Full wwPDB X-ray Structure Validation Report (i)

May 14, 2020 – 02:32 pm BST

PDB ID	:	1P1F
Title	:	Crystal structure of apo 1L-myo-inositol 1-phosphate synthase
Authors	:	Jin, X.; Geiger, J.H.
Deposited on	:	2003-04-12
Resolution	:	2.60 Å(reported)

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

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 2.60 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.
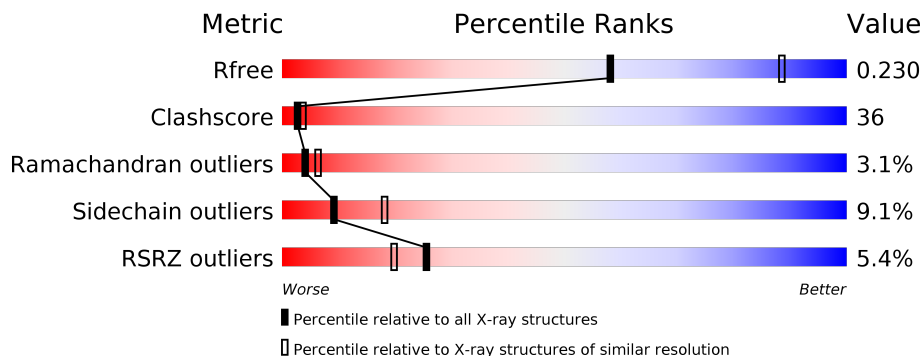
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 on 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	533	5% 43% / 44% / 7% · 6%
1	B	533	6% 40% / 45% / 8% / 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8005 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 Inositol-3-phosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total 3953	C 2519	N 661	O 757	S 16	0	0	0
1	B	496	Total 3919	C 2500	N 655	O 748	S 16	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	SEE REMARK 999	UNP P11986
A	14	VAL	LEU	SEE REMARK 999	UNP P11986
A	?	-	PHE	SEE REMARK 999	UNP P11986
A	60	LEU	GLU	SEE REMARK 999	UNP P11986
A	?	-	ALA	SEE REMARK 999	UNP P11986
A	98	GLU	LYS	SEE REMARK 999	UNP P11986
A	140	ASN	LYS	SEE REMARK 999	UNP P11986
A	141	ASP	HIS	SEE REMARK 999	UNP P11986
A	201	ASN	GLN	SEE REMARK 999	UNP P11986
A	444	PRO	ALA	SEE REMARK 999	UNP P11986
B	?	-	ARG	SEE REMARK 999	UNP P11986
B	14	VAL	LEU	SEE REMARK 999	UNP P11986
B	?	-	PHE	SEE REMARK 999	UNP P11986
B	60	LEU	GLU	SEE REMARK 999	UNP P11986
B	?	-	ALA	SEE REMARK 999	UNP P11986
B	98	GLU	LYS	SEE REMARK 999	UNP P11986
B	140	ASN	LYS	SEE REMARK 999	UNP P11986
B	141	ASP	HIS	SEE REMARK 999	UNP P11986
B	201	ASN	GLN	SEE REMARK 999	UNP P11986
B	444	PRO	ALA	SEE REMARK 999	UNP P11986

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	80	Total 80	O 80	0	0
2	B	53	Total 53	O 53	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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: Inositol-3-phosphate synthase
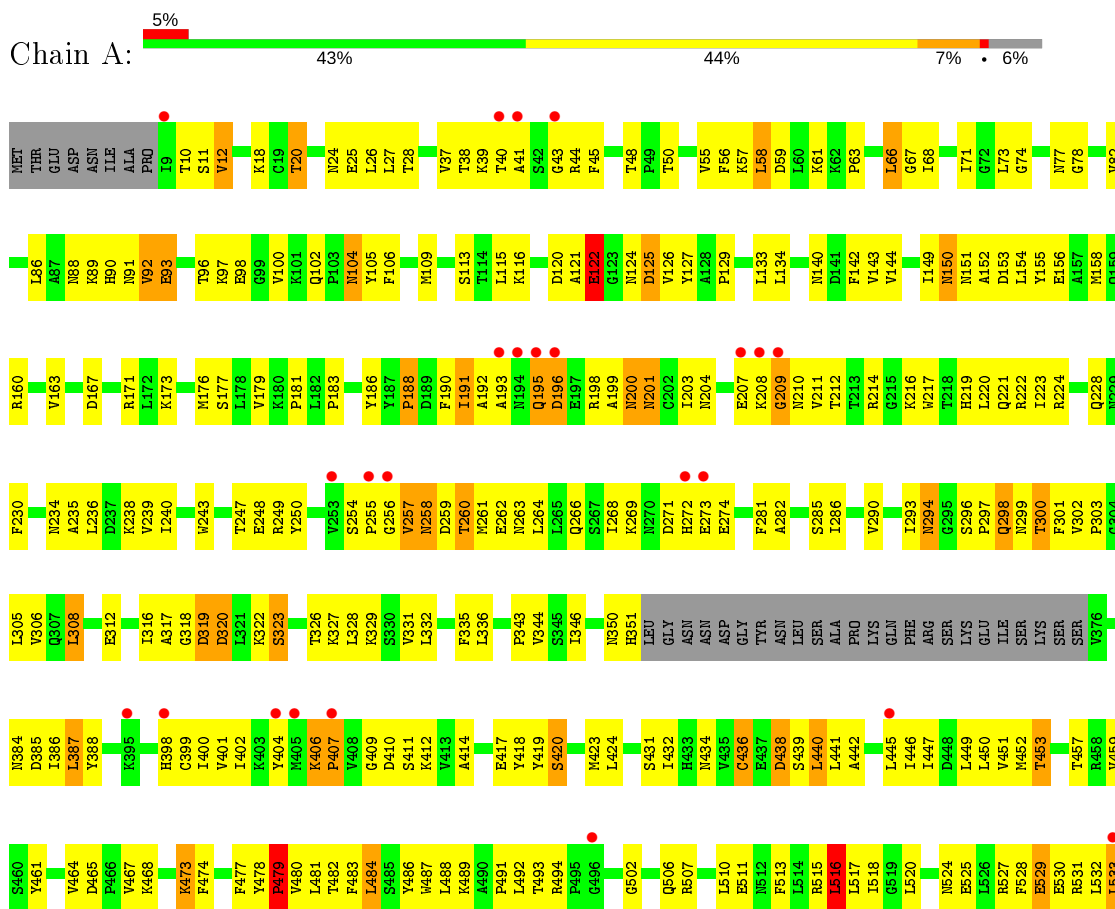
- Molecule 1: Inositol-3-phosphate synthase
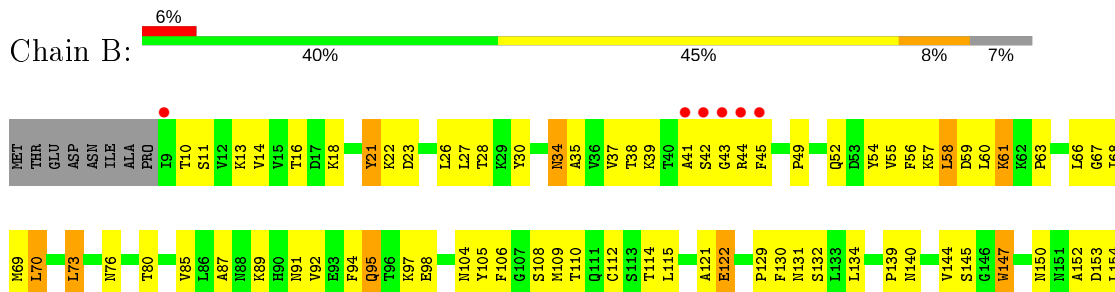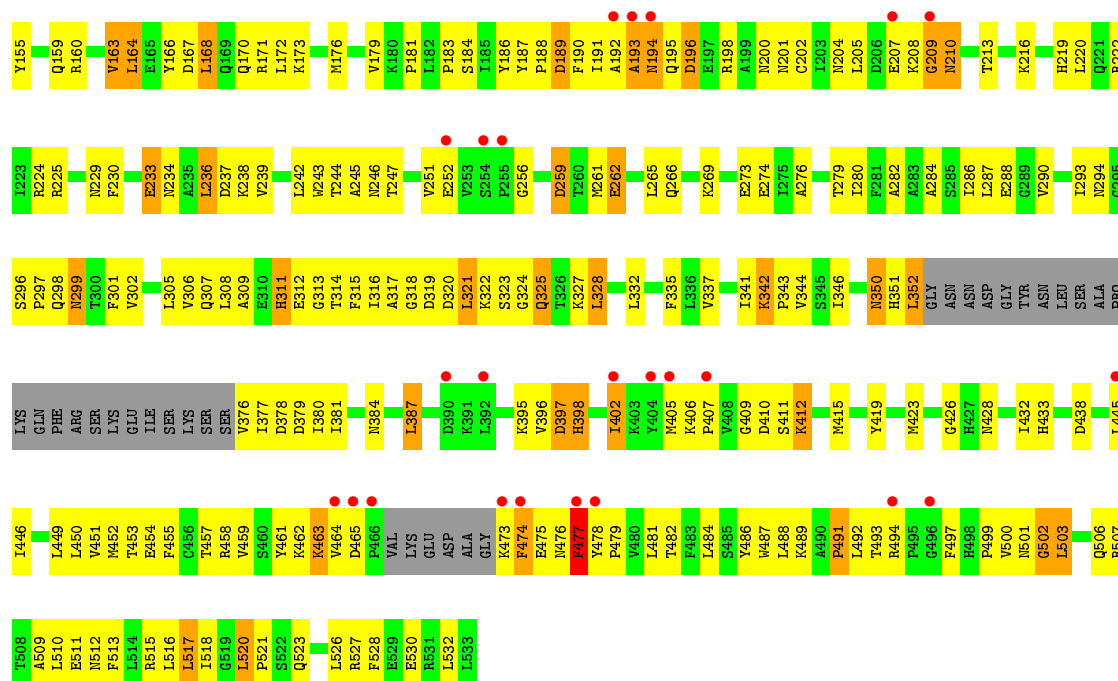
4   Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	153.54Å 97.06Å 122.06Å 90.00° 125.72° 90.00°	Depositor
Resolution (Å)	10.00 – 2.60 38.29 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.60) 91.0 (38.29-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.190 , 0.278 0.227 , 0.230	Depositor DCC
R_{free} test set	2231 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	38.3	Xtriage
Anisotropy	0.558	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 62.6	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	8005	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5 Model quality (i)

