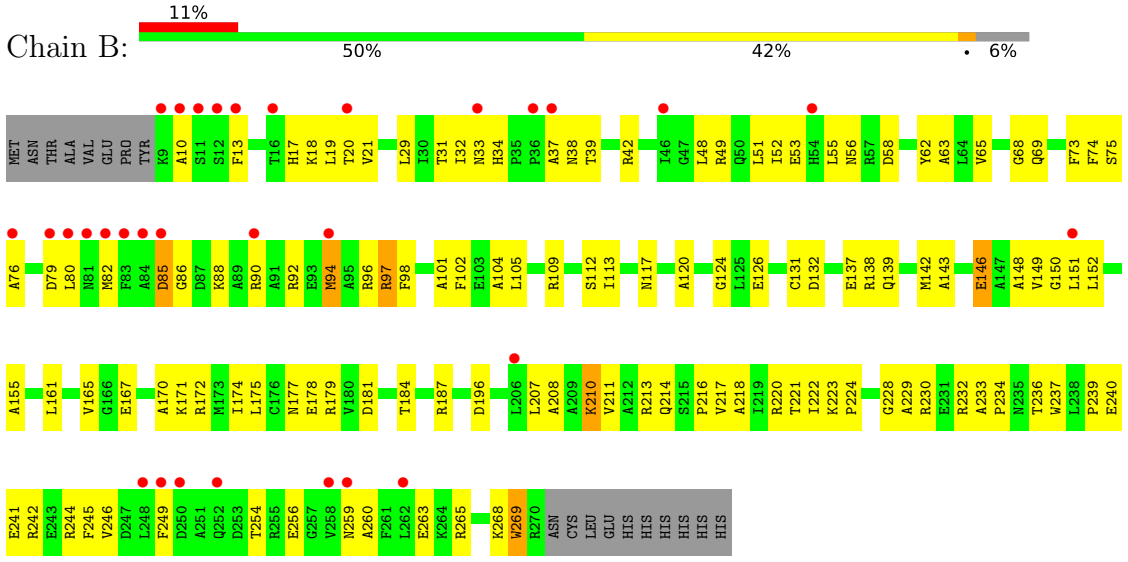
• Molecule 1: Probable enoyl-CoA hydratase/isomerase

Chain A:

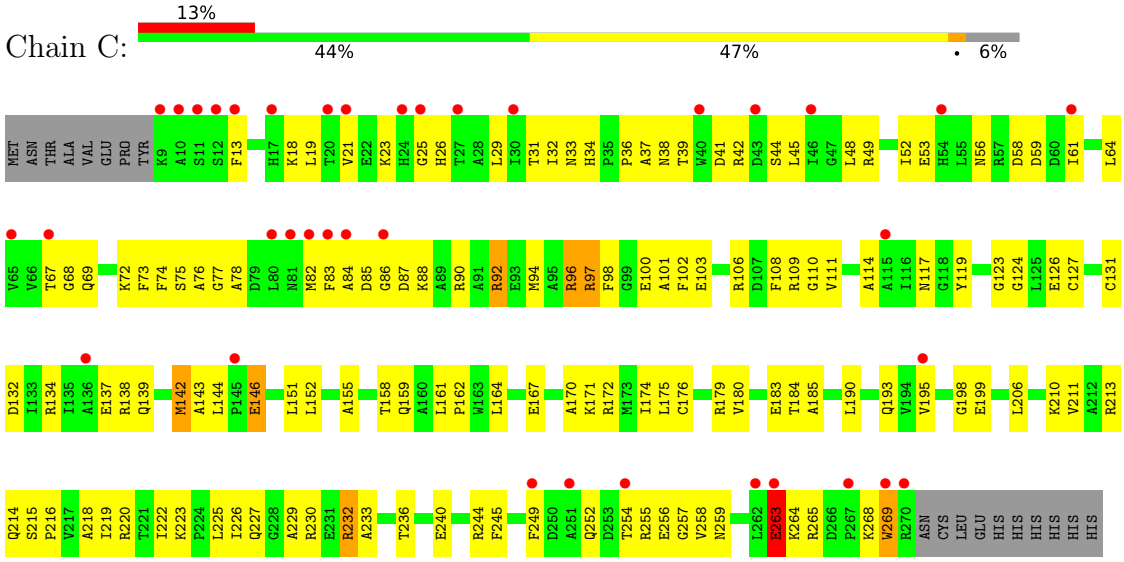


• Molecule 1: Probable enoyl-CoA hydratase/isomerase

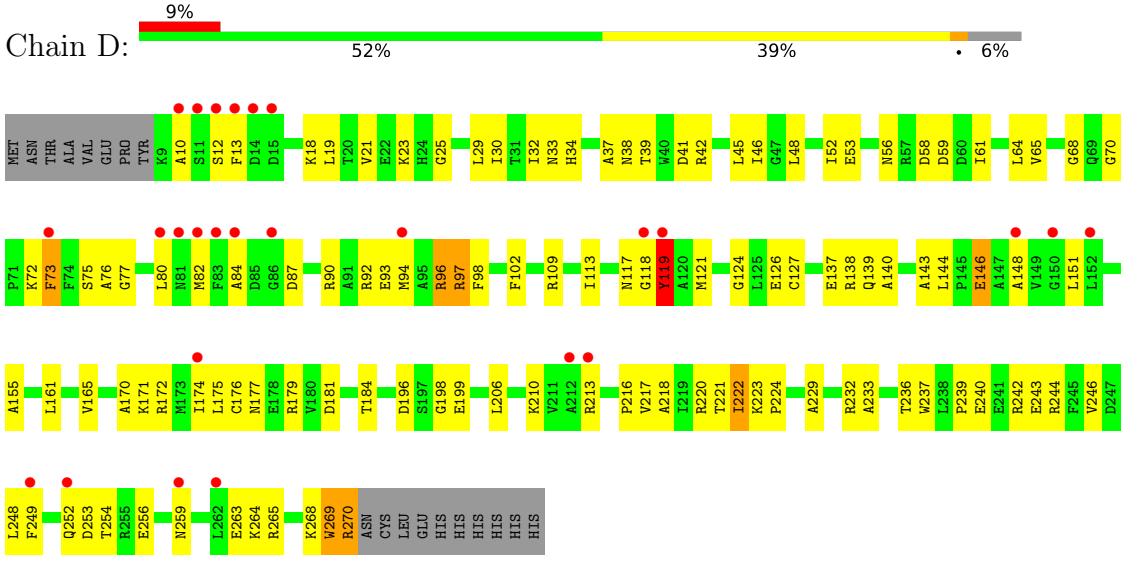
Chain B:



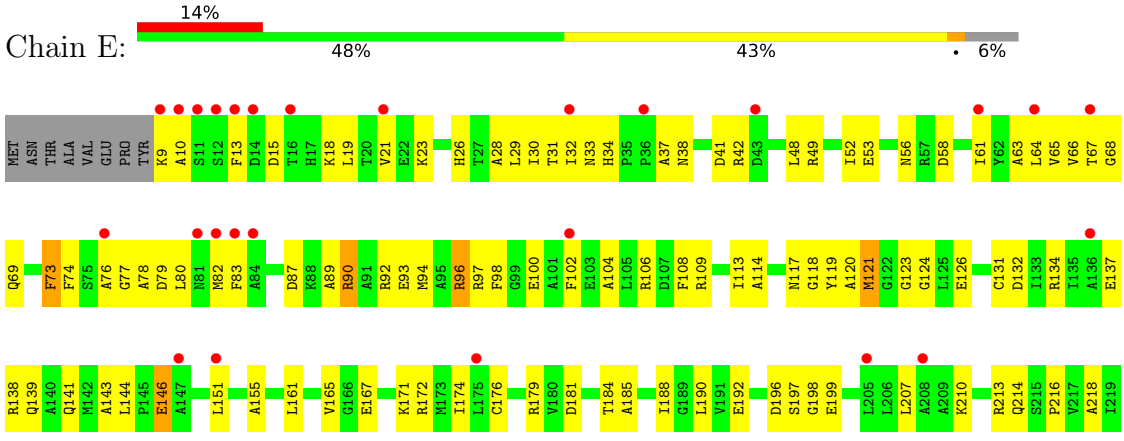
• Molecule 1: Probable enoyl-CoA hydratase/isomerase

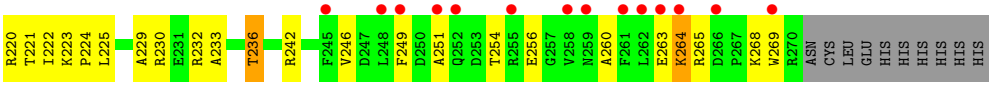


• Molecule 1: Probable enoyl-CoA hydratase/isomerase



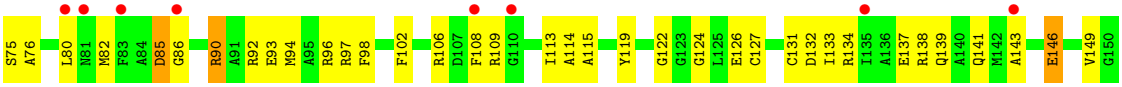
• Molecule 1: Probable enoyl-CoA hydratase/isomerase

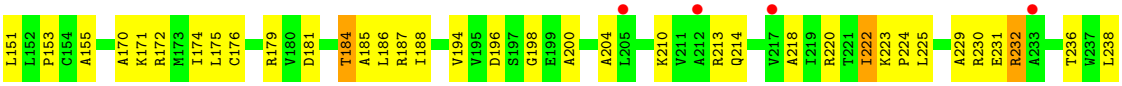


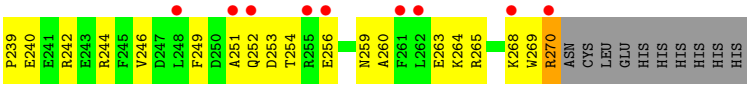


• Molecule 1: Probable enoyl-CoA hydratase/isomerase

Chain F:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	83.31Å 83.31Å 207.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.66 – 2.10 38.66 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.2 (38.66-2.10) 96.2 (38.66-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.10.1-2155_1692: ???)	Depositor
R, R_{free}	0.227 , 0.276 0.225 , 0.276	Depositor DCC
R_{free} test set	4477 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	33.9	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 24.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.073 for -h,-k,l 0.396 for h,-h-k,-l 0.074 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12387	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, IPA, PTD, MRD

