Full wwPDB X-ray Structure Validation Report (i)

May 22, 2020 – 01:25 am BST

PDB ID	:	3MXL
Title	:	Crystal structure of nitrososynthase from Micromonospora carbonacea var. africana
Authors	:	Vey, J.L.; Iverson, T.M.
Deposited on	:	2010-05-07
Resolution	:	3.15 Å(reported)

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

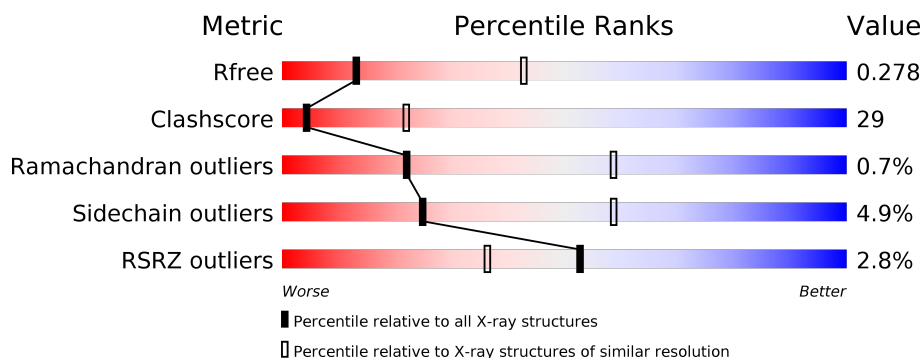|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.15 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	Percentile Ranks	Value
Rfree		0.278
Clashscore		29
Ramachandran outliers		0.7%
Sidechain outliers		4.9%
RSRZ outliers		2.8%

Worse ← → *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	395	% 54% 43% ·
1	B	395	4% 54% 37% · 6%
1	C	395	2% 52% 39% · 7%
1	D	395	3% 55% 40% · ·

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 11016 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 Nitrososynthase.

| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	0	0
			2842	1788	507	531	16			
1	B	370	Total	C	N	O	S	0	0	0
			2677	1687	474	500	16			
1	C	369	Total	C	N	O	S	0	0	0
			2666	1680	471	500	15			
1	D	391	Total	C	N	O	S	0	0	0
			2831	1782	502	531	16			

3 Residue-property plots (i)

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.
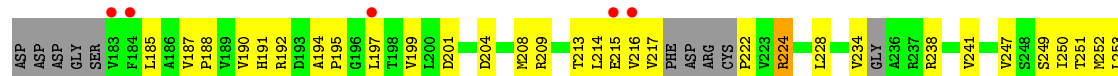
- Molecule 1: Nitrososynthase
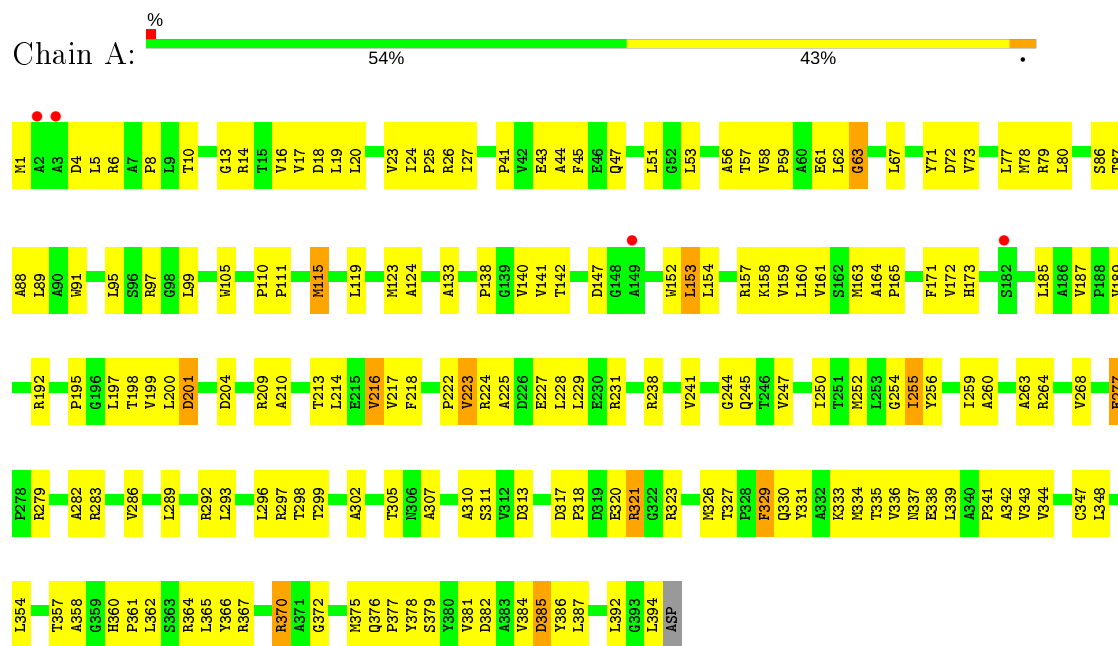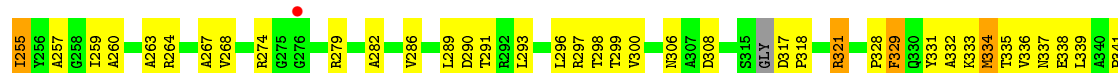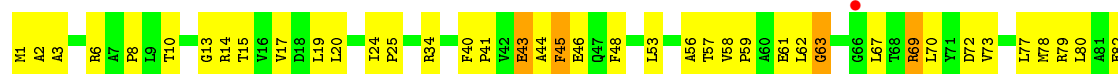