5.1 Standard geometry (i)

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	0.38	0/4030	0.65	2/5465 (0.0%)
1	B	0.50	1/3995 (0.0%)	0.70	3/5417 (0.1%)
All	All	0.45	1/8025 (0.0%)	0.68	5/10882 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	463	LYS	C-N	20.08	1.80	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	463	LYS	C-N-CA	-11.40	93.20	121.70
1	B	463	LYS	O-C-N	8.52	136.34	122.70
1	B	463	LYS	CA-C-N	-6.60	102.67	117.20
1	A	516	LEU	CA-CB-CG	6.24	129.65	115.30
1	A	319	ASP	N-CA-C	5.38	125.53	111.00

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	3953	0	3964	282	0
1	B	3919	0	3933	308	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	80	0	0	8	0
2	B	53	0	0	7	0
All	All	8005	0	7897	565	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 36.

All (565) 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:B:55:VAL:HG23	1:B:464:VAL:CG2	1.28	1.61
1:B:55:VAL:CG2	1:B:464:VAL:CG2	1.96	1.42
1:B:55:VAL:CG2	1:B:464:VAL:HG21	1.54	1.36
1:B:463:LYS:C	1:B:464:VAL:N	1.80	1.34
1:B:293:ILE:HA	1:B:317:ALA:HB2	1.33	1.10
1:A:68:ILE:HD13	1:A:450:LEU:HD13	1.41	1.01
1:A:150:ASN:HD22	1:A:151:ASN:N	1.59	1.01
1:B:115:LEU:HD22	1:B:511:GLU:HG3	1.40	1.00
1:A:12:VAL:HG11	1:A:133:LEU:HA	1.45	0.99
1:B:352:LEU:HB3	1:B:412:LYS:HG2	1.46	0.96
1:B:55:VAL:HG23	1:B:464:VAL:HG21	1.21	0.96
1:B:55:VAL:HG23	1:B:464:VAL:HG23	0.96	0.93
1:B:109:MET:HE2	1:B:507:ARG:HH11	1.29	0.93
1:B:55:VAL:HG21	1:B:464:VAL:CG2	1.95	0.93
1:B:55:VAL:HG21	1:B:464:VAL:HG21	1.51	0.93
1:A:150:ASN:ND2	1:A:152:ALA:H	1.68	0.92
1:B:463:LYS:C	1:B:464:VAL:CA	2.38	0.92
1:A:449:LEU:O	1:A:453:THR:HG23	1.71	0.89
1:A:153:ASP:OD2	1:A:177:SER:HA	1.76	0.86
1:B:160:ARG:HD3	1:B:198:ARG:NH2	1.91	0.86
1:A:293:ILE:HD11	1:A:453:THR:HG21	1.59	0.84
1:B:501:ASN:O	1:B:503:LEU:N	2.09	0.84
1:B:294:ASN:H	1:B:317:ALA:CB	1.90	0.84
1:B:87:ALA:HA	1:B:92:VAL:HG12	1.58	0.84
1:B:160:ARG:HD2	2:B:585:HOH:O	1.76	0.84
1:A:527:ARG:NH2	1:B:500:VAL:HG21	1.92	0.83
1:B:222:ARG:HD2	1:B:222:ARG:O	1.79	0.83
1:A:109:MET:O	1:A:113:SER:HB3	1.80	0.82
1:A:115:LEU:HD22	1:A:511:GLU:HG3	1.62	0.80
1:A:200:ASN:H	1:A:200:ASN:HD22	1.26	0.79
1:B:247:THR:HG23	1:B:297:PRO:HG2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:LEU:HD13	1:B:60:LEU:HD23	1.63	0.79
1:B:68:ILE:HD12	1:B:450:LEU:HD13	1.65	0.79
1:A:104:ASN:ND2	1:A:106:PHE:H	1.81	0.78
1:A:350:ASN:OD1	1:A:402:ILE:HG12	1.84	0.78
1:A:104:ASN:HD22	1:A:106:PHE:H	1.31	0.77
1:A:417:GLU:OE2	1:A:431:SER:HB3	1.85	0.77
1:B:486:TYR:HA	1:B:506:GLN:NE2	2.00	0.77
1:A:67:GLY:HA3	1:A:236:LEU:HD13	1.66	0.77
1:B:55:VAL:CG2	1:B:464:VAL:HG23	1.85	0.76
1:B:261:MET:H	1:B:307:GLN:NE2	1.84	0.75
1:B:342:LYS:HB2	1:B:387:LEU:HG	1.67	0.75
1:B:89:LYS:CA	1:B:140:ASN:HD22	1.99	0.74
1:B:76:ASN:O	1:B:80:THR:HG23	1.85	0.74
1:A:150:ASN:HD22	1:A:150:ASN:C	1.86	0.74
1:A:533:LEU:OXT	1:A:533:LEU:HD22	1.88	0.74
1:A:183:PRO:HB2	1:A:203:ILE:HG23	1.69	0.74
1:B:168:LEU:HD22	1:B:168:LEU:O	1.88	0.73
1:A:447:ILE:O	1:A:451:VAL:HG23	1.87	0.73
1:B:186:TYR:HE1	1:B:191:ILE:HD11	1.54	0.73
1:A:318:GLY:O	1:A:488:LEU:HD22	1.88	0.73
1:A:193:ALA:O	1:A:196:ASP:HB3	1.88	0.72
1:A:298:GLN:HE21	1:A:298:GLN:H	1.34	0.72
1:A:224:ARG:O	1:A:228:GLN:HG3	1.89	0.72
1:B:352:LEU:HD23	1:B:352:LEU:H	1.52	0.72
1:A:533:LEU:H	1:A:533:LEU:HD13	1.55	0.72
1:B:160:ARG:HD3	1:B:198:ARG:HH22	1.54	0.71
1:A:453:THR:O	1:A:457:THR:HG23	1.89	0.71
1:A:150:ASN:HA	1:A:200:ASN:ND2	2.06	0.71
1:A:328:LEU:HD11	1:B:332:LEU:HD21	1.72	0.71
1:B:377:ILE:O	1:B:381:ILE:HG12	1.90	0.71
1:A:323:SER:H	1:A:489:LYS:NZ	1.89	0.71
1:A:158:MET:HE1	1:A:176:MET:HG3	1.72	0.70
1:B:220:LEU:HD12	1:B:284:ALA:HB2	1.72	0.70
1:B:412:LYS:HB2	1:B:438:ASP:HB2	1.75	0.69
1:A:293:ILE:HG23	1:A:317:ALA:HB3	1.74	0.69
1:B:261:MET:O	1:B:265:LEU:HD23	1.92	0.69
1:A:39:LYS:HG3	1:A:40:THR:H	1.55	0.69
1:B:44:ARG:HB3	1:B:44:ARG:HH11	1.58	0.69
1:A:258:ASN:H	1:A:258:ASN:HD22	1.40	0.69
1:A:12:VAL:O	1:A:12:VAL:HG13	1.92	0.68
1:A:531:ARG:HD3	1:B:482:THR:HB	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:THR:HG23	1:A:27:LEU:HB2	1.76	0.68
1:A:154:LEU:HD22	1:A:179:VAL:HG11	1.74	0.68
1:B:230:PHE:HA	1:B:233:GLU:OE2	1.94	0.68
1:A:154:LEU:HD22	1:A:179:VAL:CG1	2.23	0.68
1:B:293:ILE:CA	1:B:317:ALA:HB2	2.19	0.67
1:B:478:TYR:OH	1:B:494:ARG:HB3	1.95	0.67
1:A:258:ASN:H	1:A:258:ASN:ND2	1.92	0.67
1:A:322:LYS:HA	1:A:489:LYS:HG3	1.76	0.67
1:B:152:ALA:HB3	1:B:160:ARG:HH22	1.59	0.67
1:A:55:VAL:HG23	1:A:464:VAL:HG21	1.77	0.67
1:B:282:ALA:CB	1:B:305:LEU:HD21	2.24	0.67
1:A:343:PRO:HA	1:A:420:SER:HA	1.75	0.66
1:B:89:LYS:HA	1:B:140:ASN:HD22	1.59	0.66
1:B:134:LEU:HD11	1:B:518:ILE:HG23	1.76	0.66
1:B:299:ASN:HD22	1:B:299:ASN:N	1.94	0.66
1:B:282:ALA:HB3	1:B:305:LEU:HD21	1.77	0.66
1:A:58:LEU:HD12	1:A:134:LEU:HD13	1.78	0.66
1:A:25:GLU:OE2	1:A:57:LYS:HD2	1.97	0.65
1:B:134:LEU:HD22	1:B:517:LEU:HD23	1.77	0.65
1:B:484:LEU:O	1:B:488:LEU:HD23	1.97	0.65
1:A:150:ASN:HA	1:A:200:ASN:HD21	1.61	0.65
1:A:183:PRO:HB2	1:A:203:ILE:CG2	2.27	0.65
1:A:533:LEU:CD1	1:A:533:LEU:H	2.09	0.65
1:A:478:TYR:CE1	1:A:494:ARG:HB3	2.32	0.65
1:A:12:VAL:CG1	1:A:133:LEU:HA	2.25	0.65