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	0.56	0/2057	0.77	4/2783 (0.1%)
1	B	0.55	0/2068	0.81	2/2798 (0.1%)
1	C	0.60	2/2057 (0.1%)	0.80	4/2783 (0.1%)
1	D	0.65	4/2057 (0.2%)	0.83	3/2783 (0.1%)
1	E	0.54	0/2057	0.74	2/2783 (0.1%)
1	F	0.55	0/2057	0.77	1/2783 (0.0%)
All	All	0.58	6/12353 (0.0%)	0.79	16/16713 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	263	GLU	CD-OE1	-7.63	1.17	1.25
1	D	264	LYS	CG-CD	-6.24	1.31	1.52
1	C	263	GLU	CD-OE2	-5.71	1.19	1.25
1	D	264	LYS	CE-NZ	5.58	1.62	1.49
1	D	119	TYR	CB-CG	5.47	1.59	1.51
1	D	73	PHE	CE1-CZ	-5.40	1.27	1.37

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	85	ASP	CB-CG-OD1	12.54	129.59	118.30
1	D	270	ARG	NE-CZ-NH1	-9.36	115.62	120.30
1	D	270	ARG	NE-CZ-NH2	8.47	124.53	120.30
1	B	85	ASP	CB-CG-OD2	-8.32	110.82	118.30
1	E	90	ARG	NE-CZ-NH2	-8.11	116.24	120.30
1	A	42	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	C	232	ARG	NE-CZ-NH2	6.52	123.56	120.30
1	C	263	GLU	OE1-CD-OE2	6.36	130.94	123.30
1	C	263	GLU	CA-CB-CG	5.96	126.51	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	90	ARG	NH1-CZ-NH2	5.75	125.72	119.40
1	C	232	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	F	232	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	A	82	MET	CG-SD-CE	-5.19	91.90	100.20
1	A	232	ARG	NE-CZ-NH2	5.13	122.86	120.30
1	A	176	CYS	CA-CB-SG	-5.11	104.80	114.00
1	D	73	PHE	CB-CG-CD2	5.08	124.35	120.80

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	2020	0	2005	123	0
1	B	2030	0	2011	117	1
1	C	2020	0	2005	149	0
1	D	2020	0	2005	125	1
1	E	2020	0	2005	109	0
1	F	2020	0	2005	121	0
2	A	7	0	8	1	0
2	D	6	0	7	0	0
2	E	7	0	8	0	0
3	B	4	0	8	0	0
3	C	8	0	16	0	0
3	E	4	0	8	0	0
3	F	12	0	24	3	0
4	C	8	0	14	3	0
5	F	8	0	14	0	0
6	A	30	0	0	4	0
6	B	32	0	0	5	0
6	C	36	0	0	16	0
6	D	29	0	0	3	0
6	E	33	0	0	4	0
6	F	33	0	0	12	0
All	All	12387	0	12143	705	1

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 29.

