



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 3, 2023 – 10:42 AM EDT

PDB ID : 3SS4
Title : Crystal structure of mouse Glutaminase C, phosphate-bound form
Authors : Ambrosio, A.L.B.; Dias, S.M.G.; Cerione, R.A.
Deposited on : 2011-07-07
Resolution : 2.85 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 ⓘ 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 ⓘ](#)) 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 : 2.35
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) : 2.35

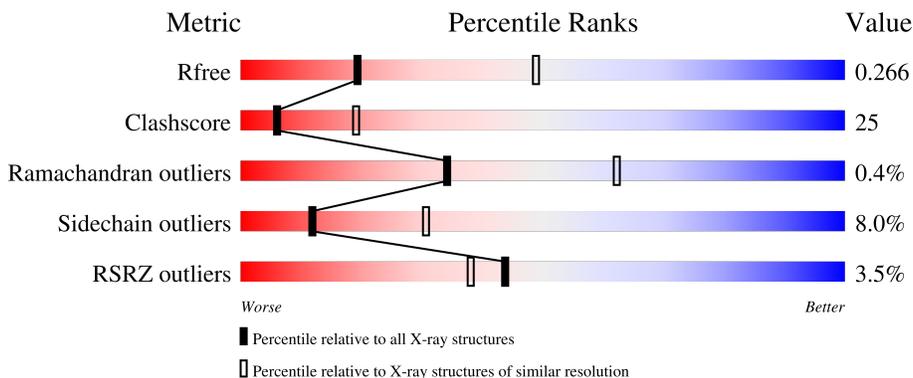
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 $\leq 5\%$. 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	479	
1	B	479	
1	C	479	
1	D	479	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 12470 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.

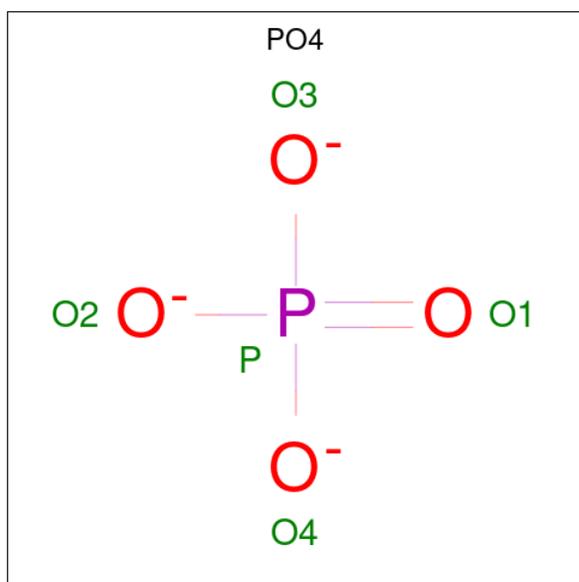
- Molecule 1 is a protein called Glutaminase C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	390	3051	1952	513	558	28	4	0	0
1	B	388	3036	1941	511	556	28	4	0	0
1	C	394	3083	1970	519	566	28	5	0	0
1	D	387	3025	1930	510	557	28	4	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	125	GLY	-	expression tag	UNP Q69ZX9
A	126	SER	-	expression tag	UNP Q69ZX9
A	127	HIS	-	expression tag	UNP Q69ZX9
B	125	GLY	-	expression tag	UNP Q69ZX9
B	126	SER	-	expression tag	UNP Q69ZX9
B	127	HIS	-	expression tag	UNP Q69ZX9
C	125	GLY	-	expression tag	UNP Q69ZX9
C	126	SER	-	expression tag	UNP Q69ZX9
C	127	HIS	-	expression tag	UNP Q69ZX9
D	125	GLY	-	expression tag	UNP Q69ZX9
D	126	SER	-	expression tag	UNP Q69ZX9
D	127	HIS	-	expression tag	UNP Q69ZX9

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

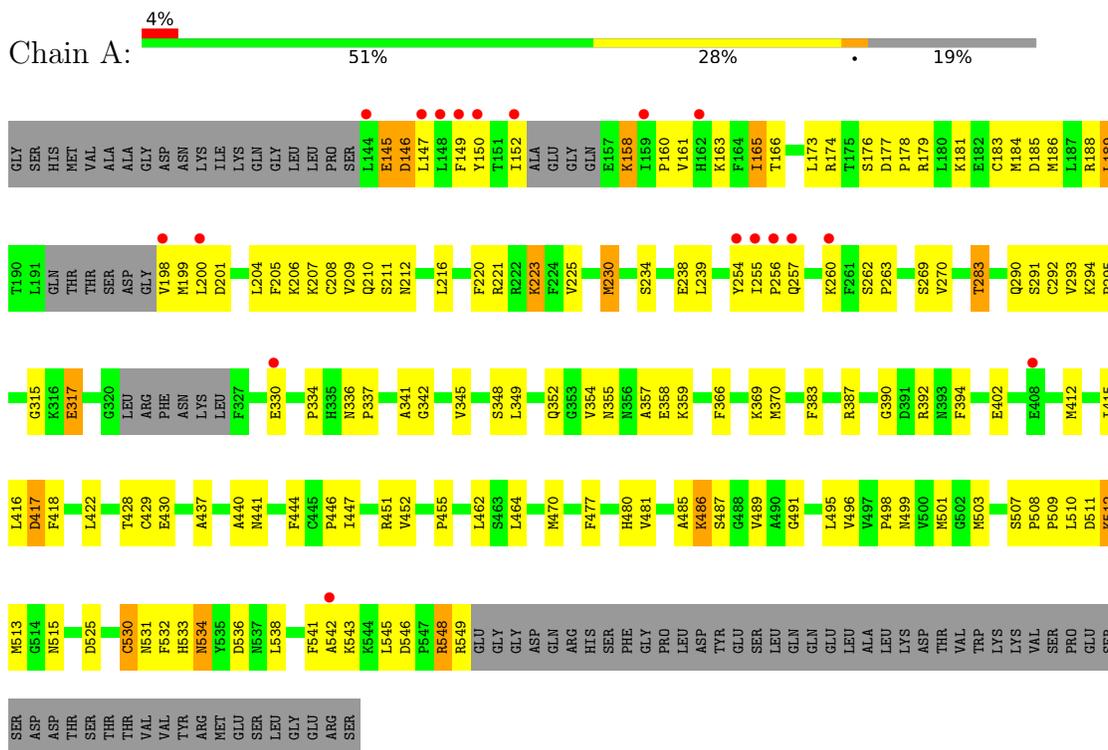
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	63	Total	O	0	0
			63	63		
3	B	71	Total	O	0	0
			71	71		
3	C	53	Total	O	0	0
			53	53		
3	D	68	Total	O	0	0
			68	68		

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: Glutaminase C



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.72Å 136.28Å 176.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.91 – 2.85 37.55 – 2.85	Depositor EDS
% Data completeness (in resolution range)	93.3 (19.91-2.85) 93.0 (37.55-2.85)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.85Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.227 , 0.270 0.222 , 0.266	Depositor DCC
R_{free} test set	2640 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	44.8	Xtrriage
Anisotropy	0.321	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12470	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.35 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.9224e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: PO4

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	0.65	3/3118 (0.1%)	0.53	0/4205
1	B	0.57	2/3101 (0.1%)	0.53	0/4179
1	C	0.62	3/3150 (0.1%)	0.55	1/4249 (0.0%)
1	D	0.59	0/3089	0.53	1/4164 (0.0%)
All	All	0.61	8/12458 (0.1%)	0.54	2/16797 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	225	VAL	CB-CG2	-5.57	1.41	1.52
1	B	489	VAL	CB-CG1	-5.54	1.41	1.52
1	C	362	TYR	CE2-CZ	-5.38	1.31	1.38
1	C	362	TYR	CD2-CE2	-5.32	1.31	1.39
1	A	225	VAL	CB-CG1	-5.22	1.41	1.52
1	B	225	VAL	CB-CG2	-5.19	1.42	1.52
1	C	362	TYR	CE1-CZ	-5.14	1.31	1.38
1	A	317	GLU	CG-CD	-5.04	1.44	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	200	LEU	CA-CB-CG	5.10	127.03	115.30
1	D	200	LEU	CA-CB-CG	5.07	126.97	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3051	0	3036	147	0
1	B	3036	0	3017	131	0
1	C	3083	0	3066	176	0
1	D	3025	0	3001	159	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	63	0	0	0	0
3	B	71	0	0	0	0
3	C	53	0	0	2	0
3	D	68	0	0	0	0
All	All	12470	0	12120	603	0

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 25.