1:B:328:LEU:HD22	1:B:332:LEU:HD12	1.79	0.65
1:B:463:LYS:CA	1:B:464:VAL:N	2.60	0.64
1:A:207:GLU:H	1:A:207:GLU:CD	2.01	0.64
1:B:207:GLU:CD	1:B:207:GLU:H	2.00	0.64
1:B:352:LEU:HD23	1:B:352:LEU:N	2.12	0.64
1:A:259:ASP:OD2	1:A:260:THR:HG22	1.97	0.64
1:A:332:LEU:O	1:A:336:LEU:HD13	1.98	0.63
1:B:477:PHE:HZ	1:B:513:PHE:CZ	2.16	0.63
1:A:50:THR:HG22	2:A:604:HOH:O	1.98	0.63
1:B:350:ASN:O	1:B:402:ILE:HA	1.97	0.63
1:B:376:VAL:HG13	1:B:377:ILE:HD12	1.79	0.63
1:B:299:ASN:HD22	1:B:299:ASN:H	1.45	0.63
1:A:41:ALA:N	2:A:581:HOH:O	2.32	0.63
1:A:328:LEU:HD13	1:B:335:PHE:CE1	2.34	0.63
1:A:480:VAL:HG11	1:A:492:LEU:O	1.98	0.62
1:A:92:VAL:O	1:A:92:VAL:CG2	2.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ASN:ND2	1:B:114:THR:HG23	2.14	0.62
1:A:109:MET:HE3	1:A:486:TYR:CE1	2.34	0.62
1:B:92:VAL:HG11	1:B:172:LEU:HD21	1.80	0.62
1:A:150:ASN:ND2	1:A:150:ASN:C	2.53	0.62
1:A:82:VAL:HG22	1:A:144:VAL:HG11	1.81	0.62
1:B:321:LEU:HD11	1:B:446:ILE:HG12	1.82	0.62
1:B:87:ALA:HA	1:B:92:VAL:CG1	2.29	0.61
1:B:213:THR:HG22	2:B:580:HOH:O	1.99	0.61
1:A:346:ILE:O	1:A:398:HIS:HA	2.00	0.61
1:A:511:GLU:O	1:A:515:ARG:HG3	1.99	0.61
1:A:115:LEU:HD22	1:A:511:GLU:CG	2.30	0.61
1:A:77:ASN:HD21	1:A:439:SER:HA	1.66	0.61
1:B:70:LEU:HD12	1:B:242:LEU:HB3	1.82	0.61
1:A:502:GLY:O	1:A:506:GLN:HG3	2.01	0.61
1:A:533:LEU:HB3	1:B:494:ARG:NH2	2.16	0.61
1:A:323:SER:H	1:A:489:LYS:HZ1	1.48	0.60
1:B:238:LYS:HZ3	1:B:457:THR:HG21	1.66	0.60
1:A:39:LYS:HE2	1:A:43:GLY:HA2	1.83	0.60
1:A:96:THR:HG22	1:A:98:GLU:H	1.64	0.60
1:A:453:THR:HG22	1:A:484:LEU:HD21	1.83	0.60
1:B:97:LYS:HB2	1:B:97:LYS:NZ	2.16	0.60
1:A:301:PHE:CE2	1:A:316:ILE:HB	2.37	0.60
1:A:92:VAL:O	1:A:92:VAL:HG23	2.00	0.60
1:A:104:ASN:HD21	1:B:423:MET:HA	1.67	0.60
1:A:254:SER:H	1:A:258:ASN:HD21	1.48	0.60
1:B:294:ASN:H	1:B:317:ALA:HB2	1.63	0.60
1:B:34:ASN:ND2	1:B:35:ALA:H	1.98	0.60
1:A:332:LEU:CD2	1:B:328:LEU:HD21	2.32	0.60
1:B:186:TYR:CZ	1:B:188:PRO:HB3	2.37	0.60
1:B:301:PHE:CE2	1:B:316:ILE:HB	2.36	0.60
1:A:191:ILE:HG22	1:A:247:THR:O	2.03	0.59
1:A:300:THR:O	1:A:305:LEU:HD23	2.02	0.59
1:A:478:TYR:HE1	1:A:494:ARG:HB3	1.68	0.59
1:B:89:LYS:N	1:B:140:ASN:HD22	1.99	0.59
1:A:467:VAL:HG23	1:A:468:LYS:N	2.18	0.59
1:A:478:TYR:CD2	1:A:479:PRO:HD2	2.38	0.59
1:B:154:LEU:HD22	1:B:179:VAL:HG11	1.85	0.59
1:B:109:MET:HE2	1:B:507:ARG:HD2	1.84	0.59
1:B:115:LEU:CD2	1:B:511:GLU:HG3	2.25	0.59
1:A:318:GLY:HA2	1:A:492:LEU:HB2	1.84	0.59
1:B:131:ASN:HA	2:B:577:HOH:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ILE:O	1:A:199:ALA:HA	2.03	0.59
1:A:282:ALA:HB3	1:A:305:LEU:HD21	1.84	0.59
1:A:286:ILE:HG21	1:A:308:LEU:HD22	1.85	0.58
1:A:104:ASN:HD22	1:A:105:TYR:N	2.02	0.58
1:A:328:LEU:HD11	1:B:332:LEU:CD2	2.32	0.58
1:B:44:ARG:HB3	1:B:44:ARG:NH1	2.18	0.58
1:A:318:GLY:HA2	1:A:492:LEU:CB	2.34	0.58
1:B:224:ARG:HB3	1:B:288:GLU:OE1	2.03	0.58
1:A:77:ASN:ND2	1:A:439:SER:HA	2.17	0.58
1:A:88:ASN:HD21	1:A:104:ASN:CA	2.17	0.58
1:B:251:VAL:H	1:B:299:ASN:HD21	1.52	0.58
1:A:531:ARG:HD3	1:B:482:THR:CB	2.33	0.58
1:B:337:VAL:HG21	1:B:380:ILE:CG2	2.34	0.58
1:A:344:VAL:HG12	1:A:419:TYR:O	2.04	0.58
1:B:350:ASN:N	1:B:350:ASN:ND2	2.51	0.58
1:A:208:LYS:O	1:A:210:ASN:ND2	2.37	0.58
1:B:463:LYS:C	1:B:464:VAL:C	2.62	0.58
1:B:515:ARG:NH1	1:B:521:PRO:O	2.36	0.58
1:B:98:GLU:N	1:B:98:GLU:OE1	2.35	0.58
1:A:441:LEU:O	1:A:445:LEU:HD13	2.04	0.57
1:B:10:THR:HG22	1:B:132:SER:HB2	1.86	0.57
1:B:183:PRO:HA	1:B:201:ASN:ND2	2.18	0.57
1:B:238:LYS:NZ	1:B:457:THR:HG21	2.19	0.57
1:A:482:THR:HG21	1:A:493:THR:HG22	1.86	0.57
1:A:67:GLY:CA	1:A:236:LEU:HD13	2.35	0.57
1:A:190:PHE:O	1:A:248:GLU:HA	2.05	0.57
1:B:87:ALA:CA	1:B:92:VAL:HG12	2.31	0.57
1:A:465:ASP:OD1	1:A:467:VAL:HG22	2.05	0.56
1:B:322:LYS:HG2	1:B:327:LYS:HG3	1.85	0.56
1:A:489:LYS:O	1:A:491:PRO:HD3	2.04	0.56
1:B:449:LEU:HD21	1:B:487:TRP:HB2	1.87	0.56
1:A:163:VAL:HG22	1:A:410:ASP:OD1	2.05	0.56
1:B:376:VAL:O	1:B:376:VAL:HG22	2.05	0.56
1:B:402:ILE:HD13	1:B:402:ILE:C	2.26	0.56
1:B:406:LYS:HB3	1:B:407:PRO:HD3	1.88	0.56
1:B:473:LYS:HD3	1:B:475:GLU:HB3	1.87	0.56
1:B:22:LYS:HG2	1:B:23:ASP:H	1.71	0.56
1:A:10:THR:HG21	1:A:129:PRO:HD2	1.88	0.56
1:B:109:MET:CE	1:B:507:ARG:HD2	2.36	0.56
1:B:26:LEU:O	1:B:57:LYS:HA	2.04	0.56
1:A:191:ILE:HG13	1:A:192:ALA:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ASN:N	1:A:200:ASN:HD22	1.93	0.56
1:B:14:VAL:HG21	1:B:518:ILE:HD12	1.89	0.55
1:B:321:LEU:HD23	1:B:487:TRP:O	2.06	0.55
1:B:528:PHE:C	1:B:530:GLU:H	2.08	0.55
1:B:187:TYR:OH	1:B:216:LYS:HG2	2.06	0.55
1:A:351:HIS:O	1:A:412:LYS:HG2	2.06	0.55
1:B:14:VAL:O	1:B:16:THR:HG22	2.07	0.55
1:B:89:LYS:HA	1:B:140:ASN:ND2	2.22	0.55
1:A:150:ASN:ND2	1:A:152:ALA:N	2.49	0.55
1:B:216:LYS:HA	1:B:219:HIS:CD2	2.42	0.55
1:A:328:LEU:HD13	1:B:335:PHE:CD1	2.40	0.55
1:A:125:ASP:OD1	1:A:527:ARG:NH2	2.39	0.55
1:A:329:LYS:HG3	1:A:418:TYR:OH	2.06	0.55
1:B:57:LYS:HD3	1:B:474:PHE:CE1	2.42	0.54
1:A:515:ARG:HB3	1:A:520:LEU:HB2	1.89	0.54
1:B:402:ILE:O	1:B:402:ILE:HG23	2.08	0.54
1:B:92:VAL:HG13	1:B:92:VAL:O	2.07	0.54
1:B:152:ALA:HB3	1:B:160:ARG:NH2	2.22	0.54
1:B:30:TYR:CD2	1:B:516:LEU:HB2	2.42	0.54
1:B:473:LYS:HE2	1:B:475:GLU:HA	1.90	0.54