All (705) 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:C:259:ASN:O	1:C:263:GLU:OE1	1.55	1.24
1:C:259:ASN:O	1:C:263:GLU:CD	1.95	1.04
1:C:45:LEU:O	6:C:402:HOH:O	1.73	1.04
1:E:119:TYR:HB3	1:E:121:MET:HE1	1.38	1.02
1:F:184:THR:HG22	1:F:187:ARG:HH21	1.24	0.99
1:D:210:LYS:HD3	1:D:213:ARG:HH22	1.29	0.96
1:C:82:MET:HE3	1:C:94:MET:HB3	1.49	0.94
1:F:137:GLU:OE2	1:F:139:GLN:NE2	2.02	0.92
1:C:110:GLY:O	6:C:403:HOH:O	1.88	0.92
1:C:143:ALA:HB2	1:C:179:ARG:HA	1.52	0.91
1:F:38:ASN:O	6:F:401:HOH:O	1.88	0.91
1:D:206:LEU:O	1:D:210:LYS:NZ	2.04	0.90
1:D:42:ARG:NH2	1:D:93:GLU:OE1	2.04	0.90
1:A:111:VAL:HG11	1:A:211:VAL:HG21	1.54	0.89
1:A:245:PHE:HB2	1:B:152:LEU:HD11	1.54	0.89
1:F:252:GLN:HE22	1:F:270:ARG:CZ	1.85	0.89
1:C:137:GLU:OE2	1:C:139:GLN:NE2	2.05	0.88
1:B:109:ARG:HD2	1:B:220:ARG:HD3	1.55	0.88
1:C:36:PRO:HG3	6:C:432:HOH:O	1.72	0.88
1:E:119:TYR:HB3	1:E:121:MET:CE	2.04	0.87
1:E:138:ARG:NH1	1:E:196:ASP:OD1	2.07	0.87
1:A:137:GLU:OE2	1:A:139:GLN:NE2	2.07	0.86
1:F:76:ALA:O	6:F:402:HOH:O	1.94	0.86
1:B:137:GLU:OE2	1:B:139:GLN:NE2	2.08	0.86
1:E:109:ARG:HD2	1:E:220:ARG:HD3	1.56	0.85
1:C:263:GLU:OE1	1:C:263:GLU:N	2.09	0.85
1:D:23:LYS:NZ	1:D:25:GLY:O	2.09	0.85
1:B:63:ALA:HB2	1:B:211:VAL:HG11	1.59	0.84
1:A:109:ARG:HD2	1:A:220:ARG:HD3	1.60	0.84
1:C:68:GLY:O	1:C:117:ASN:ND2	2.09	0.84
1:B:263:GLU:HG3	1:B:265:ARG:HG2	1.58	0.84
1:E:137:GLU:OE2	1:E:139:GLN:NE2	2.13	0.81
1:D:199:GLU:OE1	6:D:401:HOH:O	1.97	0.81
1:E:42:ARG:HE	1:E:94:MET:HE1	1.46	0.81
4:C:303:MPD:HO2	4:C:303:MPD:HO4	1.17	0.81
1:F:143:ALA:HB2	1:F:179:ARG:HA	1.63	0.81
1:A:143:ALA:HB2	1:A:179:ARG:HA	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:PHE:HE2	1:C:88:LYS:HA	1.48	0.79
1:D:82:MET:HE3	1:D:94:MET:HB3	1.65	0.79
1:F:30:ILE:HB	1:F:66:VAL:HG12	1.64	0.78
1:F:184:THR:HG22	1:F:187:ARG:NH2	1.97	0.78
1:E:143:ALA:HB2	1:E:179:ARG:HA	1.66	0.77
1:C:109:ARG:HD2	1:C:220:ARG:HD3	1.66	0.77
1:B:249:PHE:CE2	1:C:88:LYS:HA	2.19	0.77
1:D:249:PHE:HA	1:D:254:THR:HG21	1.67	0.77
1:A:226:ILE:O	6:A:401:HOH:O	2.02	0.77
1:E:18:LYS:NZ	1:E:41:ASP:OD2	2.16	0.77
1:B:37:ALA:HB1	1:B:76:ALA:HB2	1.66	0.76
1:E:94:MET:SD	1:E:94:MET:N	2.58	0.76
1:A:152:LEU:HD11	1:C:245:PHE:HB2	1.67	0.76
1:B:245:PHE:HB2	1:C:152:LEU:HD11	1.68	0.76
1:E:138:ARG:NH1	1:E:197:SER:H	1.83	0.76
1:A:233:ALA:HB1	1:B:230:ARG:O	1.85	0.76
1:F:210:LYS:HG2	1:F:213:ARG:HH22	1.51	0.76
1:D:98:PHE:HD1	1:D:102:PHE:CE2	2.04	0.75
1:A:102:PHE:CD2	1:A:155:ALA:HB1	2.21	0.75
1:E:37:ALA:HB1	1:E:76:ALA:HB2	1.67	0.74
1:B:10:ALA:HA	1:B:13:PHE:HD2	1.52	0.74
1:D:143:ALA:HB2	1:D:179:ARG:HA	1.68	0.74
1:A:172:ARG:HH22	1:C:193:GLN:HB2	1.50	0.74
1:B:242:ARG:NH2	1:C:103:GLU:OE1	2.20	0.74
1:D:263:GLU:HG3	1:D:265:ARG:HG2	1.70	0.73
1:A:266:ASP:OD1	6:A:402:HOH:O	2.06	0.73
1:A:247:ASP:OD2	1:D:96:ARG:NH1	2.20	0.73
1:A:18:LYS:HD3	1:A:34:HIS:HD2	1.55	0.72
1:F:119:TYR:HA	6:F:404:HOH:O	1.89	0.72
1:F:146:GLU:HB2	1:F:151:LEU:O	1.90	0.72
1:D:210:LYS:HD3	1:D:213:ARG:NH2	2.03	0.71
1:F:98:PHE:HD1	1:F:102:PHE:CE2	2.08	0.71
1:F:141:GLN:N	6:F:404:HOH:O	2.18	0.71
1:B:42:ARG:N	1:B:82:MET:SD	2.64	0.71
1:D:109:ARG:HD2	1:D:220:ARG:HD3	1.73	0.71
1:D:10:ALA:HB1	1:D:13:PHE:HE1	1.56	0.70
1:E:132:ASP:OD2	1:E:223:LYS:NZ	2.23	0.70
1:E:210:LYS:O	1:E:214:GLN:NE2	2.23	0.70
1:A:230:ARG:O	1:C:233:ALA:HB1	1.92	0.70
1:C:259:ASN:O	1:C:263:GLU:OE2	2.09	0.70
1:D:218:ALA:O	1:D:222:ILE:HD13	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:37:ALA:HB1	1:F:76:ALA:HB2	1.73	0.70
1:C:170:ALA:O	1:C:174:ILE:HG22	1.92	0.69
1:D:216:PRO:O	1:D:220:ARG:HG3	1.92	0.69
1:F:170:ALA:O	1:F:174:ILE:HG22	1.92	0.69
1:D:252:GLN:HG3	1:D:270:ARG:HH21	1.57	0.69
1:A:72:LYS:NZ	2:A:301:PTD:O5	2.19	0.69
1:A:146:GLU:HB2	1:A:151:LEU:O	1.93	0.69
1:D:84:ALA:HB3	1:D:90:ARG:HH12	1.56	0.68
1:E:33:ASN:OD1	6:E:401:HOH:O	2.12	0.68
1:F:113:ILE:HD12	1:F:133:ILE:HB	1.76	0.68
1:C:111:VAL:HG11	1:C:211:VAL:HG21	1.76	0.68
1:A:137:GLU:OE1	6:A:403:HOH:O	2.12	0.68
1:B:120:ALA:HB3	1:B:142:MET:HG2	1.76	0.68
1:F:141:GLN:O	6:F:404:HOH:O	2.12	0.67
1:F:231:GLU:OE2	6:F:403:HOH:O	2.10	0.67
1:D:119:TYR:HD1	1:D:119:TYR:H	1.42	0.67
1:F:263:GLU:HG3	1:F:265:ARG:HG2	1.75	0.67
1:B:233:ALA:HB1	1:C:230:ARG:O	1.93	0.67
1:F:214:GLN:N	1:F:214:GLN:OE1	2.28	0.67
1:C:97:ARG:HD2	1:C:97:ARG:N	2.09	0.67
1:D:259:ASN:O	1:D:263:GLU:HG2	1.94	0.67
1:E:249:PHE:HA	1:E:254:THR:HG21	1.76	0.67
1:E:218:ALA:O	1:E:222:ILE:HG13	1.95	0.67
1:E:126:GLU:CD	1:E:155:ALA:HB3	2.14	0.67
1:D:137:GLU:OE2	1:D:139:GLN:NE2	2.28	0.67
1:B:260:ALA:HB1	1:B:265:ARG:O	1.95	0.66
1:D:98:PHE:HD1	1:D:102:PHE:HE2	1.44	0.66
1:F:137:GLU:OE1	6:F:405:HOH:O	2.14	0.66
1:A:254:THR:HG22	1:B:150:GLY:O	1.95	0.66
1:F:114:ALA:HB2	1:F:131:CYS:SG	2.36	0.66
1:C:72:LYS:HE3	4:C:303:MPD:HM2	1.77	0.66
1:D:146:GLU:HB2	1:D:151:LEU:O	1.96	0.65
1:A:263:GLU:HG3	1:A:265:ARG:HG2	1.76	0.65
1:E:139:GLN:NE2	1:E:197:SER:OG	2.29	0.65
1:A:242:ARG:O	1:A:246:VAL:HG23	1.96	0.65
1:C:34:HIS:HB3	1:C:38:ASN:HA	1.77	0.65
1:D:53:GLU:OE1	6:D:402:HOH:O	2.14	0.65
1:E:93:GLU:O	1:E:97:ARG:HG2	1.96	0.65
1:F:90:ARG:HD3	1:F:94:MET:SD	2.37	0.65
1:C:37:ALA:HB1	1:C:76:ALA:HB2	1.78	0.65
1:A:102:PHE:HD2	1:A:155:ALA:HB1	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:GLU:CD	1:C:155:ALA:HB3	2.17	0.65
1:B:90:ARG:NH1	1:B:94:MET:SD	2.66	0.65
1:A:85:ASP:CG	1:A:86:GLY:HA2	2.17	0.65
1:C:49:ARG:N	6:C:402:HOH:O	2.24	0.65
1:C:223:LYS:HE3	6:C:403:HOH:O	1.97	0.65
1:A:256:GLU:HG2	1:A:268:LYS:O	1.97	0.64
1:D:242:ARG:O	1:D:246:VAL:HG23	1.97	0.64
1:F:82:MET:HE2	1:F:94:MET:HB3	1.79	0.64
1:B:210:LYS:HG3	1:B:213:ARG:HH22	1.63	0.64
1:E:256:GLU:HG3	6:E:412:HOH:O	1.97	0.64
1:F:16:THR:HG22	1:F:18:LYS:H	1.61	0.64
1:F:210:LYS:HG2	1:F:213:ARG:NH2	2.13	0.64
1:E:121:MET:CE	1:E:141:GLN:O	2.46	0.64
1:F:137:GLU:CD	1:F:198:GLY:H	2.01	0.64
1:B:102:PHE:CD2	1:B:155:ALA:HB1	2.33	0.64
1:B:126:GLU:CD	1:B:155:ALA:HB3	2.18	0.64
1:E:67:THR:OG1	1:E:117:ASN:ND2	2.31	0.64
1:F:146:GLU:HG3	1:F:153:PRO:HG3	1.80	0.64
1:C:195:VAL:HG12	1:C:199:GLU:HB2	1.80	0.64
1:B:63:ALA:HB2	1:B:211:VAL:CG1	2.27	0.63
1:A:82:MET:HE3	1:A:94:MET:HB3	1.79	0.63
1:C:84:ALA:O	6:C:404:HOH:O	2.15	0.63
1:D:72:LYS:HG2	1:D:73:PHE:HD1	1.63	0.63
1:C:41:ASP:N	1:C:44:SER:OG	2.21	0.63
1:D:252:GLN:HG3	1:D:270:ARG:HE	1.62	0.62
1:B:218:ALA:O	1:B:222:ILE:HG13	1.99	0.62
1:A:218:ALA:O	1:A:222:ILE:HG13	1.99	0.62
1:D:102:PHE:CD2	1:D:155:ALA:HB1	2.34	0.62
1:F:102:PHE:HE1	1:F:127:CYS:HB2	1.62	0.62
1:B:187:ARG:O	6:B:401:HOH:O	2.16	0.62
1:D:87:ASP:CG	1:D:90:ARG:HG3	2.19	0.62
1:F:42:ARG:NH2	1:F:90:ARG:HH22	1.97	0.62
1:C:98:PHE:HD1	1:C:102:PHE:CE2	2.17	0.62
1:B:259:ASN:O	1:B:263:GLU:HG2	1.99	0.62
1:C:146:GLU:HB2	1:C:151:LEU:O	1.99	0.62
1:C:37:ALA:O	1:C:76:ALA:HB2	1.99	0.62
1:F:252:GLN:HG3	1:F:253:ASP:N	2.14	0.62
1:C:102:PHE:CD2	1:C:155:ALA:HB1	2.35	0.62
1:D:98:PHE:CD1	1:D:102:PHE:HE2	2.18	0.62
1:E:233:ALA:O	1:E:236:THR:HG23	1.99	0.62
1:A:41:ASP:OD1	1:A:42:ARG:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ALA:O	1:A:174:ILE:HG22	2.00	0.61
1:D:30:ILE:HD13	1:D:64:LEU:HG	1.83	0.61
1:E:138:ARG:HH12	1:E:197:SER:H	1.47	0.61
1:F:30:ILE:O	1:F:66:VAL:HA	2.00	0.61
1:A:234:PRO:HD2	1:B:230:ARG:O	2.00	0.61
1:B:216:PRO:O	1:B:220:ARG:HG3	2.01	0.61
1:E:141:GLN:HB2	1:E:179:ARG:HH21	1.65	0.61
1:B:242:ARG:O	1:B:246:VAL:HG23	2.01	0.61
1:D:210:LYS:CD	1:D:213:ARG:HH22	2.09	0.61
1:A:98:PHE:HD1	1:A:102:PHE:CE2	2.20	0.60
1:D:221:THR:HG21	1:D:248:LEU:HD21	1.83	0.60
1:C:98:PHE:CD1	1:C:102:PHE:CE2	2.89	0.60
1:E:181:ASP:OD1	1:E:184:THR:OG1	2.15	0.60
3:F:302:IPA:H33	3:F:303:IPA:O2	2.01	0.60