- Molecule 1: Nitrososynthase

• Molecule 1: Nitrososynthase

Chain C:

• Molecule 1: Nitrososynthase

Chain D:
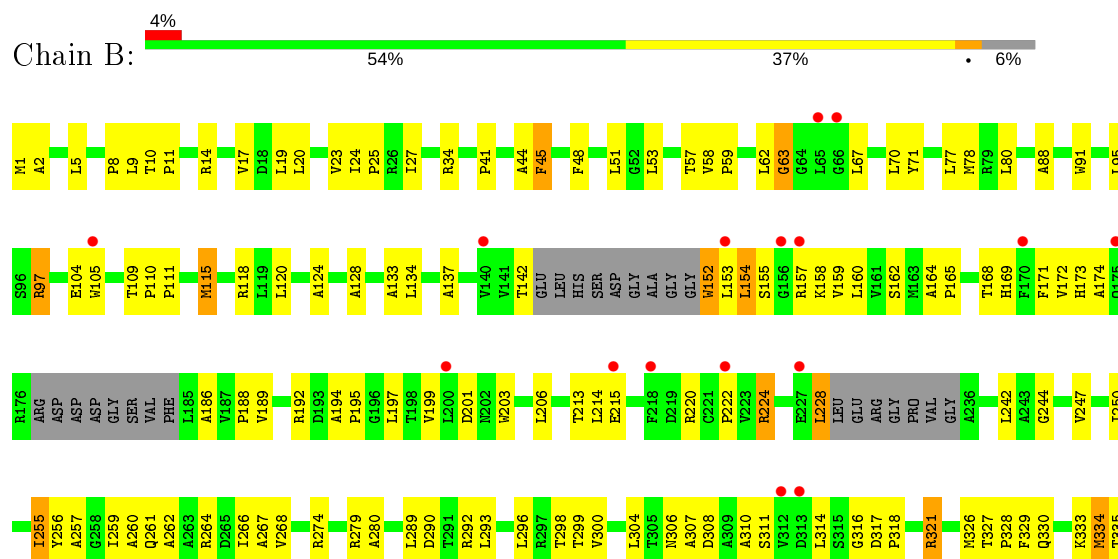
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	103.81Å 103.81Å 295.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.15 48.98 – 3.14	Depositor EDS
% Data completeness (in resolution range)	95.9 (50.00-3.15) 95.5 (48.98-3.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 3.12Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.242 , 0.281 0.243 , 0.278	Depositor DCC
R_{free} test set	2896 reflections (9.34%)	wwPDB-VP
Wilson B-factor (Å^2)	102.5	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 69.0	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.057 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11016	wwPDB-VP
Average B, all atoms (Å^2)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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	0.34	0/2895	0.58	0/3949
1	B	0.38	0/2724	0.56	0/3716
1	C	0.35	0/2711	0.57	0/3694
1	D	0.35	0/2882	0.55	0/3928
All	All	0.36	0/11212	0.57	0/15287

There are no bond length outliers.

There are no bond angle outliers.

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	2842	0	2804	177	0
1	B	2677	0	2643	159	0
1	C	2666	0	2638	157	0
1	D	2831	0	2796	179	0
All	All	11016	0	10881	636	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 29.