1:A:449:LEU:O	1:A:453:THR:CG2	2.50	0.54
1:A:158:MET:CE	1:A:176:MET:HG3	2.38	0.54
1:B:159:GLN:HG2	2:B:555:HOH:O	2.07	0.54
1:B:346:ILE:O	1:B:398:HIS:HA	2.07	0.54
1:A:258:ASN:HD22	1:A:258:ASN:N	2.00	0.53
1:A:183:PRO:HD2	2:A:595:HOH:O	2.07	0.53
1:A:25:GLU:HG2	1:A:59:ASP:HA	1.90	0.53
1:A:296:SER:HB3	1:A:298:GLN:HE22	1.72	0.53
1:A:113:SER:OG	1:A:507:ARG:NH1	2.42	0.53
1:A:58:LEU:CD1	1:A:134:LEU:HD13	2.38	0.53
1:A:55:VAL:CG2	1:A:464:VAL:HG21	2.39	0.53
1:B:332:LEU:HD13	1:B:432:ILE:HD12	1.90	0.53
1:A:527:ARG:CZ	1:B:500:VAL:HG21	2.38	0.53
1:B:155:TYR:CE2	1:B:173:LYS:HE3	2.44	0.53
1:B:462:LYS:HG2	1:B:474:PHE:CE2	2.43	0.53
1:B:67:GLY:HA3	1:B:239:VAL:HG22	1.91	0.53
1:A:203:ILE:HD12	1:A:222:ARG:HG2	1.91	0.53
1:A:196:ASP:C	1:A:196:ASP:OD2	2.48	0.52
1:A:73:LEU:HD23	1:A:181:PRO:HB3	1.91	0.52
1:B:243:TRP:CZ2	1:B:245:ALA:HB3	2.45	0.52
1:A:125:ASP:CG	1:A:527:ARG:HH22	2.13	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:LEU:CD1	1:A:221:GLN:HE21	2.22	0.52
1:B:192:ALA:O	1:B:193:ALA:O	2.26	0.52
1:A:105:TYR:OH	1:A:140:ASN:ND2	2.42	0.52
1:A:417:GLU:CD	1:A:431:SER:HB3	2.30	0.52
1:B:296:SER:HB3	1:B:297:PRO:HD2	1.90	0.52
1:A:88:ASN:HD21	1:A:104:ASN:HA	1.73	0.52
1:B:163:VAL:HB	1:B:410:ASP:OD1	2.08	0.52
1:A:387:LEU:HD12	1:B:106:PHE:CE1	2.44	0.52
1:A:525:GLU:O	1:B:509:ALA:HB2	2.09	0.52
1:A:96:THR:HG22	1:A:97:LYS:N	2.25	0.52
1:B:415:MET:HA	1:B:432:ILE:O	2.10	0.52
1:A:71:ILE:HG21	1:A:243:TRP:CE3	2.45	0.52
1:A:446:ILE:O	1:A:450:LEU:HG	2.09	0.52
1:B:301:PHE:CE1	1:B:317:ALA:HB3	2.44	0.52
1:A:272:HIS:HD2	1:A:273:GLU:N	2.08	0.52
1:B:324:GLY:HA2	1:B:327:LYS:HD3	1.92	0.52
1:A:200:ASN:H	1:A:200:ASN:ND2	2.02	0.52
1:B:129:PRO:HB2	1:B:132:SER:HB3	1.91	0.52
1:B:493:THR:HG21	1:B:499:PRO:HB3	1.92	0.52
1:A:24:ASN:HB3	1:A:61:LYS:HG3	1.92	0.51
1:B:153:ASP:OD2	1:B:155:TYR:HB3	2.10	0.51
1:B:276:ALA:O	1:B:279:THR:HB	2.10	0.51
1:B:52:GLN:HG3	1:B:54:TYR:CE1	2.45	0.51
1:B:28:THR:O	1:B:55:VAL:HA	2.10	0.51
1:A:223:ILE:HD12	1:A:281:PHE:CE2	2.45	0.51
1:A:96:THR:C	1:A:98:GLU:H	2.11	0.51
1:A:96:THR:C	1:A:98:GLU:N	2.64	0.51
1:A:320:ASP:HB3	1:A:489:LYS:HB2	1.92	0.51
1:A:438:ASP:O	1:A:441:LEU:N	2.41	0.51
1:A:120:ASP:OD1	1:A:124:ASN:N	2.42	0.51
1:A:286:ILE:CG2	1:A:308:LEU:HD22	2.41	0.51
1:A:186:TYR:O	1:A:204:ASN:ND2	2.41	0.51
1:A:247:THR:HG23	1:A:297:PRO:HG2	1.93	0.51
1:A:329:LYS:HB2	1:A:329:LYS:NZ	2.26	0.51
1:B:172:LEU:HB3	1:B:176:MET:HG2	1.91	0.51
1:A:299:ASN:O	1:A:299:ASN:CG	2.50	0.51
1:A:533:LEU:HD13	1:A:533:LEU:N	2.25	0.51
1:B:332:LEU:HD13	1:B:432:ILE:CD1	2.41	0.51
1:B:453:THR:HG23	1:B:481:LEU:CD1	2.41	0.51
1:A:18:LYS:O	1:A:28:THR:HA	2.11	0.51
1:B:195:GLN:HA	1:B:195:GLN:NE2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:LEU:HD13	1:B:308:LEU:O	2.10	0.51
1:B:39:LYS:HD3	1:B:45:PHE:CZ	2.46	0.51
1:A:515:ARG:O	1:A:518:ILE:HG12	2.11	0.50
1:B:516:LEU:HD12	1:B:517:LEU:N	2.26	0.50
1:A:262:GLU:CD	1:A:262:GLU:H	2.14	0.50
1:A:134:LEU:HD11	1:A:517:LEU:HB2	1.93	0.50
1:A:293:ILE:HG23	1:A:317:ALA:CB	2.41	0.50
1:A:93:GLU:HB3	1:A:102:GLN:NE2	2.26	0.50
1:B:168:LEU:O	1:B:172:LEU:HG	2.11	0.50
1:A:449:LEU:HD21	1:A:487:TRP:HB2	1.94	0.50
1:A:298:GLN:H	1:A:298:GLN:NE2	2.07	0.50
1:B:307:GLN:C	1:B:309:ALA:N	2.65	0.50
1:B:344:VAL:HG22	1:B:419:TYR:O	2.12	0.50
1:B:513:PHE:O	1:B:516:LEU:HG	2.12	0.50
1:A:93:GLU:HB3	1:A:102:GLN:HE22	1.75	0.49
1:B:27:LEU:HA	1:B:56:PHE:O	2.12	0.49
1:A:256:GLY:C	1:A:263:ASN:HD22	2.15	0.49
1:B:134:LEU:HD22	1:B:455:PHE:HZ	1.77	0.49
1:B:452:MET:HB3	1:B:484:LEU:HD22	1.93	0.49
1:B:59:ASP:O	1:B:458:ARG:HD2	2.11	0.49
1:A:153:ASP:OD1	1:A:156:GLU:HG3	2.12	0.49
1:A:256:GLY:HA2	1:A:263:ASN:HD22	1.78	0.49
1:A:480:VAL:CG1	1:A:492:LEU:O	2.60	0.49
1:B:491:PRO:O	1:B:493:THR:HG23	2.13	0.49
1:B:67:GLY:HA3	1:B:239:VAL:CG2	2.42	0.49
1:B:89:LYS:N	1:B:140:ASN:ND2	2.60	0.49
1:B:66:LEU:HD22	1:B:454:GLU:HG3	1.94	0.49
1:B:473:LYS:HE2	1:B:475:GLU:CA	2.43	0.49
1:B:464:VAL:HG12	1:B:465:ASP:N	2.27	0.49
1:B:73:LEU:HD13	1:B:181:PRO:HG3	1.95	0.49
1:B:311:HIS:O	1:B:313:GLY:N	2.46	0.49
1:B:321:LEU:HD11	1:B:446:ILE:CG1	2.42	0.49
1:B:69:MET:HA	1:B:145:SER:O	2.13	0.49
1:A:255:PRO:HA	1:A:259:ASP:OD1	2.13	0.48
1:A:473:LYS:C	1:A:473:LYS:HD2	2.34	0.48
1:A:68:ILE:HD12	1:A:142:PHE:CD1	2.48	0.48
1:B:239:VAL:HG12	1:B:290:VAL:HG11	1.95	0.48
1:B:350:ASN:N	1:B:350:ASN:HD22	2.09	0.48
1:A:120:ASP:HB3	1:A:126:VAL:CG2	2.43	0.48
1:A:116:LYS:HB2	1:A:127:TYR:CE2	2.48	0.48
1:A:257:VAL:HG11	1:A:274:GLU:OE2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:LYS:N	1:A:407:PRO:CD	2.76	0.48
1:B:14:VAL:HG11	1:B:520:LEU:HD13	1.95	0.48
1:A:440:LEU:HD23	1:B:426:GLY:HA3	1.95	0.48
1:A:120:ASP:C	1:A:122:GLU:H	2.16	0.48
1:B:287:LEU:HD21	1:B:308:LEU:HD21	1.96	0.48
1:B:337:VAL:HG21	1:B:380:ILE:HG23	1.95	0.48
1:B:58:LEU:HD23	1:B:459:VAL:HG22	1.95	0.48
1:B:109:MET:HE2	1:B:507:ARG:NH1	2.13	0.48
1:B:266:GLN:O	1:B:269:LYS:HB3	2.14	0.48
1:B:489:LYS:C	1:B:491:PRO:HD3	2.33	0.48
1:B:85:VAL:HG13	1:B:139:PRO:O	2.13	0.48
1:A:272:HIS:HD2	1:A:273:GLU:H	1.61	0.48
1:A:483:PHE:O	1:A:510:LEU:HD21	2.13	0.48
1:B:395:LYS:HD3	1:B:396:VAL:N	2.28	0.48