All (603) 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:200:LEU:HD12	1:A:204:LEU:CD2	1.62	1.28
1:C:148:LEU:HD13	1:C:148:LEU:O	1.41	1.18
1:C:387:ARG:HG2	1:C:387:ARG:HH11	1.01	1.15
1:A:200:LEU:HD12	1:A:204:LEU:HD21	1.19	1.14
1:A:548:ARG:HG3	1:A:548:ARG:HH11	1.08	1.13
1:A:161:VAL:HG23	1:A:200:LEU:HD21	1.33	1.09
1:C:512:LYS:H	1:C:512:LYS:HD2	0.97	1.08
1:B:145:GLU:HG3	1:B:206:LYS:HG3	1.41	1.03
1:D:152:ILE:HG22	1:D:163:LYS:NZ	1.74	1.02
1:C:512:LYS:H	1:C:512:LYS:CD	1.71	0.99
1:D:283:THR:CG2	1:D:430:GLU:HG2	1.92	0.99
1:C:202:LYS:HG3	1:C:203:ASP:OD2	1.63	0.98
1:A:283:THR:CG2	1:A:430:GLU:HG3	1.94	0.98
1:D:145:GLU:HG3	1:D:206:LYS:CG	1.94	0.97
1:C:158:LYS:HB3	1:C:199:MET:SD	2.05	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:LYS:H	1:A:512:LYS:HD2	1.32	0.95
1:D:152:ILE:HG22	1:D:163:LYS:HZ2	1.28	0.95
1:A:283:THR:HG23	1:A:430:GLU:HG3	1.48	0.95
1:D:228:ASP:OD2	1:D:231:SER:HB3	1.67	0.94
1:C:512:LYS:HD2	1:C:512:LYS:N	1.82	0.94
1:A:221:ARG:O	1:A:223:LYS:HD2	1.68	0.94
1:A:200:LEU:HD12	1:A:204:LEU:HD22	1.49	0.93
1:A:185:ASP:HA	1:A:188:ARG:HD2	1.53	0.90
1:C:202:LYS:HG3	1:C:203:ASP:H	1.36	0.90
1:A:541:PHE:HE1	1:A:549:ARG:HH12	1.13	0.90
1:A:512:LYS:H	1:A:512:LYS:CD	1.83	0.89
1:D:145:GLU:HG3	1:D:206:LYS:HG3	1.54	0.88
1:A:383:PHE:HZ	1:A:387:ARG:NH2	1.70	0.88
1:D:283:THR:CG2	1:D:430:GLU:CG	2.52	0.87
1:B:198:VAL:O	1:B:198:VAL:HG13	1.75	0.86
1:C:387:ARG:HG2	1:C:387:ARG:NH1	1.78	0.86
1:C:387:ARG:HH11	1:C:387:ARG:CG	1.88	0.84
1:A:200:LEU:CD1	1:A:204:LEU:CD2	2.54	0.84
1:A:145:GLU:HG3	1:A:206:LYS:HD3	1.58	0.84
1:A:270:VAL:HG22	1:A:503:MET:HE2	1.59	0.84
1:A:161:VAL:HG23	1:A:200:LEU:CD2	2.07	0.83
1:C:283:THR:HG21	1:C:430:GLU:HG3	1.61	0.83
1:C:159:ILE:HD11	1:C:163:LYS:HE2	1.59	0.83
1:A:383:PHE:CZ	1:A:387:ARG:NH2	2.47	0.82
1:A:383:PHE:HZ	1:A:387:ARG:HH21	1.22	0.82
1:A:548:ARG:HG3	1:A:548:ARG:NH1	1.87	0.82
1:A:200:LEU:CD1	1:A:204:LEU:HD21	2.07	0.81
1:A:239:LEU:HD22	1:A:525:ASP:HB3	1.61	0.81
1:A:412:MET:HE3	1:A:416:LEU:CD1	2.10	0.81
1:A:204:LEU:C	1:A:204:LEU:HD23	2.01	0.80
1:D:228:ASP:OD2	1:D:231:SER:CB	2.29	0.80
1:C:370:MET:HG3	1:C:452:VAL:HG11	1.63	0.80
1:C:451:ARG:HH12	1:C:455:PRO:HD3	1.47	0.80
1:D:145:GLU:CG	1:D:206:LYS:HG3	2.11	0.79
1:D:283:THR:HG23	1:D:430:GLU:HG2	1.64	0.79
1:D:283:THR:HG21	1:D:430:GLU:HG2	1.63	0.79
1:A:541:PHE:HE1	1:A:549:ARG:NH1	1.79	0.79
1:B:270:VAL:HG22	1:B:503:MET:HE2	1.63	0.79
1:D:145:GLU:HG3	1:D:206:LYS:HG2	1.63	0.79
1:A:161:VAL:CG2	1:A:200:LEU:HD21	2.13	0.78
1:B:387:ARG:HH11	1:B:387:ARG:CG	1.96	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:LYS:HD2	1:A:512:LYS:N	1.99	0.78
1:A:204:LEU:O	1:A:207:LYS:HB3	1.84	0.77
1:D:146:ASP:OD2	1:D:146:ASP:N	2.18	0.76
1:B:387:ARG:HH11	1:B:387:ARG:HG2	1.50	0.76
1:A:511:ASP:HB2	1:A:512:LYS:HD2	1.68	0.76
1:B:354:VAL:HG12	1:B:358:GLU:HB2	1.68	0.76
1:A:541:PHE:CE1	1:A:549:ARG:NH1	2.54	0.75
1:B:159:ILE:HG22	1:B:159:ILE:O	1.86	0.74
1:C:167:ALA:HB1	1:C:220:PHE:HE2	1.52	0.74
1:D:144:LEU:HB2	1:D:145:GLU:OE1	1.86	0.74
1:C:161:VAL:HG22	1:C:200:LEU:HD11	1.68	0.73
1:B:158:LYS:HD3	1:B:201:ASP:HB3	1.70	0.73
1:A:412:MET:HE3	1:A:416:LEU:HD11	1.71	0.73
1:B:548:ARG:HH11	1:B:548:ARG:HG3	1.52	0.72
1:D:181:LYS:HE2	1:D:185:ASP:OD2	1.89	0.71
1:B:151:THR:OG1	1:B:221:ARG:NH2	2.22	0.71
1:C:159:ILE:HD12	1:C:160:PRO:HD2	1.72	0.71
1:A:200:LEU:CD1	1:A:204:LEU:HD22	2.19	0.71
1:B:239:LEU:HD22	1:B:525:ASP:HB3	1.73	0.71
1:C:255:ILE:HB	1:C:385:SER:OG	1.90	0.71
1:A:256:PRO:O	1:A:260:LYS:HG3	1.90	0.71
1:C:209:VAL:CG1	1:C:213:ILE:HD13	2.20	0.70
1:C:148:LEU:HD13	1:C:148:LEU:C	2.11	0.70
1:A:283:THR:HG21	1:A:430:GLU:HG3	1.72	0.70
1:B:144:LEU:HB2	1:B:145:GLU:OE1	1.92	0.70
1:A:418:PHE:CE1	1:A:422:LEU:HD11	2.27	0.69
1:A:546:ASP:OD1	1:A:548:ARG:NH1	2.26	0.69
1:D:144:LEU:N	1:D:146:ASP:OD2	2.25	0.69
1:D:527:VAL:O	1:D:544:LYS:HE2	1.93	0.69
1:C:206:LYS:O	1:C:210:GLN:HG3	1.93	0.68
1:C:269:SER:OG	1:C:283:THR:HG23	1.94	0.68
1:B:542:ALA:HB2	1:D:455:PRO:HG2	1.76	0.68
1:D:283:THR:CG2	1:D:283:THR:O	2.40	0.68
1:A:216:LEU:O	1:A:220:PHE:HD1	1.77	0.68
1:A:336:ASN:HB2	1:A:337:PRO:HD2	1.76	0.68
1:C:148:LEU:O	1:C:148:LEU:CD1	2.32	0.67
1:A:199:MET:C	1:A:200:LEU:HD22	2.15	0.67
1:B:354:VAL:CG1	1:B:358:GLU:HB2	2.25	0.67
1:C:336:ASN:HB2	1:C:337:PRO:HD2	1.76	0.67
1:D:336:ASN:O	1:D:342:GLY:HA3	1.94	0.67
1:C:337:PRO:CG	1:C:464:LEU:HD13	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:VAL:HG12	1:D:213:ILE:HD13	1.77	0.66