1:B:68:GLY:O	1:B:117:ASN:ND2	2.34	0.60
1:B:143:ALA:HB2	1:B:179:ARG:HA	1.82	0.60
1:D:58:ASP:O	1:D:109:ARG:NH2	2.33	0.60
1:D:137:GLU:CD	1:D:198:GLY:H	2.05	0.60
1:B:146:GLU:HA	1:B:149:VAL:HG12	1.84	0.60
1:C:72:LYS:HZ1	1:C:119:TYR:HE1	1.50	0.60
1:F:42:ARG:HH22	1:F:93:GLU:CD	2.05	0.60
1:A:72:LYS:HD2	1:A:73:PHE:CE1	2.36	0.59
1:B:181:ASP:O	1:B:184:THR:OG1	2.18	0.59
1:C:218:ALA:O	1:C:222:ILE:HG13	2.02	0.59
1:E:207:LEU:HD12	1:E:210:LYS:HD2	1.84	0.59
1:F:249:PHE:HA	1:F:254:THR:HG21	1.84	0.59
1:B:48:LEU:O	1:B:52:ILE:HG12	2.02	0.59
1:B:170:ALA:O	1:B:174:ILE:HG22	2.01	0.59
1:B:172:ARG:NE	1:B:178:GLU:OE1	2.36	0.59
1:F:98:PHE:HD1	1:F:102:PHE:HE2	1.49	0.59
1:B:230:ARG:NH2	1:C:167:GLU:OE2	2.36	0.59
1:B:234:PRO:HD2	1:C:230:ARG:HA	1.83	0.59
1:A:151:LEU:HD21	1:C:258:VAL:HG13	1.83	0.59
1:F:15:ASP:O	6:F:406:HOH:O	2.17	0.59
1:F:131:CYS:O	1:F:134:ARG:NH1	2.36	0.59
1:C:38:ASN:ND2	1:C:69:GLN:O	2.35	0.59
1:F:252:GLN:HE22	1:F:270:ARG:NH2	2.00	0.59
1:C:102:PHE:CE2	1:C:155:ALA:HB1	2.38	0.58
1:C:159:GLN:O	1:C:162:PRO:HG2	2.03	0.58
1:C:249:PHE:HA	1:C:254:THR:HG21	1.84	0.58
1:F:122:GLY:HA2	1:F:146:GLU:OE1	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:GLU:CD	1:A:155:ALA:HB3	2.23	0.58
1:B:98:PHE:HD1	1:B:102:PHE:CE2	2.21	0.58
1:D:18:LYS:NZ	1:D:41:ASP:OD2	2.26	0.58
1:F:126:GLU:CD	1:F:155:ALA:HB3	2.24	0.58
1:E:146:GLU:HB2	1:E:151:LEU:O	2.03	0.58
1:F:98:PHE:CD1	1:F:102:PHE:HE2	2.21	0.58
1:B:146:GLU:HB2	1:B:151:LEU:O	2.03	0.58
1:E:9:LYS:N	1:E:23:LYS:HB2	2.18	0.58
1:E:139:GLN:OE1	1:E:139:GLN:N	2.34	0.58
1:F:85:ASP:OD1	1:F:85:ASP:N	2.30	0.58
1:C:216:PRO:O	1:C:220:ARG:HG3	2.03	0.58
1:A:18:LYS:NZ	1:A:41:ASP:OD2	2.37	0.57
1:C:18:LYS:NZ	1:C:41:ASP:OD2	2.37	0.57
1:D:170:ALA:O	1:D:174:ILE:HG22	2.04	0.57
1:E:121:MET:HE2	1:E:141:GLN:O	2.04	0.57
1:C:92:ARG:HD3	1:C:92:ARG:C	2.25	0.57
1:F:181:ASP:OD1	1:F:184:THR:OG1	2.16	0.57
1:A:38:ASN:ND2	1:A:69:GLN:O	2.35	0.57
1:D:82:MET:CE	1:D:94:MET:HB3	2.33	0.57
1:B:21:VAL:HA	1:B:29:LEU:O	2.05	0.57
1:E:21:VAL:HA	1:E:29:LEU:O	2.04	0.57
1:C:73:PHE:CD1	1:C:119:TYR:HB2	2.39	0.57
1:C:86:GLY:O	6:C:405:HOH:O	2.17	0.57
1:F:263:GLU:OE2	1:F:265:ARG:NE	2.38	0.57
1:E:96:ARG:HD2	1:E:100:GLU:OE2	2.04	0.57
1:D:19:LEU:HD23	1:D:32:ILE:HA	1.86	0.57
1:F:34:HIS:O	1:F:38:ASN:HA	2.05	0.57
1:B:37:ALA:HB1	1:B:76:ALA:CB	2.35	0.56
1:E:260:ALA:HB1	1:E:265:ARG:O	2.06	0.56
1:C:42:ARG:HG2	1:C:94:MET:SD	2.45	0.56
1:D:10:ALA:HB1	1:D:13:PHE:CE1	2.40	0.56
1:E:41:ASP:HA	1:E:82:MET:SD	2.44	0.56
1:F:67:THR:HA	1:F:74:PHE:CE1	2.40	0.56
1:C:138:ARG:NH1	1:C:183:GLU:OE2	2.39	0.56
1:C:98:PHE:CD1	1:C:102:PHE:HE2	2.24	0.56
1:E:78:ALA:HB1	1:E:83:PHE:HE2	1.71	0.56
1:F:21:VAL:HA	1:F:29:LEU:O	2.06	0.56
1:F:259:ASN:O	1:F:263:GLU:HG2	2.06	0.56
1:A:105:LEU:HD23	1:A:130:ALA:HB3	1.88	0.56
1:D:42:ARG:HB2	1:D:94:MET:HE1	1.88	0.56
1:E:78:ALA:CB	1:E:83:PHE:HE2	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:PHE:HD1	1:E:102:PHE:CE2	2.24	0.55
1:D:97:ARG:N	1:D:97:ARG:HD2	2.20	0.55
1:D:252:GLN:HG3	1:D:270:ARG:NH2	2.21	0.55
1:D:252:GLN:NE2	6:D:406:HOH:O	2.38	0.55
1:F:68:GLY:HA3	1:F:74:PHE:HA	1.89	0.55
1:D:196:ASP:HB3	1:D:199:GLU:CD	2.27	0.55
1:D:256:GLU:HG2	1:D:268:LYS:O	2.06	0.55
1:A:85:ASP:OD1	1:A:86:GLY:HA2	2.07	0.55
1:C:158:THR:O	1:C:162:PRO:HG3	2.07	0.55
1:D:171:LYS:O	1:D:175:LEU:HB2	2.07	0.55
1:E:121:MET:HE1	1:E:141:GLN:O	2.07	0.55
1:F:33:ASN:ND2	6:F:408:HOH:O	2.39	0.55
1:A:9:LYS:N	1:A:23:LYS:HB2	2.21	0.55
1:A:80:LEU:O	1:A:84:ALA:N	2.39	0.55
1:C:240:GLU:O	1:C:244:ARG:HG3	2.06	0.55
1:E:10:ALA:HB1	1:E:13:PHE:HE1	1.71	0.55
1:E:134:ARG:NH2	1:E:192:GLU:OE2	2.40	0.55
1:C:18:LYS:O	1:C:33:ASN:HB3	2.07	0.55
1:C:137:GLU:CD	1:C:198:GLY:H	2.10	0.55
1:C:225:LEU:HD11	1:C:244:ARG:HD3	1.89	0.55
1:E:102:PHE:CD2	1:E:155:ALA:HB1	2.42	0.55
1:A:216:PRO:O	1:A:220:ARG:HG3	2.07	0.55
1:A:265:ARG:NH1	1:A:268:LYS:HE3	2.22	0.55
1:C:206:LEU:HD13	1:C:210:LYS:HE3	1.88	0.55
1:A:47:GLY:O	1:A:51:LEU:N	2.32	0.54
1:B:51:LEU:O	1:B:55:LEU:HG	2.07	0.54
1:B:265:ARG:HH12	1:B:268:LYS:HE3	1.71	0.54
1:D:265:ARG:HH12	1:D:268:LYS:HE3	1.70	0.54
1:F:23:LYS:NZ	1:F:25:GLY:O	2.31	0.54
1:C:32:ILE:O	1:C:69:GLN:HB2	2.08	0.54
1:E:256:GLU:HG2	1:E:268:LYS:O	2.08	0.54
1:F:32:ILE:HG21	6:F:401:HOH:O	2.08	0.54
1:F:102:PHE:CD2	1:F:155:ALA:HB1	2.43	0.54
1:B:217:VAL:O	1:B:221:THR:HG23	2.07	0.54
1:B:167:GLU:O	1:B:171:LYS:HG3	2.08	0.54
1:B:239:PRO:HA	1:B:242:ARG:NH1	2.22	0.54
1:F:34:HIS:HB3	1:F:38:ASN:HA	1.89	0.54
1:A:139:GLN:HG3	1:E:264:LYS:HD2	1.90	0.54
1:C:68:GLY:HA3	1:C:74:PHE:HA	1.90	0.54
1:C:102:PHE:HE1	1:C:127:CYS:HB2	1.71	0.54
1:D:72:LYS:HG2	1:D:73:PHE:CD1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:PRO:HA	1:D:242:ARG:NH1	2.23	0.54
1:F:42:ARG:HH21	1:F:90:ARG:HH22	1.56	0.54
1:B:229:ALA:HA	1:B:232:ARG:O	2.08	0.53
1:B:139:GLN:HB2	1:F:264:LYS:HE2	1.90	0.53
1:D:34:HIS:HB3	1:D:38:ASN:HA	1.90	0.53
1:A:235:ASN:HA	1:A:238:LEU:HD23	1.89	0.53
1:B:230:ARG:HH21	1:C:167:GLU:CD	2.11	0.53
1:D:240:GLU:O	1:D:244:ARG:HG2	2.09	0.53
1:E:119:TYR:C	1:E:121:MET:HE3	2.29	0.53
1:B:18:LYS:O	1:B:33:ASN:N	2.42	0.53
1:C:167:GLU:HA	6:C:411:HOH:O	2.08	0.53
1:C:254:THR:O	1:C:258:VAL:HG22	2.09	0.53
1:B:120:ALA:O	1:B:142:MET:HA	2.09	0.53
1:D:102:PHE:HE1	1:D:127:CYS:HB2	1.73	0.53
1:E:90:ARG:O	1:E:93:GLU:N	2.41	0.53
1:E:223:LYS:HB3	1:E:224:PRO:HD3	1.91	0.53
1:F:106:ARG:HD2	1:F:230:ARG:NH1	2.24	0.53
1:D:232:ARG:NH2	1:D:237:TRP:CZ3	2.77	0.53
1:B:52:ILE:HG21	1:B:104:ALA:O	2.09	0.52
1:C:103:GLU:HG2	1:C:106:ARG:HH21	1.73	0.52
1:A:232:ARG:NE	1:A:236:THR:OG1	2.40	0.52
1:B:92:ARG:HG3	1:D:92:ARG:HG3	1.90	0.52
1:C:252:GLN:HG2	6:C:426:HOH:O	2.08	0.52
1:D:252:GLN:OE1	1:D:252:GLN:N	2.42	0.52
1:A:79:ASP:O	1:A:82:MET:HB3	2.10	0.52
1:B:34:HIS:HB3	1:B:38:ASN:HA	1.91	0.52
1:A:79:ASP:OD1	1:A:80:LEU:N	2.43	0.52
1:C:162:PRO:CB	6:C:411:HOH:O	2.56	0.52
1:E:120:ALA:N	1:E:121:MET:CE	2.73	0.52
1:C:131:CYS:O	1:C:134:ARG:NH1	2.43	0.52
1:E:42:ARG:HE	1:E:94:MET:CE	2.19	0.52
1:F:252:GLN:HE22	1:F:270:ARG:NE	2.07	0.52
1:B:10:ALA:HA	1:B:13:PHE:CD2	2.41	0.52
1:D:252:GLN:HG3	1:D:270:ARG:NE	2.25	0.52
1:E:114:ALA:HB2	1:E:131:CYS:SG	2.49	0.51
1:F:93:GLU:O	1:F:97:ARG:HG2	2.10	0.51
1:A:229:ALA:HA	1:A:232:ARG:O	2.10	0.51
1:D:171:LYS:HA	1:D:175:LEU:HD23	1.91	0.51
1:F:32:ILE:HD12	1:F:74:PHE:O	2.10	0.51
1:C:87:ASP:OD2	1:C:90:ARG:HG3	2.11	0.51
1:F:32:ILE:HD13	6:F:401:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ALA:HB1	1:A:265:ARG:O	2.11	0.51
1:B:256:GLU:HG2	1:B:268:LYS:O	2.11	0.51
1:F:109:ARG:HH21	1:F:220:ARG:NE	2.09	0.51
1:A:222:ILE:HG21	1:B:174:ILE:HD11	1.93	0.51
1:D:23:LYS:HE2	1:D:61:ILE:HD11	1.93	0.51
1:B:239:PRO:HA	1:B:242:ARG:HH11	1.74	0.51
1:A:56:ASN:HD22	1:A:109:ARG:HG2	1.76	0.51
1:E:79:ASP:OD1	1:E:80:LEU:N	2.43	0.51
1:F:16:THR:OG1	1:F:43:ASP:OD1	2.28	0.51
1:F:225:LEU:HD21	1:F:244:ARG:HD3	1.92	0.51
1:B:58:ASP:HA	6:B:414:HOH:O	2.11	0.50
1:E:185:ALA:HA	1:E:188:ILE:HG12	1.91	0.50
1:B:146:GLU:O	1:B:149:VAL:HG12	2.11	0.50
1:D:265:ARG:NH1	1:D:268:LYS:HE3	2.26	0.50
1:F:220:ARG:H	1:F:220:ARG:HD2	1.77	0.50
1:F:256:GLU:HG2	1:F:268:LYS:O	2.12	0.50
1:F:149:VAL:HG23	1:F:151:LEU:HG	1.92	0.50
1:F:108:PHE:O	1:F:223:LYS:HE2	2.10	0.50
1:F:109:ARG:HB2	1:F:220:ARG:HG3	1.92	0.50
1:D:84:ALA:HB3	1:D:90:ARG:NH1	2.26	0.50
1:D:148:ALA:HB2	1:D:177:ASN:ND2	2.26	0.50
1:D:42:ARG:HH21	1:D:93:GLU:CD	2.15	0.50
1:E:119:TYR:CB	1:E:121:MET:HE1	2.27	0.50
1:B:48:LEU:HD23	1:B:101:ALA:HB1	1.92	0.50
1:C:26:HIS:O	1:C:61:ILE:HA	2.11	0.50
1:C:96:ARG:O	1:C:100:GLU:HG3	2.12	0.50
1:D:42:ARG:NH1	1:D:97:ARG:HH22	2.10	0.50
1:F:184:THR:O	1:F:188:ILE:HG23	2.12	0.50