1:A:440:LEU:HA	1:A:440:LEU:HD12	1.74	0.48
1:B:22:LYS:CG	1:B:23:ASP:H	2.26	0.48
1:B:376:VAL:HG23	1:B:501:ASN:HB2	1.96	0.48
1:B:526:LEU:O	1:B:527:ARG:C	2.51	0.48
1:A:200:ASN:ND2	1:A:200:ASN:N	2.60	0.48
1:A:327:LYS:O	1:A:331:VAL:HG23	2.14	0.48
1:A:256:GLY:HA2	1:A:263:ASN:ND2	2.28	0.47
1:B:337:VAL:HG21	1:B:380:ILE:HG21	1.97	0.47
1:A:217:TRP:O	1:A:221:GLN:HG2	2.14	0.47
1:A:516:LEU:C	1:A:516:LEU:HD23	2.34	0.47
1:B:183:PRO:HG2	2:B:579:HOH:O	2.13	0.47
1:B:262:GLU:CD	1:B:262:GLU:H	2.16	0.47
1:B:322:LYS:NZ	1:B:506:GLN:HE22	2.13	0.47
1:A:191:ILE:HG13	1:A:192:ALA:N	2.29	0.47
1:A:220:LEU:HD13	1:A:221:GLN:HE21	1.79	0.47
1:A:11:SER:HA	2:A:535:HOH:O	2.13	0.47
1:B:35:ALA:CB	1:B:49:PRO:HA	2.45	0.47
1:A:442:ALA:O	1:A:446:ILE:HG13	2.15	0.47
1:A:318:GLY:O	1:A:488:LEU:HB3	2.14	0.47
1:B:166:TYR:O	1:B:170:GLN:HG2	2.13	0.47
1:A:409:GLY:C	1:A:411:SER:H	2.18	0.47
1:B:194:ASN:HA	1:B:196:ASP:OD1	2.15	0.47
1:B:247:THR:HG23	1:B:297:PRO:CG	2.42	0.47
1:B:225:ARG:HE	1:B:229:ASN:HB2	1.79	0.47
1:B:18:LYS:O	1:B:28:THR:HA	2.15	0.47
1:A:528:PHE:HZ	1:B:516:LEU:HD21	1.80	0.47
1:A:302:VAL:O	1:A:306:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:CYS:HB3	1:B:204:ASN:OD1	2.15	0.47
1:A:37:VAL:HG12	1:A:38:THR:N	2.29	0.46
1:B:242:LEU:HD23	1:B:244:THR:HB	1.97	0.46
1:B:464:VAL:CG1	1:B:465:ASP:N	2.78	0.46
1:B:501:ASN:O	1:B:502:GLY:C	2.52	0.46
1:A:266:GLN:HA	1:A:266:GLN:NE2	2.30	0.46
1:A:300:THR:HG21	2:A:561:HOH:O	2.13	0.46
1:B:167:ASP:O	1:B:171:ARG:HG3	2.16	0.46
1:B:59:ASP:HB3	1:B:458:ARG:HB3	1.96	0.46
1:A:104:ASN:HD22	1:A:106:PHE:N	2.08	0.46
1:B:318:GLY:HA2	1:B:492:LEU:HB3	1.98	0.46
1:A:183:PRO:HA	1:A:201:ASN:O	2.16	0.46
1:B:184:SER:O	1:B:202:CYS:HA	2.16	0.46
1:A:26:LEU:O	1:A:57:LYS:HA	2.15	0.46
1:B:242:LEU:CD2	1:B:244:THR:HB	2.46	0.46
1:B:97:LYS:CB	1:B:97:LYS:NZ	2.79	0.46
1:A:191:ILE:CG1	1:A:192:ALA:H	2.28	0.46
1:A:282:ALA:CB	1:A:305:LEU:HD21	2.45	0.46
1:B:454:GLU:O	1:B:457:THR:HB	2.16	0.46
1:A:120:ASP:O	1:A:122:GLU:N	2.49	0.46
1:A:216:LYS:HD2	1:A:271:ASP:HA	1.98	0.46
1:A:404:TYR:CD1	1:A:404:TYR:C	2.89	0.46
1:A:71:ILE:HG21	1:A:243:TRP:CZ3	2.50	0.46
1:B:273:GLU:HG3	1:B:274:GLU:N	2.32	0.45
1:B:94:PHE:CD2	1:B:168:LEU:HG	2.52	0.45
1:A:412:LYS:HE3	1:A:414:ALA:HB2	1.98	0.45
1:B:286:ILE:C	1:B:288:GLU:H	2.20	0.45
1:B:37:VAL:HG12	1:B:38:THR:N	2.31	0.45
1:B:487:TRP:HH2	1:B:510:LEU:HD21	1.81	0.45
1:A:320:ASP:OD2	1:A:489:LYS:HD2	2.17	0.45
1:B:207:GLU:C	1:B:208:LYS:HD2	2.36	0.45
1:B:307:GLN:C	1:B:309:ALA:H	2.20	0.45
1:B:238:LYS:HZ1	1:B:457:THR:HB	1.81	0.45
1:A:208:LYS:O	1:A:209:GLY:C	2.55	0.45
1:A:296:SER:HB3	1:A:297:PRO:HD2	1.99	0.45
1:B:451:VAL:HG12	1:B:452:MET:HE2	1.98	0.45
1:B:501:ASN:HA	1:B:506:GLN:OE1	2.17	0.45
1:A:67:GLY:O	1:A:239:VAL:HA	2.16	0.45
1:A:82:VAL:HG21	1:A:154:LEU:HD21	1.99	0.45
1:B:186:TYR:CE1	1:B:191:ILE:HD11	2.44	0.45
1:B:44:ARG:CB	1:B:44:ARG:HH11	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ILE:HD12	1:A:142:PHE:CG	2.52	0.45
1:B:150:ASN:HA	1:B:200:ASN:OD1	2.17	0.45
1:B:205:LEU:HB3	1:B:209:GLY:O	2.17	0.45
1:A:329:LYS:HE2	1:A:398:HIS:NE2	2.31	0.44
1:A:459:VAL:HG11	1:A:513:PHE:HZ	1.82	0.44
1:B:323:SER:HB2	1:B:325:GLN:HG2	1.98	0.44
1:B:58:LEU:CD1	1:B:60:LEU:HD23	2.42	0.44
1:A:90:HIS:O	1:A:91:ASN:C	2.56	0.44
1:A:190:PHE:O	1:A:191:ILE:HG23	2.17	0.44
1:A:266:GLN:C	1:A:268:ILE:N	2.70	0.44
1:B:273:GLU:HG3	1:B:274:GLU:HG3	2.00	0.44
1:A:220:LEU:O	1:A:224:ARG:HG3	2.18	0.44
1:A:258:ASN:N	1:A:258:ASN:ND2	2.57	0.44
1:B:55:VAL:CG2	1:B:464:VAL:HG22	2.27	0.44
1:A:527:ARG:HA	1:A:529:GLU:OE2	2.17	0.44
1:B:286:ILE:HG21	1:B:308:LEU:HD13	2.00	0.44
1:B:493:THR:CG2	1:B:499:PRO:HB3	2.46	0.44
1:B:294:ASN:N	1:B:317:ALA:HB2	2.30	0.44
1:B:528:PHE:CD2	1:B:532:LEU:HD13	2.53	0.44
1:A:20:THR:HG22	2:A:586:HOH:O	2.17	0.44
1:A:399:CYS:SG	1:A:399:CYS:O	2.76	0.44
1:B:415:MET:HG2	1:B:433:HIS:HD2	1.82	0.44
1:A:350:ASN:HB2	1:A:412:LYS:HD3	1.99	0.44
1:B:239:VAL:HG12	1:B:290:VAL:CG1	2.48	0.44
1:A:143:VAL:O	1:A:230:PHE:HZ	2.01	0.43
1:A:298:GLN:HE21	1:A:298:GLN:N	2.10	0.43
1:A:302:VAL:HB	1:A:303:PRO:HD2	2.01	0.43
1:A:335:PHE:CD2	1:A:336:LEU:HD12	2.53	0.43
1:B:220:LEU:HA	1:B:280:ILE:CG2	2.48	0.43
1:A:109:MET:HE3	1:A:486:TYR:CD1	2.53	0.43
1:A:477:PHE:HZ	1:A:513:PHE:CZ	2.37	0.43
1:B:477:PHE:HB3	1:B:478:TYR:H	1.57	0.43
1:A:74:GLY:HA3	2:A:550:HOH:O	2.18	0.43
1:B:121:ALA:HB3	1:B:122:GLU:OE2	2.18	0.43
1:B:194:ASN:HA	1:B:194:ASN:HD22	1.55	0.43
1:B:314:THR:HG22	1:B:315:PHE:H	1.82	0.43
1:B:352:LEU:CB	1:B:412:LYS:HG2	2.33	0.43
1:B:477:PHE:HZ	1:B:513:PHE:HZ	1.61	0.43
1:B:500:VAL:HG12	1:B:501:ASN:N	2.34	0.43
1:B:55:VAL:HG21	1:B:464:VAL:HG22	1.90	0.43
1:A:104:ASN:HD22	1:A:104:ASN:C	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:GLN:HB3	1:A:195:GLN:HE21	1.57	0.43
1:A:186:TYR:OH	1:A:196:ASP:HA	2.18	0.43
1:A:188:PRO:HD3	1:A:211:VAL:HG11	2.01	0.43
1:A:294:ASN:ND2	1:A:296:SER:H	2.16	0.43
1:A:322:LYS:NZ	1:A:506:GLN:OE1	2.48	0.43
1:B:163:VAL:HG22	1:B:164:LEU:HD13	2.01	0.43
1:B:252:GLU:HB3	1:B:274:GLU:OE2	2.18	0.43
1:A:257:VAL:HG13	1:A:272:HIS:ND1	2.34	0.43
1:A:467:VAL:HG23	1:A:468:LYS:H	1.83	0.43
1:A:143:VAL:HG21	1:A:236:LEU:HD21	2.01	0.43