1:A:200:LEU:HD22	1:A:200:LEU:N	2.09	0.66
1:C:451:ARG:NH1	1:C:455:PRO:HD3	2.09	0.66
1:B:387:ARG:HG2	1:B:387:ARG:NH1	2.10	0.66
1:D:205:PHE:O	1:D:207:LYS:N	2.29	0.66
1:A:412:MET:HE3	1:A:416:LEU:HD12	1.76	0.66
1:B:532:PHE:CZ	1:B:547:PRO:HG2	2.31	0.66
1:B:451:ARG:HH12	1:B:455:PRO:HD3	1.61	0.65
1:B:148:LEU:HD22	1:B:213:ILE:HD11	1.78	0.65
1:C:184:MET:O	1:C:188:ARG:HG3	1.96	0.65
1:D:403:LYS:C	1:D:404:LYS:HG3	2.16	0.65
1:B:387:ARG:HH11	1:B:387:ARG:CB	2.10	0.65
1:A:158:LYS:HD2	1:A:199:MET:HB3	1.79	0.65
1:C:161:VAL:CG2	1:C:200:LEU:HD11	2.26	0.65
1:D:541:PHE:HD2	1:D:544:LYS:O	1.78	0.64
1:C:283:THR:CG2	1:C:430:GLU:HG3	2.27	0.64
1:D:283:THR:HG23	1:D:283:THR:O	1.98	0.64
1:A:269:SER:HB2	1:A:429:CYS:HB3	1.79	0.64
1:B:548:ARG:HG3	1:B:548:ARG:NH1	2.12	0.64
1:D:152:ILE:HG22	1:D:163:LYS:HZ3	1.61	0.64
1:D:348:SER:OG	1:D:407:PRO:HD2	1.98	0.63
1:A:418:PHE:O	1:A:422:LEU:HD13	1.98	0.63
1:C:159:ILE:HG23	1:C:159:ILE:O	1.98	0.63
1:D:336:ASN:HB2	1:D:337:PRO:HD2	1.79	0.63
1:D:152:ILE:CG2	1:D:163:LYS:NZ	2.57	0.63
1:D:200:LEU:HD22	1:D:205:PHE:HA	1.80	0.63
1:A:437:ALA:HB1	1:A:446:PRO:HG3	1.81	0.63
1:D:172:GLY:HA3	1:D:229:PHE:CD2	2.34	0.63
1:B:336:ASN:HB2	1:B:337:PRO:HD2	1.81	0.62
1:D:145:GLU:CG	1:D:206:LYS:CG	2.72	0.62
1:D:283:THR:HG21	1:D:430:GLU:OE2	1.99	0.62
1:B:284:LYS:NZ	1:B:430:GLU:OE2	2.32	0.62
1:A:178:PRO:HA	1:A:181:LYS:HE3	1.80	0.62
1:C:270:VAL:HG22	1:C:503:MET:HE1	1.82	0.62
1:C:392:ARG:O	1:C:396:ILE:HG13	1.99	0.62
1:C:328:LEU:HD13	1:C:332:ASP:O	1.98	0.62
1:B:397:GLY:HA3	1:B:412:MET:CE	2.30	0.62
1:C:541:PHE:N	1:C:541:PHE:CD1	2.68	0.62
1:C:512:LYS:CD	1:C:512:LYS:N	2.52	0.61
1:D:418:PHE:CE1	1:D:422:LEU:HD11	2.35	0.61
1:B:149:PHE:CE1	1:B:159:ILE:HD12	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:ASP:O	1:C:202:LYS:C	2.35	0.61
1:A:221:ARG:O	1:A:223:LYS:CD	2.45	0.61
1:C:146:ASP:OD2	1:C:147:LEU:N	2.33	0.61
1:D:170:SER:HA	1:D:230:MET:SD	2.40	0.61
1:A:451:ARG:HH12	1:A:455:PRO:HD3	1.65	0.61
1:A:412:MET:CE	1:A:416:LEU:CD1	2.79	0.61
1:A:530:CYS:HA	1:A:545:LEU:O	2.00	0.61
1:C:470:MET:HG3	1:C:477:PHE:CG	2.36	0.61
1:B:229:PHE:O	1:B:233:THR:HG23	2.00	0.61
1:A:387:ARG:NH2	1:A:417:ASP:OD2	2.33	0.61
1:A:451:ARG:NH1	1:A:455:PRO:HD3	2.16	0.61
1:D:202:LYS:H	1:D:202:LYS:HD2	1.65	0.61
1:D:370:MET:HG3	1:D:452:VAL:HG11	1.83	0.61
1:D:201:ASP:OD1	1:D:201:ASP:C	2.38	0.60
1:A:412:MET:CE	1:A:416:LEU:HD12	2.31	0.60
1:C:257:GLN:HE21	1:C:381:ALA:HB1	1.66	0.60
1:D:158:LYS:HB3	1:D:199:MET:SD	2.41	0.60
1:B:167:ALA:HB1	1:B:220:PHE:HE2	1.67	0.60
1:B:305:LEU:HD13	1:B:309:TYR:CE2	2.36	0.60
1:A:334:PRO:HG2	1:A:345:VAL:HG21	1.83	0.60
1:A:336:ASN:O	1:A:342:GLY:HA3	2.02	0.60
1:B:394:PHE:HA	1:B:416:LEU:HD11	1.83	0.60
1:B:165:ILE:HG22	1:B:166:THR:N	2.16	0.59
1:C:202:LYS:HG3	1:C:203:ASP:N	2.13	0.59
1:D:200:LEU:HD23	1:D:204:LEU:HG	1.84	0.59
1:C:269:SER:OG	1:C:429:CYS:HB3	2.02	0.59
1:C:164:PHE:HD2	1:C:165:ILE:HD13	1.66	0.59
1:C:165:ILE:HG22	1:C:166:THR:N	2.16	0.59
1:D:222:ARG:HH21	1:D:222:ARG:HG3	1.67	0.59
1:D:530:CYS:HA	1:D:545:LEU:O	2.03	0.59
1:B:455:PRO:HG2	1:D:542:ALA:HB2	1.84	0.59
1:D:541:PHE:CD2	1:D:544:LYS:O	2.55	0.59
1:A:546:ASP:OD1	1:A:548:ARG:HG3	2.01	0.58
1:C:146:ASP:OD2	1:C:146:ASP:C	2.40	0.58
1:D:152:ILE:CG2	1:D:163:LYS:HZ3	2.16	0.58
1:B:355:ASN:C	1:B:355:ASN:OD1	2.42	0.58
1:D:283:THR:HG21	1:D:430:GLU:CG	2.29	0.58
1:A:145:GLU:HB2	1:A:206:LYS:HB2	1.85	0.58
1:C:225:VAL:HG22	1:C:274:ASP:OD2	2.04	0.58
1:C:345:VAL:O	1:C:348:SER:HB3	2.04	0.58
1:D:200:LEU:HA	1:D:204:LEU:HD23	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:LEU:CB	1:B:145:GLU:OE1	2.51	0.58
1:C:437:ALA:CB	1:C:446:PRO:HG3	2.34	0.58
1:B:269:SER:O	1:B:503:MET:HB2	2.02	0.57
1:D:229:PHE:O	1:D:233:THR:HG23	2.03	0.57
1:D:345:VAL:O	1:D:348:SER:HB3	2.04	0.57
1:C:209:VAL:HG11	1:C:213:ILE:HD13	1.84	0.57
1:B:174:ARG:O	1:B:177:ASP:HB2	2.05	0.57
1:D:412:MET:O	1:D:412:MET:HG2	2.02	0.57
1:A:295:PRO:HD3	1:A:486:LYS:HG3	1.86	0.57
1:A:470:MET:HE1	1:A:487:SER:HB3	1.86	0.57
1:B:200:LEU:CD2	1:B:204:LEU:HG	2.35	0.56
1:B:202:LYS:O	1:B:203:ASP:C	2.42	0.56
1:C:254:TYR:CD1	1:C:255:ILE:HG23	2.40	0.56
1:A:337:PRO:HD2	1:A:464:LEU:HD13	1.85	0.56
1:A:354:VAL:HG12	1:A:358:GLU:HB2	1.87	0.56
1:C:159:ILE:HD12	1:C:160:PRO:CD	2.34	0.56
1:D:183:CYS:HB3	1:D:212:ASN:OD1	2.05	0.56
1:B:185:ASP:OD1	1:B:188:ARG:NH2	2.37	0.56
1:B:477:PHE:CE1	1:B:481:VAL:HG21	2.41	0.56