All (636) 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:D:376:GLN:HE22	1:D:379:SER:HB2	1.10	1.15
1:B:321:ARG:HH21	1:B:321:ARG:HB2	1.16	1.05
1:A:321:ARG:HH21	1:A:321:ARG:HB2	1.19	1.04
1:A:296:LEU:HD11	1:A:336:VAL:HG23	1.41	1.02
1:C:298:THR:HG22	1:D:298:THR:HG22	1.44	0.99
1:C:376:GLN:HE22	1:C:379:SER:HB2	1.28	0.98
1:A:298:THR:HG22	1:B:298:THR:HG22	1.47	0.96
1:A:133:ALA:HB1	1:A:158:LYS:HG3	1.45	0.95
1:A:298:THR:HG21	1:B:299:THR:HA	1.49	0.94
1:B:354:LEU:O	1:B:357:THR:HG22	1.67	0.94
1:A:376:GLN:HE22	1:A:379:SER:HB2	1.32	0.93
1:C:133:ALA:HB1	1:C:158:LYS:HG3	1.51	0.92
1:C:354:LEU:O	1:C:357:THR:HG22	1.70	0.92
1:C:386:TYR:HD2	1:C:387:LEU:HD12	1.34	0.92
1:B:376:GLN:HE22	1:B:379:SER:HB2	1.33	0.91
1:D:8:PRO:HG3	1:D:17:VAL:HG21	1.53	0.91
1:D:376:GLN:NE2	1:D:379:SER:HB2	1.87	0.90
1:C:250:ILE:HA	1:C:329:PHE:CE2	2.06	0.89
1:A:147:ASP:HB3	1:A:153:LEU:HD11	1.52	0.89
1:C:157:ARG:HB3	1:C:217:VAL:HG12	1.54	0.89
1:C:201:ASP:HA	1:C:214:LEU:HD22	1.53	0.88
1:A:8:PRO:HG3	1:A:17:VAL:HG21	1.56	0.87
1:B:296:LEU:HD11	1:B:336:VAL:HG23	1.54	0.87
1:A:372:GLY:HA2	1:A:375:MET:HE2	1.56	0.87
1:A:159:VAL:HG23	1:A:160:LEU:HD23	1.56	0.87
1:A:157:ARG:HB3	1:A:217:VAL:HG12	1.55	0.87
1:A:321:ARG:HB2	1:A:321:ARG:NH2	1.90	0.85
1:D:354:LEU:O	1:D:357:THR:HG22	1.77	0.85
1:B:267:ALA:HB1	1:B:350:LEU:HD23	1.60	0.84
1:B:11:PRO:HB3	1:B:14:ARG:HH21	1.41	0.84
1:D:264:ARG:NH1	1:D:268:VAL:HG21	1.92	0.84
1:B:159:VAL:HG12	1:B:215:GLU:HG3	1.59	0.83
1:A:376:GLN:NE2	1:A:379:SER:HB2	1.93	0.82
1:B:201:ASP:HA	1:B:214:LEU:HD22	1.62	0.82
1:B:11:PRO:HA	1:B:14:ARG:HE	1.44	0.82
1:A:357:THR:HG23	1:A:360:HIS:H	1.46	0.81
1:D:257:ALA:HA	1:D:296:LEU:HD21	1.63	0.81
1:D:133:ALA:HB1	1:D:158:LYS:HG3	1.63	0.81
1:C:298:THR:HG21	1:D:299:THR:HA	1.63	0.80
1:A:317:ASP:OD2	1:A:318:PRO:HD2	1.83	0.79
1:C:63:GLY:HA3	1:C:124:ALA:HB1	1.66	0.78
1:C:41:PRO:HG3	1:C:87:THR:HG22	1.64	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:ARG:H	1:C:224:ARG:HD3	1.48	0.77
1:D:282:ALA:O	1:D:286:VAL:HG12	1.85	0.76
1:D:63:GLY:HA3	1:D:124:ALA:HB1	1.66	0.76
1:C:376:GLN:NE2	1:C:379:SER:HB2	2.00	0.76
1:B:63:GLY:HA3	1:B:124:ALA:HB1	1.65	0.76
1:D:201:ASP:HA	1:D:214:LEU:HD22	1.67	0.76
1:A:73:VAL:O	1:A:77:LEU:HD13	1.85	0.75