1:A:208:LYS:O	1:A:210:ASN:N	2.52	0.43
1:B:234:ASN:CB	1:B:236:LEU:HD22	2.49	0.43
1:B:323:SER:C	1:B:325:GLN:H	2.22	0.43
1:B:352:LEU:N	1:B:352:LEU:CD2	2.80	0.43
1:B:376:VAL:O	1:B:379:ASP:OD2	2.37	0.43
1:B:144:VAL:HG12	1:B:145:SER:N	2.34	0.43
1:B:301:PHE:CZ	1:B:317:ALA:HB3	2.54	0.43
1:B:449:LEU:HD21	1:B:488:LEU:CD2	2.49	0.43
1:A:260:THR:HG23	1:A:263:ASN:CG	2.40	0.43
1:B:415:MET:HG2	1:B:433:HIS:CD2	2.53	0.43
1:A:385:ASP:HA	1:A:388:TYR:O	2.19	0.43
1:A:66:LEU:HD11	1:A:240:ILE:HD12	2.00	0.43
1:B:13:LYS:HA	1:B:13:LYS:HD2	1.80	0.43
1:A:423:MET:CE	1:A:424:LEU:HD12	2.48	0.42
1:B:105:TYR:O	1:B:108:SER:HB3	2.19	0.42
1:B:85:VAL:HA	1:B:105:TYR:OH	2.18	0.42
1:B:57:LYS:HB2	1:B:474:PHE:CZ	2.54	0.42
1:B:147:TRP:N	1:B:147:TRP:CE3	2.87	0.42
1:B:282:ALA:O	1:B:286:ILE:HG13	2.19	0.42
1:B:95:GLN:CA	1:B:95:GLN:HE21	2.32	0.42
1:A:272:HIS:CD2	1:A:273:GLU:N	2.86	0.42
1:A:527:ARG:HG2	1:A:527:ARG:NH1	2.34	0.42
1:A:533:LEU:HD12	1:B:478:TYR:CD1	2.55	0.42
1:A:63:PRO:HG3	1:A:238:LYS:HE2	2.00	0.42
1:B:104:ASN:OD1	1:B:106:PHE:CG	2.72	0.42
1:B:154:LEU:HB2	1:B:179:VAL:HB	2.01	0.42
1:B:34:ASN:ND2	1:B:35:ALA:N	2.66	0.42
1:B:351:HIS:ND1	1:B:405:MET:HG3	2.35	0.42
1:B:484:LEU:HA	1:B:487:TRP:CE3	2.54	0.42
1:A:266:GLN:NE2	1:A:269:LYS:HD2	2.35	0.42
1:A:528:PHE:O	1:A:532:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:LEU:HD22	1:B:511:GLU:CG	2.29	0.42
1:B:296:SER:HB3	1:B:298:GLN:OE1	2.20	0.42
1:B:311:HIS:C	1:B:313:GLY:H	2.23	0.42
1:A:212:THR:C	1:A:214:ARG:H	2.23	0.42
1:A:56:PHE:CE1	1:A:461:TYR:HB3	2.55	0.42
1:B:216:LYS:HA	1:B:219:HIS:HD2	1.84	0.42
1:B:220:LEU:CD1	1:B:284:ALA:HB2	2.46	0.42
1:B:487:TRP:C	1:B:488:LEU:HD22	2.39	0.42
1:A:68:ILE:CD1	1:A:450:LEU:HD13	2.30	0.42
1:A:532:LEU:HG	1:B:461:TYR:CE2	2.54	0.42
1:B:261:MET:O	1:B:265:LEU:CD2	2.64	0.42
1:B:247:THR:CG2	1:B:297:PRO:HG2	2.44	0.42
1:B:302:VAL:O	1:B:306:VAL:HG23	2.20	0.42
1:A:196:ASP:C	1:A:198:ARG:H	2.22	0.42
1:B:163:VAL:HG13	2:B:576:HOH:O	2.19	0.42
1:B:21:TYR:CD1	1:B:21:TYR:N	2.86	0.42
1:B:395:LYS:NZ	1:B:397:ASP:HA	2.35	0.42
1:B:188:PRO:C	1:B:190:PHE:H	2.23	0.42
1:B:299:ASN:ND2	1:B:299:ASN:H	2.13	0.42
1:B:61:LYS:HE3	1:B:61:LYS:HB3	1.96	0.42
1:A:134:LEU:HD11	1:A:517:LEU:CB	2.49	0.42
1:A:78:GLY:O	1:A:82:VAL:HG23	2.20	0.42
1:B:104:ASN:HB3	2:B:538:HOH:O	2.18	0.42
1:B:317:ALA:O	1:B:492:LEU:HD13	2.20	0.42
1:A:151:ASN:O	1:A:152:ALA:C	2.58	0.41
1:A:285:SER:OG	1:A:290:VAL:HG23	2.20	0.41
1:A:326:THR:OG1	1:A:489:LYS:HE3	2.20	0.41
1:A:452:MET:HG2	1:A:487:TRP:CH2	2.56	0.41
1:B:110:THR:HG22	1:B:130:PHE:CE2	2.55	0.41
1:A:247:THR:HG22	1:A:248:GLU:O	2.20	0.41
1:A:318:GLY:HA3	1:A:492:LEU:H	1.85	0.41
1:A:44:ARG:HG3	1:B:11:SER:OG	2.20	0.41
1:B:186:TYR:O	1:B:188:PRO:HD3	2.20	0.41
1:B:63:PRO:HG3	1:B:238:LYS:HD3	2.01	0.41
1:B:34:ASN:HD22	1:B:35:ALA:N	2.18	0.41
1:B:463:LYS:O	1:B:464:VAL:C	2.58	0.41
1:A:524:ASN:HA	1:B:512:ASN:ND2	2.36	0.41
1:A:152:ALA:HB3	1:A:160:ARG:NH2	2.35	0.41
1:A:318:GLY:HA2	1:A:492:LEU:HB3	2.02	0.41
1:A:473:LYS:HD2	1:A:474:PHE:O	2.20	0.41
1:B:243:TRP:CE2	1:B:245:ALA:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:ILE:O	1:B:343:PRO:CD	2.69	0.41
1:B:462:LYS:HG2	1:B:474:PHE:HE2	1.85	0.41
1:A:527:ARG:HH21	1:B:500:VAL:HG21	1.80	0.41
1:A:327:LYS:NZ	1:A:445:LEU:HD21	2.35	0.41
1:B:41:ALA:O	1:B:43:GLY:N	2.53	0.41
1:A:73:LEU:HG	1:A:154:LEU:HD11	2.03	0.41
1:A:234:ASN:O	1:A:235:ALA:HB3	2.21	0.41
1:A:250:TYR:HD1	1:A:299:ASN:OD1	2.02	0.41
1:B:318:GLY:HA2	1:B:492:LEU:CB	2.51	0.41
1:A:220:LEU:O	1:A:220:LEU:HD22	2.21	0.41
1:A:39:LYS:HE3	1:A:45:PHE:CE1	2.55	0.41
1:A:40:THR:HG23	1:A:44:ARG:O	2.21	0.41
1:A:436:CYS:HB3	1:B:428:ASN:ND2	2.36	0.41
1:B:445:LEU:HG	1:B:487:TRP:HD1	1.86	0.41
1:B:478:TYR:CD1	1:B:479:PRO:HD2	2.56	0.41
1:B:58:LEU:CD1	1:B:134:LEU:HD23	2.51	0.41
1:B:187:TYR:CE1	1:B:216:LYS:HE2	2.55	0.41
1:B:409:GLY:C	1:B:411:SER:H	2.24	0.41
1:A:104:ASN:C	1:A:104:ASN:ND2	2.74	0.41
1:A:167:ASP:O	1:A:171:ARG:HG3	2.21	0.41
1:A:219:HIS:O	1:A:223:ILE:HG12	2.20	0.41
1:A:256:GLY:CA	1:A:263:ASN:HD22	2.32	0.41
1:A:89:LYS:HD2	2:A:540:HOH:O	2.21	0.41
1:B:110:THR:HA	1:B:130:PHE:CD2	2.55	0.41
1:B:528:PHE:C	1:B:530:GLU:N	2.73	0.41
1:A:109:MET:O	1:A:113:SER:CB	2.59	0.41
1:A:308:LEU:O	1:A:312:GLU:HG2	2.21	0.41
1:A:386:ILE:HG21	1:B:112:CYS:HA	2.03	0.41
1:A:533:LEU:HB3	1:B:494:ARG:HH22	1.85	0.41
1:B:315:PHE:CG	1:B:481:LEU:HD21	2.56	0.41
1:B:63:PRO:HD3	1:B:238:LYS:HD2	2.01	0.40
1:B:463:LYS:C	1:B:464:VAL:O	2.60	0.40
1:B:335:PHE:CD2	1:B:335:PHE:C	2.94	0.40
1:A:11:SER:CB	1:B:44:ARG:HG3	2.51	0.40
1:B:381:ILE:HD11	1:B:396:VAL:HG21	2.04	0.40
1:A:316:ILE:HD11	1:A:480:VAL:HG22	2.04	0.40
1:B:154:LEU:HD22	1:B:179:VAL:CG1	2.50	0.40
1:A:155:TYR:CD1	1:A:173:LYS:HA	2.57	0.40
1:A:400:ILE:HG22	1:A:401:VAL:N	2.36	0.40
1:B:256:GLY:N	1:B:259:ASP:OD1	2.55	0.40
1:B:306:VAL:O	1:B:309:ALA:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:HIS:C	1:B:313:GLY:N	2.75	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	497/533 (93%)	427 (86%)	55 (11%)	15 (3%)	4	7
1	B	490/533 (92%)	409 (84%)	65 (13%)	16 (3%)	4	6
All	All	987/1066 (93%)	836 (85%)	120 (12%)	31 (3%)	4	6