1:C:145:GLU:OE1	1:C:206:LYS:HE3	2.05	0.56
1:D:149:PHE:CE2	1:D:202:LYS:HG3	2.40	0.56
1:C:346:VAL:HA	1:C:349:LEU:HD22	1.88	0.56
1:C:354:VAL:CG1	1:C:358:GLU:HB2	2.36	0.56
1:A:204:LEU:HD23	1:A:205:PHE:N	2.20	0.56
1:A:387:ARG:NH2	1:A:417:ASP:OD1	2.39	0.56
1:B:531:ASN:HB2	1:B:536:ASP:HB3	1.87	0.56
1:A:531:ASN:HB2	1:A:536:ASP:HB3	1.86	0.56
1:C:160:PRO:HB3	1:C:162:HIS:CE1	2.41	0.56
1:C:530:CYS:HA	1:C:545:LEU:O	2.05	0.56
1:D:160:PRO:HD2	1:D:163:LYS:HD3	1.88	0.56
1:A:437:ALA:CB	1:A:446:PRO:HG3	2.36	0.56
1:C:541:PHE:HZ	1:C:549:ARG:NH2	2.04	0.56
1:D:451:ARG:HH12	1:D:455:PRO:HD3	1.70	0.55
1:B:198:VAL:O	1:B:198:VAL:CG1	2.48	0.55
1:D:216:LEU:O	1:D:220:PHE:HD1	1.88	0.55
1:D:283:THR:CG2	1:D:430:GLU:OE2	2.54	0.55
1:A:209:VAL:HG13	1:A:216:LEU:HD12	1.86	0.55
1:A:444:PHE:HE1	1:A:451:ARG:NH2	2.03	0.55
1:C:283:THR:O	1:C:428:THR:HB	2.06	0.55
1:B:467:SER:O	1:B:474:SER:HB3	2.07	0.55
1:C:198:VAL:O	1:C:198:VAL:HG12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:LEU:HD13	1:C:293:VAL:HG23	1.88	0.55
1:C:201:ASP:O	1:C:202:LYS:O	2.25	0.55
1:B:530:CYS:HA	1:B:545:LEU:O	2.06	0.55
1:C:437:ALA:HB3	1:C:446:PRO:HG3	1.86	0.55
1:A:146:ASP:OD2	1:A:146:ASP:N	2.36	0.55
1:D:189:LEU:O	1:D:193:THR:HG23	2.07	0.54
1:C:227:PRO:HD2	1:C:547:PRO:O	2.07	0.54
1:D:269:SER:O	1:D:503:MET:HB2	2.06	0.54
1:A:283:THR:CG2	1:A:430:GLU:OE2	2.55	0.54
1:B:224:PHE:HA	1:B:274:ASP:OD2	2.07	0.54
1:B:334:PRO:HG2	1:B:345:VAL:HG21	1.90	0.54
1:C:348:SER:HA	1:C:415:ILE:HD12	1.90	0.54
1:C:467:SER:O	1:C:474:SER:HB3	2.07	0.54
1:D:205:PHE:O	1:D:208:CYS:N	2.37	0.54
1:A:283:THR:CG2	1:A:430:GLU:CG	2.78	0.54
1:B:331:ASP:O	1:B:332:ASP:HB2	2.06	0.54
1:C:255:ILE:HD13	1:C:386:GLU:OE2	2.08	0.54
1:D:148:LEU:HD12	1:D:205:PHE:CZ	2.42	0.54
1:A:283:THR:HG21	1:A:430:GLU:CG	2.38	0.54
1:A:290:GLN:O	1:A:293:VAL:HG12	2.07	0.54
1:C:266:TRP:HA	1:C:506:TRP:O	2.07	0.54
1:A:441:ASN:O	1:C:540:HIS:HD2	1.90	0.54
1:B:209:VAL:CG1	1:B:213:ILE:HD13	2.37	0.54
1:A:369:LYS:HB3	1:A:452:VAL:HG22	1.89	0.54
1:B:218:GLN:HG3	1:B:223:LYS:HB2	1.90	0.53
1:B:336:ASN:O	1:B:342:GLY:HA3	2.08	0.53
1:D:378:PHE:CE1	1:D:424:SER:HB2	2.43	0.53
1:A:348:SER:HA	1:A:415:ILE:HD12	1.91	0.53
1:B:512:LYS:CD	1:B:512:LYS:H	2.20	0.53
1:D:179:ARG:HG3	1:D:447:ILE:O	2.09	0.53
1:D:387:ARG:NH1	1:D:417:ASP:OD1	2.40	0.53
1:B:387:ARG:HH11	1:B:387:ARG:HB3	1.73	0.53
1:C:397:GLY:HA3	1:C:412:MET:CE	2.38	0.53
1:D:209:VAL:CG1	1:D:213:ILE:HD13	2.38	0.53
1:A:354:VAL:HG13	1:A:358:GLU:OE1	2.08	0.53
1:B:548:ARG:HH11	1:B:548:ARG:CG	2.21	0.53
1:C:200:LEU:HA	1:C:204:LEU:HD23	1.91	0.53
1:D:315:GLY:O	1:D:336:ASN:HA	2.08	0.53
1:A:206:LYS:O	1:A:210:GLN:HB2	2.08	0.53
1:B:149:PHE:CD1	1:B:159:ILE:HD12	2.43	0.53
1:B:534:ASN:OD1	1:D:534:ASN:OD1	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:LEU:C	1:C:148:LEU:CD1	2.74	0.53
1:D:149:PHE:CD2	1:D:202:LYS:HG3	2.43	0.53
1:D:527:VAL:O	1:D:544:LYS:CE	2.56	0.53
1:D:298:TYR:OH	1:D:460:ASN:HB3	2.09	0.53
1:B:337:PRO:CG	1:B:464:LEU:HD13	2.39	0.53
1:B:451:ARG:NH1	1:B:455:PRO:HD3	2.23	0.53
1:C:187:LEU:HD23	1:C:208:CYS:SG	2.49	0.53
1:C:209:VAL:HG13	1:C:216:LEU:HD12	1.91	0.53
1:D:213:ILE:HG23	1:D:214:VAL:N	2.24	0.53
1:C:485:ALA:HB2	1:C:495:LEU:HD12	1.89	0.52
1:D:451:ARG:NH1	1:D:455:PRO:HD3	2.24	0.52
1:A:160:PRO:HG2	1:A:163:LYS:HB3	1.90	0.52
1:A:387:ARG:HH21	1:A:417:ASP:CG	2.12	0.52
1:A:455:PRO:HG2	1:C:542:ALA:HB2	1.91	0.52
1:A:534:ASN:OD1	1:C:534:ASN:OD1	2.27	0.52
1:B:532:PHE:HZ	1:B:547:PRO:HG2	1.74	0.52
1:D:354:VAL:HG12	1:D:358:GLU:HB2	1.90	0.52
1:C:161:VAL:CG2	1:C:200:LEU:CD1	2.87	0.52
1:A:283:THR:HG21	1:A:430:GLU:OE2	2.09	0.52
1:B:397:GLY:HA3	1:B:412:MET:HE3	1.90	0.52
1:D:239:LEU:HD22	1:D:525:ASP:HB3	1.92	0.52
1:D:266:TRP:HA	1:D:506:TRP:O	2.08	0.52
1:B:148:LEU:CD2	1:B:213:ILE:HD11	2.38	0.52
1:C:305:LEU:HD13	1:C:309:TYR:CE2	2.44	0.52
1:D:360:PHE:CE1	1:D:421:GLN:HB3	2.45	0.52
1:B:227:PRO:HD2	1:B:547:PRO:O	2.10	0.52
1:C:336:ASN:O	1:C:342:GLY:HA3	2.10	0.52
1:B:533:HIS:HB3	1:B:536:ASP:OD2	2.10	0.52
1:C:170:SER:HA	1:C:230:MET:SD	2.49	0.52
1:D:227:PRO:HD2	1:D:547:PRO:O	2.10	0.52
1:A:354:VAL:O	1:A:359:LYS:HE3	2.10	0.51
1:B:295:PRO:HD3	1:B:486:LYS:HG2	1.92	0.51
1:C:312:ARG:O	1:C:333:LYS:HD2	2.10	0.51
1:A:387:ARG:NH2	1:A:417:ASP:CG	2.64	0.51
1:C:167:ALA:CB	1:C:220:PHE:HE2	2.23	0.51
1:B:397:GLY:HA3	1:B:412:MET:HE2	1.92	0.51
1:C:289:LEU:CD1	1:C:293:VAL:HG23	2.40	0.51
1:D:205:PHE:O	1:D:206:LYS:C	2.47	0.51