1:C:102:PHE:CE1	1:C:127:CYS:HA	2.46	0.50
1:C:172:ARG:O	1:C:176:CYS:HB2	2.12	0.50
1:E:58:ASP:O	1:E:109:ARG:NH2	2.41	0.50
1:F:260:ALA:HB1	1:F:265:ARG:O	2.11	0.50
1:B:207:LEU:HA	1:B:210:LYS:HD3	1.94	0.49
1:C:48:LEU:O	1:C:52:ILE:HG12	2.11	0.49
1:A:163:TRP:NE1	1:B:167:GLU:OE1	2.35	0.49
1:E:77:GLY:HA2	1:E:124:GLY:H	1.77	0.49
1:A:144:LEU:HD22	1:A:146:GLU:OE1	2.13	0.49
1:A:150:GLY:C	1:A:151:LEU:HD22	2.33	0.49
1:C:255:ARG:O	1:C:259:ASN:HB2	2.13	0.49
1:E:37:ALA:CB	1:E:76:ALA:HB2	2.38	0.49
1:E:68:GLY:HA3	1:E:74:PHE:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:75:SER:HB3	1:F:124:GLY:HA3	1.93	0.49
1:B:171:LYS:O	1:B:175:LEU:HB2	2.12	0.49
1:A:223:LYS:HB3	1:A:224:PRO:HD3	1.94	0.49
1:A:266:ASP:OD1	1:A:266:ASP:N	2.45	0.49
1:B:249:PHE:HA	1:B:254:THR:HG21	1.93	0.49
1:D:92:ARG:C	1:D:92:ARG:HD3	2.33	0.49
1:D:93:GLU:HG3	1:D:94:MET:N	2.28	0.49
1:E:172:ARG:O	1:E:176:CYS:HB2	2.12	0.49
1:F:251:ALA:O	1:F:254:THR:HG22	2.13	0.49
1:A:120:ALA:HB3	1:A:142:MET:HG2	1.95	0.49
1:C:195:VAL:CG1	1:C:199:GLU:HB2	2.40	0.49
1:A:40:TRP:N	1:A:77:GLY:O	2.45	0.49
1:A:265:ARG:HH12	1:A:268:LYS:HE3	1.77	0.49
1:A:74:PHE:CD1	1:A:116:ILE:HA	2.48	0.49
1:C:31:THR:HG23	1:C:67:THR:HG23	1.94	0.49
1:D:80:LEU:HD22	1:D:80:LEU:H	1.77	0.49
1:D:181:ASP:O	1:D:184:THR:OG1	2.28	0.49
1:F:64:LEU:HD21	1:F:66:VAL:HG13	1.93	0.49
1:C:72:LYS:CE	4:C:303:MPD:HM2	2.41	0.49
1:D:102:PHE:CE1	1:D:127:CYS:HB2	2.47	0.49
1:C:114:ALA:HB2	1:C:131:CYS:SG	2.53	0.49
1:D:48:LEU:O	1:D:52:ILE:HG12	2.12	0.49
1:E:102:PHE:CE2	1:E:155:ALA:HB1	2.48	0.49
1:A:120:ALA:O	1:A:142:MET:HA	2.13	0.48
1:C:39:THR:HB	1:C:76:ALA:HB3	1.95	0.48
1:F:30:ILE:HG23	6:F:414:HOH:O	2.12	0.48
1:A:152:LEU:HB3	1:C:222:ILE:HG12	1.95	0.48
1:A:215:SER:O	1:A:219:ILE:HG12	2.12	0.48
1:B:148:ALA:HB2	1:B:177:ASN:ND2	2.28	0.48
1:E:138:ARG:HH11	1:E:196:ASP:HA	1.78	0.48
1:A:249:PHE:CE1	1:B:88:LYS:HA	2.49	0.48
1:B:34:HIS:ND1	1:B:39:THR:HG22	2.28	0.48
1:C:23:LYS:HE2	1:C:61:ILE:HD11	1.94	0.48
1:C:161:LEU:N	1:C:162:PRO:HD2	2.28	0.48
1:C:259:ASN:C	1:C:263:GLU:OE2	2.51	0.48
1:F:239:PRO:HA	1:F:242:ARG:NH1	2.27	0.48
1:A:64:LEU:HD21	1:A:66:VAL:HG13	1.95	0.48
1:C:256:GLU:HG2	1:C:268:LYS:O	2.13	0.48
1:A:251:ALA:O	1:A:254:THR:OG1	2.30	0.48
1:A:259:ASN:O	1:A:263:GLU:HG2	2.14	0.48
1:B:19:LEU:HD23	1:B:32:ILE:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:MET:HE2	1:B:94:MET:HA	1.95	0.48
1:D:233:ALA:HB3	1:D:236:THR:CG2	2.44	0.48
1:C:48:LEU:HB3	6:C:402:HOH:O	2.12	0.48
1:C:64:LEU:N	1:C:111:VAL:O	2.44	0.48
1:C:97:ARG:HD2	1:C:97:ARG:H	1.76	0.48
1:C:144:LEU:HB3	1:C:146:GLU:OE1	2.14	0.48
1:E:123:GLY:HA2	1:E:126:GLU:OE1	2.14	0.48
1:F:138:ARG:NE	1:F:196:ASP:HA	2.28	0.48
1:C:75:SER:HB3	1:C:124:GLY:HA3	1.96	0.48
1:C:233:ALA:HB3	1:C:236:THR:HG23	1.96	0.48
1:E:106:ARG:HD2	1:E:230:ARG:NH1	2.28	0.48
1:A:58:ASP:O	1:A:109:ARG:NH2	2.43	0.48
1:D:41:ASP:O	1:D:45:LEU:HG	2.13	0.48
1:D:68:GLY:O	1:D:117:ASN:ND2	2.46	0.48
1:E:61:ILE:HD11	1:E:63:ALA:O	2.14	0.48
1:C:82:MET:HE2	1:C:98:PHE:HE2	1.78	0.47
1:D:21:VAL:HA	1:D:29:LEU:O	2.14	0.47
1:D:64:LEU:HD23	1:D:65:VAL:N	2.29	0.47
1:A:174:ILE:HG21	1:C:226:ILE:HD11	1.96	0.47
1:B:138:ARG:NH1	1:B:196:ASP:OD1	2.47	0.47
1:E:89:ALA:HA	6:E:420:HOH:O	2.14	0.47
1:A:92:ARG:HD3	1:A:92:ARG:C	2.35	0.47
1:B:143:ALA:HB2	1:B:179:ARG:HB3	1.96	0.47
1:B:208:ALA:O	1:B:211:VAL:HG12	2.14	0.47
1:B:241:GLU:OE2	1:C:158:THR:OG1	2.15	0.47
1:C:58:ASP:O	1:C:109:ARG:NH2	2.42	0.47
1:D:90:ARG:O	1:D:94:MET:HG2	2.14	0.47
1:F:109:ARG:HH21	1:F:220:ARG:HE	1.61	0.47
1:E:80:LEU:H	1:E:80:LEU:HD22	1.80	0.47
1:F:146:GLU:HG3	1:F:153:PRO:CG	2.42	0.47
1:D:139:GLN:OE1	1:D:139:GLN:N	2.37	0.47
1:E:119:TYR:CB	1:E:121:MET:CE	2.86	0.47
1:E:263:GLU:HG3	1:E:265:ARG:HG2	1.96	0.47
1:A:42:ARG:HH22	1:A:93:GLU:CD	2.18	0.47
1:A:171:LYS:HD3	1:C:132:ASP:HB3	1.96	0.47
1:C:263:GLU:HB2	1:C:265:ARG:HG2	1.96	0.47
1:D:37:ALA:HB1	1:D:76:ALA:HB2	1.96	0.47
1:F:14:ASP:HB3	3:F:302:IPA:H13	1.96	0.47
1:F:132:ASP:OD1	1:F:223:LYS:NZ	2.48	0.47
1:F:186:LEU:HD22	1:F:194:VAL:HG23	1.96	0.47
1:F:218:ALA:O	1:F:222:ILE:HD13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:TYR:HB3	6:B:419:HOH:O	2.14	0.47
1:D:119:TYR:CD1	1:D:140:ALA:HA	2.49	0.47
1:D:171:LYS:CA	1:D:175:LEU:HD23	2.45	0.47
1:B:161:LEU:O	1:B:165:VAL:HG22	2.15	0.47
1:C:42:ARG:HG2	1:C:94:MET:HE1	1.97	0.47
1:E:28:ALA:H	1:E:61:ILE:HD11	1.80	0.47
1:C:263:GLU:HG2	1:C:265:ARG:HE	1.78	0.47
1:D:229:ALA:HA	1:D:232:ARG:O	2.14	0.47
1:E:90:ARG:HG2	1:E:94:MET:SD	2.55	0.47
1:F:37:ALA:HB1	1:F:76:ALA:CB	2.43	0.47
1:A:263:GLU:OE2	1:A:265:ARG:NE	2.48	0.46
1:B:112:SER:OG	1:B:132:ASP:N	2.43	0.46
1:B:210:LYS:HG3	1:B:213:ARG:NH2	2.29	0.46
1:F:56:ASN:OD1	1:F:108:PHE:HD1	1.98	0.46
1:C:34:HIS:ND1	1:C:39:THR:HG22	2.31	0.46
1:C:167:GLU:CA	6:C:411:HOH:O	2.62	0.46
1:D:70:GLY:O	1:D:117:ASN:ND2	2.48	0.46
1:D:144:LEU:HB3	1:D:146:GLU:OE1	2.15	0.46
1:D:213:ARG:O	1:D:269:TRP:HZ2	1.98	0.46
1:A:21:VAL:HA	1:A:29:LEU:O	2.15	0.46
1:D:217:VAL:O	1:D:221:THR:HG22	2.15	0.46
1:F:92:ARG:C	1:F:92:ARG:HD3	2.36	0.46
1:F:185:ALA:HA	1:F:188:ILE:HG12	1.97	0.46
1:B:85:ASP:HA	1:B:86:GLY:HA2	1.60	0.46
1:C:39:THR:OG1	1:C:77:GLY:O	2.18	0.46
1:E:96:ARG:O	1:E:100:GLU:HG3	2.16	0.46
1:F:172:ARG:O	1:F:176:CYS:HB2	2.14	0.46
1:A:149:VAL:O	1:C:257:GLY:HA3	2.15	0.46
1:A:257:GLY:C	1:B:149:VAL:HG23	2.36	0.46
1:C:164:LEU:HD23	1:C:164:LEU:HA	1.78	0.46
1:C:185:ALA:HB1	1:C:190:LEU:HB3	1.98	0.46
1:E:92:ARG:NH1	1:E:96:ARG:HG3	2.30	0.46
1:E:108:PHE:O	1:E:223:LYS:HE2	2.16	0.46
1:F:220:ARG:H	1:F:220:ARG:CD	2.28	0.46
1:C:41:ASP:O	1:C:44:SER:OG	2.20	0.46
1:C:85:ASP:HA	1:C:86:GLY:HA2	1.74	0.46
1:A:222:ILE:HG12	1:B:152:LEU:HB3	1.97	0.46
1:D:73:PHE:HA	1:D:118:GLY:HA3	1.98	0.46
1:E:19:LEU:HD23	1:E:32:ILE:HA	1.97	0.46
1:E:28:ALA:N	1:E:61:ILE:HD11	2.31	0.46
1:E:221:THR:O	1:E:224:PRO:HD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:LEU:HD22	1:A:151:LEU:N	2.31	0.46
1:A:98:PHE:CD1	1:A:102:PHE:CE2	3.01	0.46
1:F:113:ILE:CD1	1:F:133:ILE:HB	2.43	0.46
1:A:257:GLY:O	1:B:149:VAL:HG23	2.16	0.46
1:D:244:ARG:HD2	1:D:244:ARG:N	2.30	0.46
1:B:38:ASN:ND2	1:B:69:GLN:O	2.42	0.45
1:C:23:LYS:HG3	1:C:61:ILE:HD11	1.98	0.45
1:C:49:ARG:O	1:C:53:GLU:HG3	2.16	0.45
1:E:249:PHE:CA	1:E:254:THR:HG21	2.44	0.45
1:A:56:ASN:ND2	1:A:108:PHE:HD1	2.14	0.45
1:D:87:ASP:OD2	1:D:90:ARG:HG3	2.15	0.45
1:F:146:GLU:HG3	1:F:153:PRO:CD	2.46	0.45
1:C:134:ARG:NH2	1:C:164:LEU:HD11	2.30	0.45
1:D:59:ASP:HA	1:D:109:ARG:NH2	2.31	0.45
1:E:13:PHE:CZ	1:E:15:ASP:HB2	2.51	0.45
1:A:142:MET:O	1:A:180:VAL:HG22	2.15	0.45
1:A:151:LEU:HD21	1:C:254:THR:HG23	1.99	0.45
1:B:58:ASP:O	1:B:109:ARG:NH2	2.48	0.45
1:B:102:PHE:HD2	1:B:155:ALA:HB1	1.80	0.45
1:D:233:ALA:HB3	1:D:236:THR:HG23	1.97	0.45
1:F:41:ASP:O	1:F:44:SER:OG	2.31	0.45
1:A:18:LYS:O	1:A:33:ASN:HB3	2.17	0.45
1:B:75:SER:HB3	1:B:124:GLY:HA3	1.98	0.45
1:B:233:ALA:O	1:B:236:THR:HG23	2.16	0.45
1:C:21:VAL:HA	1:C:29:LEU:O	2.16	0.45
1:E:119:TYR:HD1	1:E:141:GLN:H	1.64	0.45
1:F:115:ALA:HB1	1:F:200:ALA:HB1	1.97	0.45
1:A:246:VAL:HB	1:D:92:ARG:NH2	2.31	0.45
6:A:407:HOH:O	1:D:243:GLU:HA	2.16	0.45
1:D:30:ILE:HD12	1:D:30:ILE:N	2.32	0.45
1:D:56:ASN:OD1	1:D:109:ARG:HG2	2.16	0.45
1:D:126:GLU:CD	1:D:155:ALA:HB3	2.37	0.45
1:D:252:GLN:HG2	1:D:253:ASP:N	2.32	0.45
1:A:56:ASN:HD21	1:A:108:PHE:HD1	1.65	0.45
1:F:240:GLU:O	1:F:244:ARG:HG3	2.17	0.45
1:E:52:ILE:HG21	1:E:104:ALA:O	2.16	0.45
1:F:109:ARG:HB2	1:F:220:ARG:CG	2.45	0.45
1:A:257:GLY:HA3	1:B:149:VAL:O	2.16	0.45
1:D:172:ARG:O	1:D:176:CYS:HB2	2.17	0.45
1:E:64:LEU:HB2	1:E:108:PHE:CE2	2.52	0.45