1:D:97:ARG:HG3	1:D:97:ARG:HH11	1.52	0.75
1:D:381:VAL:O	1:D:384:VAL:HG12	1.85	0.75
1:A:63:GLY:HA3	1:A:124:ALA:HB1	1.67	0.74
1:B:186:ALA:HB1	1:B:228:LEU:HD11	1.68	0.74
1:D:197:LEU:HD11	1:D:216:VAL:HG23	1.70	0.73
1:A:153:LEU:HD12	1:A:153:LEU:N	2.03	0.73
1:C:250:ILE:HA	1:C:329:PHE:HE2	1.51	0.73
1:D:357:THR:HG23	1:D:360:HIS:H	1.53	0.73
1:A:360:HIS:ND1	1:A:361:PRO:HD2	2.03	0.73
1:C:376:GLN:HE22	1:C:379:SER:CB	2.00	0.73
1:A:354:LEU:O	1:A:357:THR:HG22	1.88	0.72
1:A:41:PRO:HG3	1:A:87:THR:HG22	1.71	0.72
1:B:250:ILE:HA	1:B:329:PHE:CE2	2.25	0.72
1:C:381:VAL:O	1:C:384:VAL:HG12	1.89	0.72
1:B:314:LEU:HD23	1:B:316:GLY:H	1.55	0.71
1:B:59:PRO:HD2	1:B:120:LEU:HD21	1.70	0.71
1:A:299:THR:HA	1:B:298:THR:HG21	1.72	0.71
1:A:77:LEU:HD11	1:A:95:LEU:HD12	1.73	0.71
1:C:80:LEU:HD23	1:C:88:ALA:HA	1.73	0.70
1:D:241:VAL:HG22	1:D:245:GLN:HE21	1.56	0.70
1:A:159:VAL:CG2	1:A:160:LEU:HD23	2.21	0.70
1:C:386:TYR:CD2	1:C:387:LEU:HD12	2.24	0.70
1:A:200:LEU:O	1:A:214:LEU:HB3	1.90	0.69
1:A:195:PRO:HG2	1:A:222:PRO:HD2	1.75	0.69
1:D:332:ALA:O	1:D:336:VAL:HG12	1.92	0.69
1:B:321:ARG:CB	1:B:321:ARG:HH21	1.99	0.69
1:B:115:MET:HA	1:B:118:ARG:HD3	1.74	0.69
1:A:381:VAL:O	1:A:384:VAL:HG12	1.92	0.69
1:B:317:ASP:OD2	1:B:318:PRO:HD2	1.93	0.69
1:C:333:LYS:HG2	1:C:337:ASN:HD21	1.58	0.68
1:C:296:LEU:HD11	1:C:336:VAL:HG23	1.75	0.68
1:A:154:LEU:HD11	1:A:172:VAL:HG11	1.76	0.68
1:B:70:LEU:HB2	1:B:308:ASP:OD2	1.94	0.68
1:D:164:ALA:HB3	1:D:214:LEU:HD12	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:LEU:O	1:A:297:ARG:HG3	1.94	0.68
1:B:154:LEU:HD23	1:B:154:LEU:C	2.14	0.68
1:A:333:LYS:NZ	1:A:337:ASN:HD21	1.92	0.68
1:A:86:SER:CB	1:A:210:ALA:HB3	2.25	0.67
1:D:386:TYR:HD2	1:D:387:LEU:HD12	1.59	0.67
1:D:69:ARG:O	1:D:73:VAL:HG23	1.93	0.67
1:D:86:SER:CB	1:D:210:ALA:HB3	2.24	0.67
1:A:47:GLN:O	1:A:51:LEU:HD13	1.95	0.67
1:C:299:THR:HA	1:D:298:THR:HG21	1.76	0.67
1:D:195:PRO:HG2	1:D:222:PRO:HD2	1.77	0.67
1:D:360:HIS:ND1	1:D:361:PRO:HD2	2.09	0.67
1:A:59:PRO:HB2	1:A:62:LEU:HD23	1.77	0.67
1:B:376:GLN:HE22	1:B:379:SER:CB	2.05	0.67
1:B:321:ARG:NH2	1:B:321:ARG:HB2	2.01	0.66
1:A:392:LEU:HB2	1:A:394:LEU:CD1	2.26	0.66
1:B:192:ARG:HH21	1:B:199:VAL:HG11	1.62	0.65
1:B:376:GLN:NE2	1:B:379:SER:HB2	2.10	0.65