1:B:339:VAL:HG23	1:B:342:GLY:H	1.75	0.51
1:B:253:ASP:O	1:B:254:TYR:O	2.29	0.51
1:C:229:PHE:O	1:C:233:THR:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:548:ARG:C	1:C:549:ARG:HG3	2.31	0.51
1:A:491:GLY:HA2	1:A:510:LEU:HD21	1.93	0.51
1:D:354:VAL:CG1	1:D:358:GLU:HB2	2.40	0.51
1:A:146:ASP:O	1:A:149:PHE:N	2.42	0.51
1:B:491:GLY:HA2	1:B:510:LEU:HD21	1.93	0.51
1:C:148:LEU:HD12	1:C:205:PHE:CZ	2.46	0.51
1:C:348:SER:OG	1:C:407:PRO:HD2	2.11	0.51
1:A:290:GLN:HG3	1:A:489:VAL:HG12	1.91	0.51
1:C:440:ALA:HB2	1:C:496:VAL:HG13	1.93	0.51
1:D:532:PHE:CZ	1:D:547:PRO:HG2	2.45	0.51
1:A:498:PRO:O	1:A:499:ASN:HB2	2.11	0.50
1:B:437:ALA:HB1	1:B:446:PRO:HG3	1.93	0.50
1:C:209:VAL:HG12	1:C:213:ILE:HD13	1.90	0.50
1:B:402:GLU:HG3	1:B:403:LYS:HD2	1.94	0.50
1:D:331:ASP:O	1:D:332:ASP:HB2	2.11	0.50
1:D:440:ALA:HB2	1:D:496:VAL:HG13	1.93	0.50
1:D:152:ILE:HB	1:D:159:ILE:HD13	1.94	0.50
1:D:334:PRO:HG2	1:D:345:VAL:HG21	1.93	0.50
1:D:378:PHE:HE1	1:D:424:SER:HB2	1.75	0.50
1:A:283:THR:O	1:A:428:THR:HB	2.11	0.50
1:D:283:THR:HG23	1:D:430:GLU:CG	2.30	0.50
1:D:394:PHE:HA	1:D:416:LEU:HD11	1.94	0.50
1:D:467:SER:O	1:D:474:SER:HB3	2.10	0.50
1:C:213:ILE:HG23	1:C:214:VAL:N	2.26	0.50
1:D:498:PRO:O	1:D:499:ASN:HB2	2.12	0.50
1:A:204:LEU:O	1:A:205:PHE:C	2.50	0.50
1:D:151:THR:HG22	1:D:151:THR:O	2.12	0.50
1:D:160:PRO:O	1:D:163:LYS:HB3	2.12	0.50
1:A:145:GLU:OE2	1:A:210:GLN:HA	2.11	0.50
1:C:162:HIS:O	1:C:166:THR:OG1	2.30	0.50
1:B:149:PHE:CE1	1:B:159:ILE:CD1	2.95	0.49
1:C:315:GLY:O	1:C:336:ASN:HA	2.12	0.49
1:A:486:LYS:HD2	1:A:487:SER:N	2.27	0.49
1:B:354:VAL:CG1	1:B:358:GLU:CB	2.90	0.49
1:D:305:LEU:HD13	1:D:309:TYR:CE2	2.47	0.49
1:D:312:ARG:O	1:D:333:LYS:HD2	2.12	0.49
1:D:418:PHE:O	1:D:422:LEU:HD13	2.12	0.49
1:D:184:MET:O	1:D:188:ARG:HG3	2.11	0.49
1:A:486:LYS:HD2	1:A:487:SER:H	1.77	0.49
1:C:161:VAL:HG23	1:C:200:LEU:CD1	2.42	0.49
1:C:237:ASP:OD1	1:C:280:ILE:HD12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:495:LEU:HD22	1:D:523:CYS:SG	2.52	0.49
1:D:527:VAL:O	1:D:544:LYS:NZ	2.45	0.49
1:C:294:LYS:N	1:C:295:PRO:HD2	2.28	0.49
1:B:371:ALA:O	1:B:374:GLU:HG3	2.12	0.49
1:D:228:ASP:OD2	1:D:231:SER:HB2	2.11	0.49
1:A:200:LEU:CD2	1:A:200:LEU:N	2.76	0.49
1:A:204:LEU:CD2	1:A:204:LEU:C	2.76	0.49
1:C:337:PRO:HG3	1:C:464:LEU:HD13	1.94	0.49
1:C:541:PHE:CZ	1:C:549:ARG:NH2	2.80	0.49
1:A:354:VAL:CG1	1:A:358:GLU:OE1	2.61	0.49
1:B:145:GLU:HG3	1:B:206:LYS:CG	2.29	0.49
1:A:174:ARG:O	1:A:177:ASP:HB2	2.13	0.49
1:C:444:PHE:HE1	1:C:451:ARG:NH2	2.11	0.49
1:D:188:ARG:O	1:D:192:GLN:HG3	2.12	0.49
1:A:501:MET:HE2	1:A:532:PHE:CE2	2.47	0.48
1:C:218:GLN:HG3	1:C:223:LYS:HB2	1.95	0.48
1:C:161:VAL:HG23	1:C:200:LEU:HD12	1.95	0.48
1:C:239:LEU:HD22	1:C:525:ASP:HB3	1.95	0.48
1:C:482:GLY:O	1:C:534:ASN:HB2	2.13	0.48
1:C:367:LEU:HD23	1:C:370:MET:HE3	1.95	0.48
1:D:201:ASP:O	1:D:202:LYS:C	2.52	0.48
1:B:491:GLY:HA3	1:B:507:SER:O	2.13	0.48
1:D:148:LEU:HD12	1:D:205:PHE:HZ	1.78	0.48
1:D:217:THR:O	1:D:221:ARG:HG2	2.13	0.48
1:A:254:TYR:CD1	1:A:255:ILE:HG23	2.49	0.48
1:B:162:HIS:O	1:B:165:ILE:HB	2.13	0.48
1:C:270:VAL:HG22	1:C:503:MET:CE	2.44	0.48
1:D:160:PRO:HG3	1:D:199:MET:CE	2.44	0.48
1:C:412:MET:HE1	1:C:416:LEU:HD12	1.94	0.48
1:B:148:LEU:HD22	1:B:213:ILE:CD1	2.43	0.48
1:C:541:PHE:HZ	1:C:549:ARG:HH22	1.61	0.48
1:D:365:GLN:O	1:D:369:LYS:HG3	2.13	0.48
1:A:234:SER:O	1:A:238:GLU:HG3	2.14	0.47
1:B:354:VAL:O	1:B:359:LYS:HE3	2.14	0.47
1:D:198:VAL:O	1:D:199:MET:HG2	2.13	0.47
1:A:145:GLU:HG3	1:A:206:LYS:CD	2.38	0.47
1:B:210:GLN:O	1:B:211:SER:C	2.51	0.47
1:B:200:LEU:HD23	1:B:204:LEU:HG	1.96	0.47
1:B:508:PRO:HD2	1:B:509:PRO:HD3	1.96	0.47
1:A:179:ARG:HG3	1:A:447:ILE:O	2.15	0.47
1:A:499:ASN:ND2	1:C:538:LEU:HG	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:LYS:O	1:B:210:GLN:CB	2.61	0.47
1:B:290:GLN:O	1:B:293:VAL:HG12	2.14	0.47
1:C:151:THR:HG22	1:C:151:THR:O	2.15	0.47
1:C:531:ASN:HB2	1:C:536:ASP:HB3	1.96	0.47
1:D:399:TYR:CZ	1:D:403:LYS:HE3	2.48	0.47
1:A:230:MET:HA	1:A:230:MET:CE	2.45	0.47
1:D:198:VAL:O	1:D:198:VAL:HG12	2.14	0.47
1:A:354:VAL:CG1	1:A:358:GLU:HB2	2.44	0.47
1:B:480:HIS:O	1:B:533:HIS:HD2	1.98	0.47
1:B:512:LYS:H	1:B:512:LYS:HD2	1.79	0.47
1:C:275:GLY:O	1:C:277:ARG:HG2	2.15	0.47
1:D:531:ASN:HB2	1:D:536:ASP:HB3	1.96	0.47
1:B:145:GLU:HG2	1:B:206:LYS:HE2	1.96	0.47
1:C:361:ASP:O	1:C:365:GLN:HG2	2.14	0.47
1:C:397:GLY:HA3	1:C:412:MET:HE2	1.96	0.47
1:A:291:SER:O	1:A:486:LYS:HE3	2.15	0.47