1:E:144:LEU:HD22	1:E:146:GLU:OE1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:216:PRO:O	1:E:220:ARG:HG3	2.17	0.45
1:E:225:LEU:HD23	1:E:225:LEU:HA	1.79	0.45
1:A:78:ALA:HB1	1:A:83:PHE:CE2	2.51	0.45
1:F:56:ASN:OD1	1:F:109:ARG:HG2	2.17	0.45
1:F:171:LYS:O	1:F:175:LEU:N	2.50	0.45
1:D:223:LYS:HB3	1:D:224:PRO:HD3	1.99	0.44
1:B:143:ALA:HB1	6:B:409:HOH:O	2.16	0.44
1:D:82:MET:HE3	1:D:94:MET:CE	2.47	0.44
1:D:143:ALA:HB2	1:D:179:ARG:CA	2.42	0.44
1:A:51:LEU:O	1:A:55:LEU:HG	2.17	0.44
1:A:56:ASN:ND2	1:A:109:ARG:HG2	2.33	0.44
1:A:263:GLU:HG2	1:A:263:GLU:H	1.32	0.44
1:B:65:VAL:HA	1:B:113:ILE:O	2.17	0.44
1:B:210:LYS:O	1:B:214:GLN:NE2	2.48	0.44
1:C:34:HIS:O	1:C:38:ASN:N	2.48	0.44
1:C:142:MET:O	1:C:180:VAL:HG22	2.17	0.44
1:C:215:SER:O	1:C:219:ILE:HG12	2.18	0.44
1:A:78:ALA:HB2	1:A:98:PHE:CZ	2.53	0.44
1:A:105:LEU:HD21	1:A:131:CYS:SG	2.57	0.44
1:A:233:ALA:HB3	1:A:236:THR:HG23	1.98	0.44
1:C:41:ASP:OD1	1:C:42:ARG:N	2.48	0.44
1:C:225:LEU:HA	1:C:225:LEU:HD23	1.76	0.44
1:A:92:ARG:NH2	1:D:246:VAL:HB	2.33	0.44
1:A:235:ASN:HA	1:A:238:LEU:CD2	2.47	0.44
1:C:82:MET:HE2	1:C:98:PHE:CE2	2.52	0.44
1:E:30:ILE:N	1:E:30:ILE:HD12	2.33	0.44
1:F:223:LYS:HB3	1:F:224:PRO:HD3	2.00	0.44
1:B:79:ASP:OD1	1:B:80:LEU:N	2.51	0.44
1:F:34:HIS:O	1:F:38:ASN:N	2.50	0.44
1:C:218:ALA:HB2	6:C:412:HOH:O	2.18	0.43
1:E:49:ARG:O	1:E:53:GLU:HG3	2.17	0.43
1:F:242:ARG:O	1:F:246:VAL:HG22	2.18	0.43
1:B:56:ASN:O	1:B:109:ARG:CZ	2.66	0.43
1:E:65:VAL:HA	1:E:113:ILE:O	2.19	0.43
1:A:102:PHE:CE2	1:A:155:ALA:HB1	2.52	0.43
1:A:137:GLU:HG3	1:A:200:ALA:HB2	2.01	0.43
1:B:171:LYS:O	1:B:175:LEU:N	2.50	0.43
1:F:102:PHE:CE2	1:F:155:ALA:HB1	2.53	0.43
1:C:37:ALA:CB	1:C:76:ALA:HB2	2.47	0.43
1:E:229:ALA:HA	1:E:232:ARG:O	2.19	0.43
1:B:105:LEU:HD21	1:B:131:CYS:SG	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:115:ALA:HB2	1:F:204:ALA:HB2	2.00	0.43
1:E:48:LEU:O	1:E:52:ILE:HG12	2.19	0.43
1:A:56:ASN:HD21	1:A:109:ARG:H	1.66	0.43
1:C:167:GLU:N	6:C:411:HOH:O	2.51	0.43
1:A:16:THR:HG21	1:A:44:SER:HA	2.00	0.43
1:A:68:GLY:O	1:A:117:ASN:ND2	2.36	0.43
1:A:213:ARG:NH2	1:A:213:ARG:HB3	2.34	0.43
1:B:20:THR:OG1	1:B:31:THR:HB	2.18	0.43
1:C:19:LEU:HD23	1:C:32:ILE:HA	2.01	0.43
1:D:39:THR:HG22	1:D:76:ALA:HB3	2.01	0.43
1:D:252:GLN:CG	1:D:270:ARG:HH21	2.29	0.43
1:F:48:LEU:O	1:F:52:ILE:HG12	2.19	0.43
1:F:210:LYS:O	1:F:213:ARG:HB2	2.18	0.43
1:A:48:LEU:O	1:A:52:ILE:HG12	2.19	0.43
1:B:210:LYS:HA	1:B:213:ARG:NH2	2.34	0.43
1:D:12:SER:O	1:D:13:PHE:HB3	2.19	0.43
1:D:77:GLY:HA2	1:D:124:GLY:H	1.83	0.43
1:F:42:ARG:HH21	1:F:90:ARG:NH2	2.15	0.43
1:A:34:HIS:O	1:A:38:ASN:HA	2.19	0.43
1:A:139:GLN:CB	1:E:264:LYS:HG3	2.49	0.43
1:A:235:ASN:OD1	1:B:230:ARG:HB3	2.18	0.43
1:A:236:THR:HG23	1:A:236:THR:H	1.57	0.43
1:B:146:GLU:H	1:B:146:GLU:HG2	1.50	0.43
1:C:123:GLY:HA2	1:C:126:GLU:OE1	2.19	0.43
1:D:119:TYR:CD1	1:D:119:TYR:N	2.83	0.43
1:F:45:LEU:HA	1:F:45:LEU:HD23	1.75	0.43
1:B:213:ARG:O	1:B:269:TRP:HZ2	2.02	0.42
1:D:75:SER:HB3	1:D:124:GLY:CA	2.49	0.42
1:E:34:HIS:O	1:E:38:ASN:HA	2.19	0.42
1:F:69:GLN:OE1	1:F:69:GLN:HA	2.19	0.42
1:A:37:ALA:HB1	1:A:76:ALA:HB2	2.01	0.42
1:C:56:ASN:OD1	1:C:109:ARG:HG2	2.19	0.42
1:A:26:HIS:O	1:A:61:ILE:HA	2.19	0.42
1:A:171:LYS:O	1:A:175:LEU:N	2.45	0.42
1:B:223:LYS:HB3	1:B:224:PRO:HD3	2.00	0.42
1:B:224:PRO:HB2	1:B:244:ARG:HH12	1.84	0.42
1:C:42:ARG:HG2	1:C:94:MET:CE	2.49	0.42
1:C:255:ARG:HA	1:C:258:VAL:CG2	2.49	0.42
1:C:265:ARG:HH22	1:C:268:LYS:HE3	1.85	0.42
1:B:97:ARG:HD2	1:B:97:ARG:N	2.34	0.42
1:D:121:MET:HA	1:D:143:ALA:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:137:GLU:CD	1:E:198:GLY:H	2.22	0.42
1:F:236:THR:H	1:F:236:THR:HG23	1.58	0.42
1:F:263:GLU:HG2	1:F:263:GLU:H	1.60	0.42
1:A:186:LEU:HD22	1:A:194:VAL:HG23	2.00	0.42
1:B:49:ARG:O	1:B:53:GLU:HG3	2.20	0.42
1:D:18:LYS:O	1:D:33:ASN:N	2.51	0.42
1:C:227:GLN:O	6:C:407:HOH:O	2.21	0.42
1:E:210:LYS:HA	1:E:213:ARG:NH2	2.34	0.42
1:E:242:ARG:O	1:E:246:VAL:HG23	2.19	0.42
1:A:151:LEU:CD2	1:C:254:THR:HG23	2.50	0.42
1:C:48:LEU:HD23	1:C:101:ALA:HB1	2.02	0.42
1:C:78:ALA:HB1	1:C:83:PHE:HE2	1.85	0.42
1:D:248:LEU:HA	1:D:248:LEU:HD23	1.86	0.42
1:D:29:LEU:C	1:D:30:ILE:HD12	2.40	0.42
1:E:121:MET:CB	1:E:143:ALA:O	2.67	0.42
1:E:144:LEU:HD12	1:E:174:ILE:HG12	2.01	0.42
1:E:251:ALA:O	1:E:254:THR:HG22	2.20	0.42
1:A:185:ALA:HA	1:A:188:ILE:HG12	2.01	0.42
1:D:98:PHE:CD1	1:D:102:PHE:CE2	2.92	0.42
1:F:229:ALA:HA	1:F:232:ARG:O	2.20	0.42
1:C:13:PHE:O	6:C:406:HOH:O	2.21	0.42
1:A:181:ASP:OD1	1:A:184:THR:N	2.28	0.41
1:B:143:ALA:HB2	1:B:179:ARG:CA	2.48	0.41
1:D:102:PHE:CE2	1:D:155:ALA:HB1	2.55	0.41
1:E:38:ASN:ND2	1:E:69:GLN:O	2.41	0.41
1:F:14:ASP:O	3:F:302:IPA:O2	2.32	0.41
1:F:34:HIS:O	1:F:38:ASN:CA	2.68	0.41
1:B:17[A]:HIS:CD2	6:B:421:HOH:O	2.73	0.41
1:B:102:PHE:CE2	1:B:155:ALA:HB1	2.55	0.41
1:B:265:ARG:HH22	1:B:268:LYS:HE3	1.84	0.41
1:E:87:ASP:OD1	1:E:89:ALA:N	2.52	0.41
1:E:161:LEU:O	1:E:165:VAL:HG22	2.20	0.41
1:C:23:LYS:NZ	1:C:25:GLY:O	2.41	0.41
1:C:213:ARG:O	1:C:269:TRP:HZ2	2.04	0.41
1:C:229:ALA:HA	1:C:232:ARG:O	2.20	0.41
1:F:18:LYS:C	1:F:19:LEU:HD12	2.41	0.41
1:F:239:PRO:HA	1:F:242:ARG:HH11	1.86	0.41
1:B:68:GLY:HA3	1:B:74:PHE:HA	2.02	0.41
1:B:172:ARG:HH11	1:B:172:ARG:HD3	1.71	0.41
1:E:31:THR:HG23	1:E:67:THR:HG23	2.02	0.41
1:E:98:PHE:CD1	1:E:102:PHE:HE2	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:109:ARG:HE	1:F:220:ARG:HG2	1.85	0.41
1:A:167:GLU:HB3	1:A:171:LYS:HE3	2.02	0.41
1:B:38:ASN:ND2	1:B:73:PHE:O	2.49	0.41
1:B:232:ARG:HG2	1:B:236:THR:HG21	2.02	0.41
1:C:102:PHE:CE2	1:C:155:ALA:CB	3.03	0.41
1:D:65:VAL:HA	1:D:113:ILE:O	2.20	0.41
1:D:138:ARG:NH1	1:D:196:ASP:OD1	2.53	0.41
1:E:73:PHE:HA	1:E:118:GLY:HA3	2.02	0.41
1:A:144:LEU:HB3	1:A:146:GLU:OE1	2.21	0.41
1:A:196:ASP:HB3	1:A:199:GLU:CD	2.41	0.41
1:C:37:ALA:HB1	1:C:76:ALA:CB	2.50	0.41
1:F:80:LEU:HA	1:F:80:LEU:HD23	1.79	0.41
1:C:210:LYS:O	1:C:214:GLN:NE2	2.52	0.41
1:E:188:ILE:HG13	1:E:190:LEU:H	1.86	0.41
1:A:151:LEU:N	1:A:151:LEU:CD2	2.83	0.41
1:A:248:LEU:HD23	1:A:248:LEU:HA	1.94	0.41
1:C:171:LYS:O	1:C:175:LEU:HB2	2.20	0.41
1:C:236:THR:HA	1:D:232:ARG:NH1	2.35	0.41
1:D:75:SER:HB3	1:D:124:GLY:HA3	2.03	0.41
1:D:161:LEU:O	1:D:165:VAL:HG22	2.21	0.41
1:E:30:ILE:O	1:E:66:VAL:HA	2.21	0.41
1:A:68:GLY:HA3	1:A:74:PHE:HA	2.03	0.41
1:A:217:VAL:O	1:A:221:THR:HG23	2.20	0.41
1:C:19:LEU:CD2	1:C:32:ILE:HA	2.50	0.41
1:C:59:ASP:HA	1:C:109:ARG:NH2	2.36	0.41
1:C:96:ARG:HD2	1:C:100:GLU:OE2	2.21	0.41
1:D:210:LYS:O	1:D:213:ARG:HB2	2.21	0.41
1:E:167:GLU:HB3	1:E:171:LYS:HE3	2.03	0.41
1:A:88:LYS:HG2	1:C:249:PHE:CD1	2.55	0.41
1:D:42:ARG:O	1:D:46:ILE:HG12	2.20	0.41
1:E:199:GLU:N	6:E:403:HOH:O	2.53	0.41
1:F:138:ARG:HH21	1:F:196:ASP:HB2	1.86	0.41
1:F:249:PHE:O	1:F:249:PHE:CD1	2.75	0.40
1:A:61:ILE:HA	1:A:61:ILE:HD13	1.82	0.40
1:C:64:LEU:HB2	1:C:108:PHE:CE2	2.57	0.40
1:C:114:ALA:HB2	1:C:131:CYS:CB	2.51	0.40
1:D:270:ARG:H	1:D:270:ARG:HG2	1.64	0.40
1:E:56:ASN:OD1	1:E:109:ARG:HG2	2.20	0.40
1:F:29:LEU:HD12	1:F:65:VAL:O	2.21	0.40
1:B:17[A]:HIS:NE2	1:B:18:LYS:HG2	2.37	0.40
1:B:113:ILE:HD12	1:B:208:ALA:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:PHE:CE2	1:D:119:TYR:HB2	2.56	0.40
1:E:26:HIS:O	1:E:61:ILE:HD12	2.21	0.40
1:E:143:ALA:HB3	1:E:179:ARG:HG2	2.03	0.40
1:F:85:ASP:HA	1:F:86:GLY:HA2	1.76	0.40
1:F:238:LEU:HB2	1:F:239:PRO:HD3	2.02	0.40
1:A:64:LEU:CD2	1:A:66:VAL:HG13	2.52	0.40
1:B:143:ALA:HB2	1:B:179:ARG:CB	2.51	0.40
1:B:240:GLU:O	1:B:244:ARG:HG3	2.21	0.40
1:D:82:MET:HE3	1:D:94:MET:HE3	2.02	0.40
1:D:232:ARG:HG2	1:D:233:ALA:N	2.37	0.40
1:B:228:GLY:O	1:B:237:TRP:NE1	2.55	0.40
1:C:232:ARG:NH1	1:D:236:THR:HG22	2.37	0.40