1:A:142:THR:OG1	1:A:158:LYS:HE2	1.97	0.65
1:A:152:TRP:C	1:A:153:LEU:HD12	2.17	0.65
1:A:185:LEU:HD12	1:A:231:ARG:HD2	1.79	0.65
1:C:164:ALA:N	1:C:165:PRO:HD2	2.12	0.65
1:A:133:ALA:HB1	1:A:158:LYS:CG	2.24	0.65
1:A:364:ARG:HA	1:A:367:ARG:HH21	1.62	0.65
1:B:142:THR:O	1:B:174:ALA:HA	1.97	0.64
1:A:6:ARG:HD3	1:A:297:ARG:HH22	1.62	0.64
1:A:154:LEU:CD1	1:A:172:VAL:HG11	2.28	0.64
1:C:311:SER:HA	1:C:321:ARG:HH12	1.62	0.64
1:B:370:ARG:HG3	1:D:366:TYR:OH	1.98	0.64
1:A:77:LEU:HB3	1:A:255:ILE:HG22	1.80	0.64
1:B:335:THR:O	1:B:339:LEU:HB2	1.97	0.64
1:C:253:LEU:HD23	1:C:300:VAL:HG12	1.80	0.63
1:D:197:LEU:HD12	1:D:198:THR:H	1.63	0.63
1:C:62:LEU:HD21	1:C:105:TRP:CH2	2.33	0.63
1:C:292:ARG:HH21	1:C:292:ARG:HG2	1.63	0.63
1:D:195:PRO:CG	1:D:222:PRO:HD2	2.29	0.63
1:D:77:LEU:HD11	1:D:95:LEU:HD12	1.80	0.63
1:B:164:ALA:N	1:B:165:PRO:HD2	2.14	0.63
1:A:161:VAL:HG21	1:A:216:VAL:CG1	2.28	0.62
1:A:13:GLY:O	1:A:17:VAL:HG23	2.00	0.62
1:D:14:ARG:HG3	1:D:14:ARG:HH11	1.65	0.62
1:B:194:ALA:HB3	1:B:197:LEU:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:ALA:HB1	1:C:169:HIS:CD2	2.34	0.62
1:B:115:MET:CE	1:B:189:VAL:HG21	2.30	0.62
1:B:8:PRO:HG3	1:B:17:VAL:HG21	1.82	0.62
1:D:10:THR:HG23	1:D:13:GLY:H	1.65	0.62
1:D:13:GLY:O	1:D:17:VAL:HG23	2.00	0.62
1:A:10:THR:HG23	1:A:13:GLY:H	1.65	0.61
1:C:163:MET:HG2	1:C:163:MET:O	2.01	0.61
1:C:90:ALA:O	1:C:93:VAL:HG23	2.00	0.61
1:A:20:LEU:O	1:A:24:ILE:HG12	1.99	0.61
1:C:10:THR:HG23	1:C:13:GLY:H	1.65	0.61
1:A:310:ALA:O	1:A:321:ARG:NH2	2.26	0.61
1:A:160:LEU:HA	1:A:213:THR:HG22	1.83	0.61
1:D:341:PRO:HA	1:D:344:VAL:CG2	2.30	0.61
1:B:381:VAL:O	1:B:384:VAL:HG12	1.99	0.61
1:D:264:ARG:HD3	1:D:293:LEU:CD2	2.31	0.61
1:C:70:LEU:HB2	1:C:308:ASP:OD2	2.01	0.61
1:D:263:ALA:CB	1:D:344:VAL:HG12	2.31	0.61
1:C:260:ALA:HB1	1:C:343:VAL:HG21	1.82	0.61
1:D:97:ARG:NH1	1:D:97:ARG:HG3	2.12	0.61
1:A:78:MET:HG3	1:A:254:GLY:O	2.00	0.60
1:B:41:PRO:HB2	1:B:44:ALA:HB3	1.82	0.60
1:B:164:ALA:HB3	1:B:214:LEU:HD12	1.83	0.60
1:B:314:LEU:HD23	1:B:316:GLY:N	2.15	0.60
1:A:187:VAL:O	1:A:187:VAL:HG23	2.02	0.60
1:A:19:LEU:HG	1:A:51:LEU:HD23	1.82	0.60
1:B:19:LEU:HB3	1:B:53:LEU:HD11	1.84	0.60
1:D:59:PRO:HB2	1:D:62:LEU:HD23	1.84	0.60
1:A:223:VAL:HG13	1:A:223:VAL:O	2.02	0.60