1:D:275:GLY:O	1:D:277:ARG:HG2	2.15	0.47
1:A:186:MET:HB3	1:A:208:CYS:HA	1.97	0.47
1:A:548:ARG:NH1	1:A:548:ARG:CG	2.65	0.47
1:C:257:GLN:HA	1:C:260:LYS:HE2	1.96	0.47
1:D:168:LEU:HD21	1:D:180:LEU:HD13	1.97	0.47
1:D:252:ALA:HB2	1:D:489:VAL:HG22	1.97	0.47
1:B:422:LEU:HD12	1:B:422:LEU:HA	1.72	0.46
1:C:212:ASN:N	1:C:212:ASN:ND2	2.62	0.46
1:D:171:THR:O	1:D:276:GLN:HG2	2.15	0.46
1:D:174:ARG:O	1:D:177:ASP:HB2	2.15	0.46
1:A:355:ASN:OD1	1:A:357:ALA:HB3	2.15	0.46
1:B:230:MET:CE	1:B:230:MET:HA	2.46	0.46
1:B:512:LYS:HD2	1:B:512:LYS:N	2.30	0.46
1:D:345:VAL:O	1:D:349:LEU:HD13	2.16	0.46
1:A:441:ASN:HB3	1:A:444:PHE:O	2.14	0.46
1:B:251:VAL:HG22	1:B:508:PRO:HB2	1.98	0.46
1:A:150:TYR:O	1:A:152:ILE:N	2.49	0.46
1:A:390:GLY:O	1:A:394:PHE:HD2	1.99	0.46
1:B:221:ARG:HD3	1:B:221:ARG:HA	1.41	0.46
1:B:348:SER:HA	1:B:415:ILE:HD12	1.98	0.46
1:B:444:PHE:CE2	1:B:451:ARG:HB2	2.51	0.46
1:C:354:VAL:HG12	1:C:355:ASN:N	2.30	0.46
1:A:538:LEU:HG	1:C:499:ASN:OD1	2.16	0.46
1:B:165:ILE:HD12	1:B:165:ILE:HA	1.73	0.46
1:A:508:PRO:N	1:A:509:PRO:CD	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:ASN:HD21	1:B:357:ALA:HB3	1.81	0.46
1:B:489:VAL:O	1:B:489:VAL:HG12	2.14	0.46
1:C:189:LEU:O	1:C:192:GLN:HB2	2.14	0.46
1:C:202:LYS:CG	1:C:203:ASP:N	2.77	0.46
1:D:159:ILE:O	1:D:159:ILE:HG22	2.15	0.46
1:D:302:VAL:HG11	1:D:457:ALA:HA	1.98	0.46
1:B:161:VAL:HG12	1:B:162:HIS:N	2.30	0.45
1:A:477:PHE:CE1	1:A:481:VAL:HG21	2.50	0.45
1:A:444:PHE:CE1	1:A:451:ARG:NH2	2.84	0.45
1:B:200:LEU:HD23	1:B:204:LEU:HD23	1.97	0.45
1:B:204:LEU:O	1:B:207:LYS:HB3	2.16	0.45
1:D:209:VAL:HG13	1:D:216:LEU:CD1	2.46	0.45
1:B:284:LYS:NZ	1:B:430:GLU:CD	2.70	0.45
1:C:159:ILE:O	1:C:160:PRO:C	2.54	0.45
1:C:416:LEU:O	1:C:420:PHE:CD2	2.69	0.45
1:D:286:PRO:HA	1:D:427:VAL:O	2.17	0.45
1:B:186:MET:HB3	1:B:208:CYS:HA	1.99	0.45
1:A:294:LYS:N	1:A:295:PRO:HD2	2.31	0.45
1:C:149:PHE:CE2	1:C:202:LYS:N	2.85	0.45
1:D:403:LYS:O	1:D:404:LYS:HG3	2.15	0.45
1:B:315:GLY:O	1:B:336:ASN:HA	2.17	0.45
1:C:394:PHE:HA	1:C:416:LEU:HD11	1.99	0.45
1:D:481:VAL:O	1:D:527:VAL:HG21	2.17	0.45
1:D:492:GLY:HA3	1:D:504:MET:HE3	1.99	0.45
1:D:507:SER:OG	1:D:518:LYS:HD2	2.16	0.45
1:B:416:LEU:HD23	1:B:416:LEU:HA	1.84	0.45
1:B:437:ALA:CB	1:B:446:PRO:HG3	2.47	0.45
1:C:182:GLU:CD	1:C:182:GLU:H	2.20	0.45
1:C:354:VAL:HG11	1:C:358:GLU:HB2	1.99	0.45
1:A:146:ASP:O	1:A:147:LEU:C	2.53	0.44
1:B:216:LEU:O	1:B:220:PHE:HD1	1.99	0.44
1:C:172:GLY:HA3	1:C:229:PHE:CD2	2.52	0.44
1:C:507:SER:HB3	1:C:516:SER:HG	1.83	0.44
1:D:279:SER:OG	1:D:283:THR:HG21	2.16	0.44
1:D:339:VAL:HG23	1:D:342:GLY:H	1.82	0.44
1:D:444:PHE:CE2	1:D:451:ARG:HB2	2.53	0.44
1:B:200:LEU:HD23	1:B:204:LEU:CD2	2.48	0.44
1:C:202:LYS:HG3	1:C:203:ASP:CG	2.35	0.44
1:C:363:VAL:O	1:C:367:LEU:HG	2.18	0.44
1:C:444:PHE:CE1	1:C:451:ARG:NH2	2.86	0.44
1:B:156:GLN:NE2	1:B:157:GLU:H	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:387:ARG:HE	1:C:417:ASP:CG	2.21	0.44
1:D:485:ALA:HA	1:D:494:LEU:O	2.18	0.44
1:A:183:CYS:CB	1:A:212:ASN:OD1	2.66	0.44
1:B:201:ASP:O	1:B:202:LYS:C	2.54	0.44
1:B:508:PRO:CD	1:B:509:PRO:HD3	2.48	0.44
1:C:251:VAL:HG22	1:C:508:PRO:HB2	1.98	0.44
1:D:200:LEU:HD23	1:D:204:LEU:CD2	2.48	0.44
1:B:159:ILE:O	1:B:160:PRO:C	2.55	0.44
1:C:300:ILE:HG23	1:C:366:PHE:CE2	2.53	0.44
1:C:412:MET:CE	1:C:416:LEU:HD12	2.48	0.44
1:D:200:LEU:HD23	1:D:204:LEU:CG	2.46	0.44
1:A:165:ILE:HG22	1:A:166:THR:N	2.33	0.43
1:C:296:LEU:O	1:C:300:ILE:HG13	2.18	0.43
1:C:444:PHE:CE2	1:C:451:ARG:HB2	2.53	0.43
1:C:451:ARG:NH2	3:C:118:HOH:O	2.51	0.43
1:B:355:ASN:OD1	1:B:355:ASN:O	2.35	0.43
1:C:165:ILE:HD12	1:C:165:ILE:HA	1.57	0.43
1:C:265:LEU:HB3	1:C:506:TRP:CZ3	2.54	0.43
1:D:213:ILE:O	1:D:214:VAL:C	2.57	0.43
1:D:383:PHE:O	1:D:387:ARG:HB2	2.17	0.43
1:C:254:TYR:CE2	1:C:258:LEU:HD12	2.53	0.43
1:C:549:ARG:NH1	3:C:114:HOH:O	2.49	0.43
1:A:370:MET:HG2	1:A:452:VAL:HG11	2.01	0.43
1:B:292:CYS:HA	1:B:486:LYS:HG3	1.99	0.43
1:B:305:LEU:HD13	1:B:309:TYR:HE2	1.80	0.43
1:C:160:PRO:HB3	1:C:162:HIS:HE1	1.82	0.43
1:B:378:PHE:CE1	1:B:424:SER:HB2	2.54	0.43
1:B:527:VAL:CG1	1:B:533:HIS:HB2	2.49	0.43
1:C:148:LEU:HD12	1:C:205:PHE:HZ	1.84	0.43
1:C:283:THR:HG23	1:C:429:CYS:HB2	1.99	0.43
1:C:498:PRO:O	1:C:499:ASN:HB2	2.19	0.43
1:D:204:LEU:O	1:D:205:PHE:C	2.57	0.43
1:D:240:TYR:HD1	1:D:268:VAL:HG23	1.83	0.43
1:D:262:SER:O	1:D:508:PRO:HG2	2.18	0.43
1:C:164:PHE:CD2	1:C:165:ILE:HD13	2.49	0.43
1:C:545:LEU:HD12	1:C:546:ASP:N	2.34	0.43