All (1) 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:B:196:ASP:OD2	1:D:270:ARG:NH1[3_454]	2.02	0.18

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	260/280 (93%)	258 (99%)	2 (1%)	0	100	100
1	B	261/280 (93%)	256 (98%)	5 (2%)	0	100	100
1	C	260/280 (93%)	257 (99%)	3 (1%)	0	100	100
1	D	260/280 (93%)	257 (99%)	3 (1%)	0	100	100
1	E	260/280 (93%)	256 (98%)	4 (2%)	0	100	100
1	F	260/280 (93%)	255 (98%)	5 (2%)	0	100	100
All	All	1561/1680 (93%)	1539 (99%)	22 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	201/219 (92%)	198 (98%)	3 (2%)	65	71
1	B	202/219 (92%)	196 (97%)	6 (3%)	41	44
1	C	201/219 (92%)	192 (96%)	9 (4%)	27	27
1	D	201/219 (92%)	195 (97%)	6 (3%)	41	44
1	E	201/219 (92%)	194 (96%)	7 (4%)	36	38
1	F	201/219 (92%)	192 (96%)	9 (4%)	27	27
All	All	1207/1314 (92%)	1167 (97%)	40 (3%)	38	40

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	ASP
1	A	146	GLU
1	A	269	TRP
1	B	94	MET
1	B	96	ARG
1	B	97	ARG
1	B	146	GLU
1	B	210	LYS
1	B	269	TRP
1	C	92	ARG
1	C	96	ARG
1	C	97	ARG
1	C	142	MET
1	C	146	GLU
1	C	184	THR
1	C	263	GLU
1	C	264	LYS
1	C	269	TRP
1	D	96	ARG