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	GLU
1	A	191	ILE
1	B	193	ALA
1	B	210	ASN
1	B	311	HIS
1	B	476	ASN
1	B	502	GLY
1	B	503	LEU
1	A	121	ALA
1	A	209	GLY
1	A	319	ASP
1	A	323	SER
1	A	479	PRO
1	A	481	LEU
1	B	209	GLY
1	B	259	ASP
1	B	491	PRO

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Mol	Chain	Res	Type
1	A	261	MET
1	B	312	GLU
1	B	477	PHE
1	A	125	ASP
1	B	42	SER
1	B	319	ASP
1	B	320	ASP
1	A	320	ASP
1	B	189	ASP
1	A	407	PRO
1	B	342	LYS
1	A	12	VAL
1	A	257	VAL
1	A	188	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	443/471 (94%)	404 (91%)	39 (9%)	10	19
1	B	440/471 (93%)	399 (91%)	41 (9%)	9	17
All	All	883/942 (94%)	803 (91%)	80 (9%)	9	18

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	48	THR
1	A	58	LEU
1	A	66	LEU
1	A	86	LEU
1	A	92	VAL
1	A	93	GLU
1	A	100	VAL
1	A	104	ASN

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Mol	Chain	Res	Type
1	A	122	GLU
1	A	150	ASN
1	A	195	GLN
1	A	196	ASP
1	A	200	ASN
1	A	201	ASN
1	A	249	ARG
1	A	258	ASN
1	A	260	THR
1	A	264	LEU
1	A	294	ASN
1	A	298	GLN
1	A	300	THR
1	A	308	LEU
1	A	387	LEU
1	A	406	LYS
1	A	420	SER
1	A	432	ILE
1	A	434	ASN
1	A	436	CYS
1	A	438	ASP
1	A	440	LEU
1	A	453	THR
1	A	473	LYS
1	A	479	PRO
1	A	484	LEU
1	A	516	LEU
1	A	529	GLU
1	A	530	GLU
1	A	533	LEU
1	B	21	TYR
1	B	34	ASN
1	B	58	LEU
1	B	61	LYS
1	B	70	LEU
1	B	73	LEU
1	B	91	ASN
1	B	95	GLN
1	B	122	GLU
1	B	147	TRP
1	B	163	VAL
1	B	164	LEU