1:B:313:TYR:O	1:B:333:LYS:HB3	2.18	0.43
1:C:295:PRO:HD3	1:C:486:LYS:HG2	2.01	0.43
1:D:202:LYS:H	1:D:202:LYS:CD	2.29	0.43
1:D:428:THR:OG1	1:D:431:SER:HB3	2.19	0.43
1:A:542:ALA:HB2	1:C:455:PRO:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:481:VAL:O	1:B:527:VAL:HG21	2.18	0.43
1:C:507:SER:HB3	1:C:516:SER:OG	2.18	0.43
1:C:507:SER:OG	1:C:509:PRO:HD2	2.19	0.43
1:A:189:LEU:HD12	1:A:189:LEU:HA	1.83	0.43
1:B:508:PRO:N	1:B:509:PRO:CD	2.82	0.43
1:D:541:PHE:CD1	1:D:541:PHE:N	2.87	0.43
1:A:349:LEU:HA	1:A:352:GLN:HE21	1.84	0.42
1:C:340:ASN:O	1:C:344:ILE:HG13	2.19	0.42
1:B:272:THR:HA	1:B:501:MET:CB	2.50	0.42
1:B:445:CYS:HB3	1:B:448:THR:OG1	2.19	0.42
1:C:364:MET:HE1	1:C:425:ILE:HG23	2.01	0.42
1:D:212:ASN:O	1:D:213:ILE:C	2.58	0.42
1:D:233:THR:HB	1:D:278:HIS:CG	2.54	0.42
1:A:262:SER:HA	1:A:263:PRO:HD3	1.91	0.42
1:A:337:PRO:CD	1:A:464:LEU:HD13	2.49	0.42
1:D:367:LEU:HA	1:D:370:MET:HE3	2.01	0.42
1:A:204:LEU:O	1:A:207:LYS:N	2.52	0.42
1:A:295:PRO:CD	1:A:486:LYS:HG3	2.49	0.42
1:C:422:LEU:HD12	1:C:422:LEU:HA	1.58	0.42
1:A:257:GLN:CD	1:A:257:GLN:H	2.23	0.42
1:C:380:ASN:O	1:C:384:GLN:HG2	2.19	0.42
1:A:292:CYS:O	1:A:295:PRO:HD2	2.20	0.42
1:C:159:ILE:HD12	1:C:159:ILE:HA	1.82	0.42
1:C:269:SER:HG	1:C:283:THR:HG23	1.84	0.42
1:D:237:ASP:OD1	1:D:280:ILE:HD12	2.20	0.42
1:D:346:VAL:HA	1:D:349:LEU:HD22	2.02	0.42
1:A:165:ILE:HD12	1:A:165:ILE:HA	1.85	0.42
1:B:511:ASP:HB2	1:B:512:LYS:NZ	2.35	0.42
1:C:485:ALA:HA	1:C:494:LEU:O	2.20	0.42
1:D:148:LEU:CD1	1:D:205:PHE:HZ	2.33	0.42
1:A:221:ARG:O	1:A:223:LYS:CE	2.67	0.42
1:C:311:HIS:O	1:C:333:LYS:HE3	2.20	0.42
1:D:545:LEU:HD12	1:D:546:ASP:N	2.35	0.42
1:A:341:ALA:O	1:A:345:VAL:HG23	2.20	0.42
1:C:339:VAL:HG23	1:C:342:GLY:H	1.84	0.42
1:D:512:LYS:H	1:D:512:LYS:HG3	1.34	0.42
1:A:334:PRO:HG2	1:A:345:VAL:CG2	2.49	0.41
1:B:305:LEU:HB3	1:B:309:TYR:CD2	2.55	0.41
1:C:225:VAL:N	1:C:274:ASP:OD2	2.52	0.41
1:C:240:TYR:CD1	1:C:280:ILE:HG23	2.55	0.41
1:C:272:THR:HA	1:C:501:MET:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:LYS:O	1:D:210:GLN:HB2	2.20	0.41
1:A:204:LEU:O	1:A:207:LYS:CB	2.62	0.41
1:A:480:HIS:O	1:A:533:HIS:HD2	2.02	0.41
1:B:202:LYS:O	1:B:205:PHE:N	2.53	0.41
1:C:283:THR:HA	1:C:429:CYS:HB2	2.02	0.41
1:D:209:VAL:HG13	1:D:216:LEU:HD12	2.02	0.41
1:D:221:ARG:HA	1:D:221:ARG:HD3	1.84	0.41
1:A:440:ALA:HB2	1:A:496:VAL:HG13	2.01	0.41
1:A:485:ALA:HB2	1:A:495:LEU:HD12	2.02	0.41
1:B:284:LYS:HZ2	1:B:430:GLU:CD	2.24	0.41
1:D:359:LYS:HB3	1:D:418:PHE:CZ	2.55	0.41
1:B:483:LEU:HD21	1:B:532:PHE:O	2.20	0.41
1:C:173:LEU:HD12	1:C:173:LEU:HA	1.75	0.41
1:D:314:VAL:HG22	1:D:315:GLY:N	2.36	0.41
1:B:233:THR:HB	1:B:278:HIS:CG	2.55	0.41
1:B:279:SER:HB3	1:B:283:THR:OG1	2.20	0.41
1:B:527:VAL:HG13	1:B:533:HIS:HB2	2.03	0.41
1:C:507:SER:HA	1:C:508:PRO:HD3	1.94	0.41
1:D:364:MET:HE2	1:D:425:ILE:HG12	2.02	0.41
1:A:184:MET:O	1:A:188:ARG:HG3	2.20	0.41
1:B:295:PRO:CD	1:B:486:LYS:HG2	2.50	0.41
1:D:160:PRO:HG3	1:D:199:MET:HE2	2.01	0.41
1:D:294:LYS:N	1:D:295:PRO:HD2	2.36	0.41
1:D:190:THR:HG21	1:D:204:LEU:HD21	2.03	0.41
1:D:298:TYR:CZ	1:D:302:VAL:HG21	2.56	0.41
1:A:513:MET:HB2	1:A:515:ASN:ND2	2.35	0.41
1:B:149:PHE:CD1	1:B:159:ILE:CD1	3.04	0.41
1:C:254:TYR:C	1:C:255:ILE:CG2	2.90	0.41
1:C:265:LEU:HD13	1:C:506:TRP:HH2	1.86	0.41
1:D:294:LYS:HA	1:D:297:LYS:HE2	2.03	0.41
1:B:408:GLU:O	1:B:408:GLU:HG2	2.21	0.41
1:C:221:ARG:HD3	1:C:221:ARG:HA	1.88	0.41
1:C:367:LEU:HD23	1:C:370:MET:CE	2.51	0.41
1:D:151:THR:O	1:D:151:THR:CG2	2.68	0.41
1:A:315:GLY:O	1:A:336:ASN:HA	2.21	0.40
1:A:462:LEU:HB3	1:C:535:TYR:CD1	2.56	0.40
1:A:491:GLY:HA3	1:A:507:SER:O	2.21	0.40
1:A:533:HIS:HB3	1:A:536:ASP:OD2	2.20	0.40
1:C:254:TYR:C	1:C:255:ILE:HG23	2.41	0.40
1:D:205:PHE:C	1:D:207:LYS:N	2.70	0.40
1:B:234:SER:O	1:B:238:GLU:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:371:ALA:O	1:D:374:GLU:HG3	2.21	0.40
1:A:462:LEU:HD23	1:A:462:LEU:HA	1.88	0.40
1:C:159:ILE:O	1:C:159:ILE:CG2	2.67	0.40
1:C:351:LYS:HD3	1:C:351:LYS:HA	1.61	0.40
1:D:204:LEU:HD12	1:D:204:LEU:HA	1.82	0.40
1:D:470:MET:HG3	1:D:477:PHE:CG	2.55	0.40
1:A:150:TYR:C	1:A:152:ILE:N	2.74	0.40
1:A:511:ASP:HB2	1:A:512:LYS:CD	2.46	0.40
1:B:337:PRO:HG3	1:B:464:LEU:HD13	2.03	0.40
1:C:163:LYS:O	1:C:163:LYS:HG3	2.22	0.40
1:C:250:LYS:HG3	1:C:251:VAL:O	2.21	0.40
1:C:252:ALA:CB	1:C:489:VAL:HG22	2.52	0.40
1:C:396:ILE:O	1:C:400:LEU:HG	2.21	0.40
1:B:179:ARG:HG3	1:B:447:ILE:O	2.21	0.40