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Mol	Chain	Res	Type
1	D	97	ARG
1	D	119	TYR
1	D	146	GLU
1	D	222	ILE
1	D	269	TRP
1	E	73	PHE
1	E	96	ARG
1	E	121	MET
1	E	146	GLU
1	E	236	THR
1	E	264	LYS
1	E	269	TRP
1	F	61	ILE
1	F	85	ASP
1	F	90	ARG
1	F	96	ARG
1	F	146	GLU
1	F	184	THR
1	F	222	ILE
1	F	269	TRP
1	F	270	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	34	HIS
1	A	56	ASN
1	A	252	GLN
1	B	54	HIS
1	C	26	HIS
1	C	227	GLN
1	D	26	HIS
1	E	117	ASN
1	F	252	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

12 ligands are modelled in this entry.

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	PTD	E	302	-	6,6,6	0.56	0	5,5,5	0.60	0
3	IPA	B	301	-	3,3,3	0.50	0	3,3,3	0.36	0
3	IPA	F	301	-	3,3,3	0.67	0	3,3,3	0.36	0
3	IPA	E	301	-	3,3,3	0.60	0	3,3,3	0.36	0
3	IPA	C	301	-	3,3,3	0.63	0	3,3,3	0.44	0
3	IPA	F	303	-	3,3,3	0.74	0	3,3,3	0.18	0
4	MPD	C	303	-	7,7,7	0.86	0	9,10,10	1.20	1 (11%)
5	MRD	F	304	-	7,7,7	0.65	0	9,10,10	0.68	0
2	PTD	D	301	-	5,5,6	0.55	0	4,4,5	1.46	1 (25%)
3	IPA	F	302	-	3,3,3	0.72	0	3,3,3	0.09	0
2	PTD	A	301	-	6,6,6	0.48	0	5,5,5	1.19	0
3	IPA	C	302	-	3,3,3	0.44	0	3,3,3	0.74	0

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	PTD	E	302	-	-	2/2/4/4	-
4	MPD	C	303	-	-	0/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MRD	F	304	-	-	1/5/5/5	-
2	PTD	D	301	-	-	1/2/3/4	-
2	PTD	A	301	-	-	0/2/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	301	PTD	C4-C3-C2	-2.52	97.21	116.23
4	C	303	MPD	CM-C2-C3	2.13	119.87	109.96

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	302	PTD	C1-C2-C3-C4
5	F	304	MRD	C2-C3-C4-C5
2	E	302	PTD	C2-C3-C4-C5
2	D	301	PTD	C2-C3-C4-C5

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	303	IPA	1	0
4	C	303	MPD	3	0
3	F	302	IPA	3	0
2	A	301	PTD	1	0

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	262/280 (93%)	0.96	36 (13%) 3 4	21, 47, 95, 121	0
1	B	262/280 (93%)	0.85	31 (11%) 4 5	17, 44, 73, 106	0
1	C	262/280 (93%)	1.03	37 (14%) 2 3	16, 52, 82, 109	0
1	D	262/280 (93%)	0.83	26 (9%) 7 9	18, 44, 75, 104	0
1	E	262/280 (93%)	1.27	40 (15%) 2 3	24, 55, 84, 138	0
1	F	262/280 (93%)	1.05	36 (13%) 3 4	25, 55, 78, 104	0
All	All	1572/1680 (93%)	1.00	206 (13%) 3 4	16, 49, 84, 138	0

All (206) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	10	ALA	29.6
1	E	11	SER	23.2
1	C	10	ALA	17.5
1	D	11	SER	14.1
1	F	10	ALA	12.9
1	B	81	ASN	11.5
1	E	12	SER	10.8
1	B	10	ALA	10.5
1	A	11	SER	9.3
1	A	249	PHE	9.0
1	D	12	SER	9.0
1	A	10	ALA	8.6
1	E	262	LEU	8.6
1	B	11	SER	8.6
1	D	86	GLY	8.6
1	D	82	MET	8.5
1	C	25	GLY	8.4
1	D	10	ALA	8.2
1	A	12	SER	7.8

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Mol	Chain	Res	Type	RSRZ
1	A	262	LEU	7.7
1	F	11	SER	7.7
1	C	12	SER	7.6
1	B	12	SER	7.4
1	D	84	ALA	7.0
1	A	82	MET	7.0
1	E	84	ALA	6.6
1	A	81	ASN	6.4
1	C	9	LYS	6.4
1	E	81	ASN	6.2
1	C	81	ASN	6.2
1	F	252	GLN	6.1
1	F	251	ALA	6.1
1	E	249	PHE	6.1
1	C	83	PHE	6.0
1	D	14	ASP	5.9
1	B	249	PHE	5.8
1	B	82	MET	5.7
1	A	252	GLN	5.7
1	C	30	ILE	5.6
1	D	81	ASN	5.6
1	A	270	ARG	5.4
1	C	82	MET	5.4
1	E	13	PHE	5.3
1	C	11	SER	5.3
1	A	145	PRO	5.3
1	E	252	GLN	5.1
1	C	20	THR	5.1
1	D	150	GLY	5.0
1	C	17	HIS	5.0
1	F	12	SER	4.9
1	C	270	ARG	4.8
1	C	86	GLY	4.8
1	C	267	PRO	4.7
1	B	84	ALA	4.7
1	E	255	ARG	4.7
1	E	264	LYS	4.7
1	F	9	LYS	4.6
1	B	13	PHE	4.6
1	C	251	ALA	4.6
1	A	14	ASP	4.5
1	C	80	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	F	256	GLU	4.4
1	B	80	LEU	4.4
1	A	258	VAL	4.4
1	D	249	PHE	4.3
1	A	87	ASP	4.3
1	E	16	THR	4.2
1	B	9	LYS	4.1
1	D	262	LEU	4.1
1	B	79	ASP	4.0
1	E	258	VAL	3.9
1	B	16	THR	3.9
1	A	80	LEU	3.9
1	F	80	LEU	3.9
1	D	73	PHE	3.9
1	B	83	PHE	3.8
1	E	83	PHE	3.8
1	C	249	PHE	3.8
1	F	81	ASN	3.8
1	A	254	THR	3.8
1	E	82	MET	3.7
1	B	36	PRO	3.7
1	D	13	PHE	3.6
1	C	263	GLU	3.6
1	F	17	HIS	3.5
1	D	119	TYR	3.5
1	F	61	ILE	3.5
1	F	261	PHE	3.4
1	B	54	HIS	3.4
1	C	61	ILE	3.4
1	D	152	LEU	3.4
1	A	15	ASP	3.3
1	E	263	GLU	3.3
1	F	62	TYR	3.3
1	E	259	ASN	3.3
1	C	262	LEU	3.3
1	F	217	VAL	3.3
1	F	268	LYS	3.2
1	E	266	ASP	3.2
1	A	13	PHE	3.2
1	F	30	ILE	3.2
1	D	94	MET	3.1
1	A	154	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	16	THR	3.1
1	E	175	LEU	3.1
1	F	108	PHE	3.1
1	A	86	GLY	3.1
1	A	264	LYS	3.1
1	F	205	LEU	3.0
1	F	212	ALA	3.0
1	F	57	ARG	3.0
1	B	262	LEU	3.0
1	F	248	LEU	3.0
1	E	102	PHE	3.0
1	A	9	LYS	2.9
1	A	151	LEU	2.9
1	B	46	ILE	2.9
1	D	213	ARG	2.9
1	F	83	PHE	2.9
1	F	270	ARG	2.9
1	C	254	THR	2.8
1	F	29	LEU	2.8
1	E	32	ILE	2.8
1	F	255	ARG	2.8
1	A	265	ARG	2.7
1	A	36	PRO	2.7
1	E	251	ALA	2.7
1	C	65	VAL	2.7
1	E	261	PHE	2.6
1	E	269	TRP	2.6
1	E	36	PRO	2.6
1	A	98	PHE	2.6
1	E	151	LEU	2.6
1	E	147	ALA	2.6
1	E	208	ALA	2.6
1	F	16	THR	2.6
1	A	35	PRO	2.6
1	D	252	GLN	2.6
1	F	86	GLY	2.6
1	A	83	PHE	2.6
1	D	83	PHE	2.6
1	B	94	MET	2.5
1	D	212	ALA	2.5
1	E	64	LEU	2.5
1	F	43	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	61	ILE	2.5
1	E	245	PHE	2.5
1	B	248	LEU	2.5
1	A	29	LEU	2.4
1	B	85	ASP	2.4
1	B	76	ALA	2.4
1	A	267	PRO	2.4
1	B	252	GLN	2.4
1	B	259	ASN	2.4
1	C	145	PRO	2.4
1	D	118	GLY	2.4
1	D	15	ASP	2.4
1	E	67	THR	2.4
1	A	79	ASP	2.4
1	B	33	ASN	2.4
1	C	195	VAL	2.4
1	F	23	LYS	2.4
1	A	250	ASP	2.4
1	B	151	LEU	2.3
1	C	54	HIS	2.3
1	B	90	ARG	2.3
1	C	13	PHE	2.3
1	C	84	ALA	2.3
1	C	40	TRP	2.3
1	B	20	THR	2.3
1	C	115	ALA	2.3
1	C	24	HIS	2.3
1	D	148	ALA	2.2
1	B	206	LEU	2.2
1	B	250	ASP	2.2
1	F	135	ILE	2.2
1	C	136	ALA	2.2
1	E	9	LYS	2.2
1	C	46	ILE	2.2
1	A	213	ARG	2.2
1	C	21	VAL	2.2
1	C	67	THR	2.2
1	E	136	ALA	2.2
1	F	143	ALA	2.2
1	F	233	ALA	2.2
1	D	80	LEU	2.1
1	E	205	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	259	ASN	2.1
1	C	43	ASP	2.1
1	E	43	ASP	2.1
1	B	258	VAL	2.1
1	E	14	ASP	2.1
1	C	269	TRP	2.1
1	A	63	ALA	2.1
1	F	14	ASP	2.1
1	A	32	ILE	2.1
1	B	37	ALA	2.1
1	D	174	ILE	2.1
1	F	262	LEU	2.1
1	E	21	VAL	2.1
1	E	248	LEU	2.0
1	C	27	THR	2.0
1	E	76	ALA	2.0
1	F	110	GLY	2.0
1	F	15	ASP	2.0
1	A	68	GLY	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
3	IPA	E	301	4/4	0.80	0.21	10,24,38,51	0
2	PTD	D	301	6/7	0.82	0.17	33,36,38,38	0
3	IPA	B	301	4/4	0.83	0.12	10,14,17,25	0
2	PTD	A	301	7/7	0.83	0.14	21,34,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	IPA	F	302	4/4	0.83	0.17	40,41,45,54	0
2	PTD	E	302	7/7	0.85	0.13	10,22,34,35	0
4	MPD	C	303	8/8	0.88	0.15	26,39,53,54	0
3	IPA	F	301	4/4	0.89	0.27	20,21,33,46	0
3	IPA	F	303	4/4	0.90	0.24	13,26,28,33	0
3	IPA	C	301	4/4	0.90	0.10	30,37,42,43	0
3	IPA	C	302	4/4	0.91	0.09	17,19,21,31	0
5	MRD	F	304	8/8	0.93	0.10	26,34,36,39	0

6.5 Other polymers (i)

There are no such residues in this entry.