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Mol	Chain	Res	Type
1	B	168	LEU
1	B	189	ASP
1	B	194	ASN
1	B	196	ASP
1	B	210	ASN
1	B	233	GLU
1	B	236	LEU
1	B	237	ASP
1	B	246	ASN
1	B	262	GLU
1	B	299	ASN
1	B	321	LEU
1	B	325	GLN
1	B	328	LEU
1	B	350	ASN
1	B	352	LEU
1	B	378	ASP
1	B	384	ASN
1	B	387	LEU
1	B	397	ASP
1	B	398	HIS
1	B	402	ILE
1	B	412	LYS
1	B	474	PHE
1	B	477	PHE
1	B	497	PHE
1	B	517	LEU
1	B	520	LEU
1	B	523	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	76	ASN
1	A	77	ASN
1	A	88	ASN
1	A	90	HIS
1	A	91	ASN
1	A	102	GLN
1	A	104	ASN
1	A	131	ASN

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Mol	Chain	Res	Type
1	A	140	ASN
1	A	150	ASN
1	A	159	GLN
1	A	162	GLN
1	A	169	GLN
1	A	170	GLN
1	A	195	GLN
1	A	200	ASN
1	A	201	ASN
1	A	210	ASN
1	A	221	GLN
1	A	228	GLN
1	A	234	ASN
1	A	258	ASN
1	A	266	GLN
1	A	270	ASN
1	A	272	HIS
1	A	294	ASN
1	A	298	GLN
1	A	307	GLN
1	A	311	HIS
1	A	476	ASN
1	A	498	HIS
1	A	512	ASN
1	A	523	GLN
1	B	34	ASN
1	B	91	ASN
1	B	95	GLN
1	B	140	ASN
1	B	159	GLN
1	B	162	GLN
1	B	170	GLN
1	B	194	ASN
1	B	195	GLN
1	B	210	ASN
1	B	219	HIS
1	B	228	GLN
1	B	258	ASN
1	B	263	ASN
1	B	270	ASN
1	B	299	ASN
1	B	307	GLN

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Mol	Chain	Res	Type
1	B	325	GLN
1	B	350	ASN
1	B	428	ASN
1	B	433	HIS
1	B	498	HIS
1	B	506	GLN
1	B	523	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	463:LYS	C	464:VAL	N	1.80

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	501/533 (93%)	0.13	24 (4%)	30	24	13, 43, 77, 80	0
1	B	496/533 (93%)	0.21	30 (6%)	21	16	17, 44, 80, 80	0
All	All	997/1066 (93%)	0.17	54 (5%)	25	20	13, 43, 79, 80	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	404	TYR	6.6
1	B	407	PRO	5.5
1	B	464	VAL	5.1
1	A	194	ASN	4.3
1	A	195	GLN	4.1
1	B	465	ASP	4.1
1	B	44	ARG	4.1
1	B	478	TYR	4.0
1	B	473	LYS	3.9
1	A	256	GLY	3.8
1	A	208	LYS	3.7
1	B	41	ALA	3.5
1	A	193	ALA	3.5
1	B	9	ILE	3.5
1	B	477	PHE	3.3
1	B	207	GLU	3.2
1	A	41	ALA	3.2
1	B	496	GLY	3.2
1	B	404	TYR	3.0
1	B	466	PRO	2.9
1	A	398	HIS	2.8
1	B	405	MET	2.8
1	A	9	ILE	2.7
1	A	407	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	209	GLY	2.6
1	B	42	SER	2.6
1	A	40	THR	2.6
1	A	273	GLU	2.6
1	B	402	ILE	2.5
1	B	194	ASN	2.5
1	B	252	GLU	2.5
1	B	255	PRO	2.4
1	A	253	VAL	2.4
1	B	193	ALA	2.4
1	B	494	ARG	2.4
1	A	395	LYS	2.4
1	A	255	PRO	2.3
1	A	196	ASP	2.3
1	B	45	PHE	2.3
1	A	496	GLY	2.2
1	B	43	GLY	2.2
1	B	209	GLY	2.2
1	B	392	LEU	2.1
1	A	272	HIS	2.1
1	A	405	MET	2.1
1	B	390	ASP	2.1
1	A	445	LEU	2.1
1	B	192	ALA	2.1
1	B	254	SER	2.1
1	A	207	GLU	2.0
1	A	43	GLY	2.0
1	B	445	LEU	2.0
1	B	474	PHE	2.0
1	A	533	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 carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.