There are no symmetry-related clashes.

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	382/479 (80%)	366 (96%)	16 (4%)	0	100	100
1	B	378/479 (79%)	366 (97%)	10 (3%)	2 (0%)	29	57
1	C	386/479 (81%)	378 (98%)	6 (2%)	2 (0%)	29	57
1	D	377/479 (79%)	362 (96%)	13 (3%)	2 (0%)	29	57
All	All	1523/1916 (80%)	1472 (97%)	45 (3%)	6 (0%)	34	62

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	202	LYS

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Mol	Chain	Res	Type
1	C	202	LYS
1	D	205	PHE
1	D	206	LYS
1	B	211	SER
1	C	199	MET

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	339/415 (82%)	314 (93%)	25 (7%)	13	35
1	B	337/415 (81%)	308 (91%)	29 (9%)	10	27
1	C	343/415 (83%)	316 (92%)	27 (8%)	12	31
1	D	337/415 (81%)	309 (92%)	28 (8%)	11	29
All	All	1356/1660 (82%)	1247 (92%)	109 (8%)	12	31

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	GLU
1	A	146	ASP
1	A	158	LYS
1	A	165	ILE
1	A	173	LEU
1	A	176	SER
1	A	189	LEU
1	A	198	VAL
1	A	201	ASP
1	A	211	SER
1	A	223	LYS
1	A	230	MET
1	A	283	THR
1	A	317	GLU
1	A	330	GLU
1	A	366	PHE

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Mol	Chain	Res	Type
1	A	392	ARG
1	A	402	GLU
1	A	417	ASP
1	A	486	LYS
1	A	512	LYS
1	A	530	CYS
1	A	534	ASN
1	A	543	LYS
1	A	548	ARG
1	B	146	ASP
1	B	147	LEU
1	B	158	LYS
1	B	161	VAL
1	B	165	ILE
1	B	173	LEU
1	B	176	SER
1	B	189	LEU
1	B	203	ASP
1	B	211	SER
1	B	212	ASN
1	B	218	GLN
1	B	225	VAL
1	B	230	MET
1	B	254	TYR
1	B	317	GLU
1	B	319	SER
1	B	355	ASN
1	B	366	PHE
1	B	387	ARG
1	B	392	ARG
1	B	404	LYS
1	B	412	MET
1	B	417	ASP
1	B	422	LEU
1	B	512	LYS
1	B	534	ASN
1	B	541	PHE
1	B	548	ARG
1	C	144	LEU
1	C	146	ASP
1	C	165	ILE
1	C	166	THR

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Mol	Chain	Res	Type
1	C	173	LEU
1	C	199	MET
1	C	203	ASP
1	C	211	SER
1	C	218	GLN
1	C	225	VAL
1	C	230	MET
1	C	260	LYS
1	C	293	VAL
1	C	308	GLU
1	C	317	GLU
1	C	327	PHE
1	C	351	LYS
1	C	366	PHE
1	C	387	ARG
1	C	402	GLU
1	C	412	MET
1	C	417	ASP
1	C	422	LEU
1	C	512	LYS
1	C	541	PHE
1	C	543	LYS
1	C	545	LEU
1	D	146	ASP
1	D	173	LEU
1	D	176	SER
1	D	183	CYS
1	D	191	LEU
1	D	199	MET
1	D	201	ASP
1	D	202	LYS
1	D	221	ARG
1	D	222	ARG
1	D	230	MET
1	D	234	SER
1	D	250	LYS
1	D	253	ASP
1	D	261	PHE
1	D	282	ASP
1	D	283	THR
1	D	319	SER
1	D	327	PHE

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Mol	Chain	Res	Type
1	D	332	ASP
1	D	366	PHE
1	D	402	GLU
1	D	404	LYS
1	D	412	MET
1	D	512	LYS
1	D	534	ASN
1	D	541	PHE
1	D	545	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	335	HIS
1	B	156	GLN
1	C	540	HIS

5.3.3 RNA [i](#)

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](#)

4 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	PO4	A	1	-	4,4,4	0.87	0	6,6,6	0.48	0
2	PO4	D	4	-	4,4,4	0.85	0	6,6,6	0.47	0
2	PO4	C	3	-	4,4,4	0.87	0	6,6,6	0.38	0
2	PO4	B	2	-	4,4,4	0.88	0	6,6,6	0.40	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95th 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	390/479 (81%)	0.01	18 (4%) 32 27	26, 40, 75, 88	4 (1%)
1	B	388/479 (81%)	0.01	15 (3%) 39 34	26, 40, 78, 94	4 (1%)
1	C	394/479 (82%)	0.05	15 (3%) 40 35	24, 43, 82, 105	4 (1%)
1	D	387/479 (80%)	0.02	6 (1%) 72 70	24, 41, 77, 95	4 (1%)
All	All	1559/1916 (81%)	0.02	54 (3%) 44 38	24, 41, 78, 105	16 (1%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	150	TYR	6.8
1	A	150	TYR	5.9
1	C	149	PHE	5.7
1	A	200	LEU	4.7
1	A	257	GLN	4.6
1	D	150	TYR	4.6
1	C	200	LEU	4.1
1	A	148	LEU	3.9
1	B	262	SER	3.6
1	A	147	LEU	3.5
1	C	254	TYR	3.3
1	A	159	ILE	3.1
1	C	256	PRO	3.1
1	A	255	ILE	3.1
1	A	542	ALA	3.1
1	A	408	GLU	3.0
1	A	260	LYS	3.0
1	D	144	LEU	2.9
1	B	259	ALA	2.9
1	B	353	GLY	2.8
1	C	205	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	147	LEU	2.8
1	C	162	HIS	2.8
1	B	218	GLN	2.8
1	C	156	GLN	2.8
1	A	254	TYR	2.7
1	A	330	GLU	2.7
1	C	330	GLU	2.7
1	A	198	VAL	2.6
1	C	150	TYR	2.6
1	A	162	HIS	2.5
1	B	158	LYS	2.5
1	C	144	LEU	2.5
1	C	163	LYS	2.4
1	B	151	THR	2.4
1	D	221	ARG	2.4
1	A	144	LEU	2.4
1	B	191	LEU	2.3
1	A	256	PRO	2.3
1	B	260	LYS	2.3
1	B	254	TYR	2.3
1	A	152	ILE	2.2
1	B	152	ILE	2.2
1	D	164	PHE	2.2
1	C	332	ASP	2.2
1	C	255	ILE	2.2
1	B	214	VAL	2.2
1	C	259	ALA	2.1
1	D	332	ASP	2.1
1	C	159	ILE	2.1
1	A	149	PHE	2.1
1	B	217	THR	2.1
1	D	162	HIS	2.0
1	B	144	LEU	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, 95th 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	PO4	D	4	5/5	0.94	0.12	43,52,68,84	0
2	PO4	A	1	5/5	0.96	0.13	40,49,56,71	0
2	PO4	C	3	5/5	0.97	0.11	45,49,58,74	0
2	PO4	B	2	5/5	0.98	0.08	49,50,67,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.