1:C:59:PRO:HB2	1:C:62:LEU:HD23	1.84	0.60
1:A:8:PRO:HG2	1:A:14:ARG:HD2	1.84	0.59
1:D:41:PRO:HB2	1:D:44:ALA:HB3	1.83	0.59
1:C:357:THR:HG23	1:C:360:HIS:H	1.67	0.59
1:C:41:PRO:HB2	1:C:44:ALA:HB3	1.84	0.59
1:C:372:GLY:HA2	1:C:375:MET:HE2	1.85	0.59
1:D:321:ARG:HH21	1:D:321:ARG:HB2	1.68	0.59
1:D:41:PRO:HG3	1:D:87:THR:CG2	2.33	0.59
1:A:24:ILE:N	1:A:25:PRO:HD2	2.17	0.59
1:B:292:ARG:HG2	1:B:292:ARG:HH21	1.67	0.59
1:D:394:LEU:HD12	1:D:394:LEU:N	2.17	0.59
1:A:241:VAL:HG22	1:A:245:GLN:HE21	1.67	0.58
1:C:300:VAL:O	1:C:304:LEU:HG	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:LEU:HD11	1:D:216:VAL:CG2	2.33	0.58
1:D:58:VAL:HG13	1:D:120:LEU:HD11	1.84	0.58
1:C:157:ARG:CB	1:C:217:VAL:HG12	2.31	0.58
1:A:157:ARG:NH1	1:A:217:VAL:HG11	2.19	0.58
1:A:163:MET:HG2	1:A:163:MET:O	2.03	0.58
1:A:198:THR:HB	1:A:217:VAL:CG2	2.33	0.58
1:A:357:THR:HG22	1:A:360:HIS:HB2	1.85	0.58
1:C:274:ARG:HA	1:C:274:ARG:HE	1.68	0.58
1:D:335:THR:O	1:D:339:LEU:HB2	2.03	0.58
1:B:259:ILE:HG23	1:B:365:LEU:HD22	1.85	0.58
1:D:164:ALA:N	1:D:165:PRO:HD2	2.18	0.58
1:D:78:MET:O	1:D:82:GLU:HG3	2.03	0.58
1:C:394:LEU:H	1:C:394:LEU:HD12	1.68	0.58
1:A:171:PHE:CE1	1:A:189:VAL:HG22	2.39	0.57
1:D:394:LEU:HD12	1:D:394:LEU:H	1.69	0.57
1:B:71:TYR:HA	1:B:304:LEU:HD13	1.84	0.57
1:B:91:TRP:CE2	1:B:95:LEU:HD11	2.38	0.57
1:D:228:LEU:HD12	1:D:228:LEU:N	2.20	0.57
1:D:58:VAL:HG13	1:D:120:LEU:CD1	2.34	0.57
1:A:357:THR:CG2	1:A:360:HIS:HB2	2.34	0.57
1:A:41:PRO:HB2	1:A:44:ALA:HB3	1.86	0.57
1:A:384:VAL:HG11	1:C:281:GLY:HA3	1.87	0.57
1:A:335:THR:O	1:A:339:LEU:HB2	2.05	0.57
1:D:56:ALA:O	1:D:58:VAL:HG23	2.04	0.57
1:C:360:HIS:CE1	1:C:362:LEU:HB2	2.40	0.57
1:C:394:LEU:HD12	1:C:394:LEU:N	2.19	0.57
1:B:154:LEU:HD23	1:B:155:SER:N	2.19	0.57
1:A:296:LEU:HD11	1:A:336:VAL:CG2	2.27	0.56
1:B:296:LEU:CD1	1:B:336:VAL:HG23	2.30	0.56
1:D:86:SER:HB2	1:D:210:ALA:HB3	1.86	0.56
1:C:48:PHE:CD1	1:C:53:LEU:HD22	2.41	0.56
1:A:326:MET:O	1:A:330:GLN:HG2	2.06	0.56
1:B:115:MET:HE1	1:B:189:VAL:HG21	1.87	0.56
1:C:340:ALA:O	1:C:343:VAL:HG22	2.06	0.56
1:D:176:ARG:O	1:D:183:VAL:HG13	2.06	0.56
1:C:306:ASN:ND2	1:C:328:PRO:HG3	2.20	0.56
1:C:290:ASP:HB3	1:D:331:TYR:CE1	2.41	0.56
1:C:307:ALA:O	1:C:311:SER:HB2	2.06	0.56
1:C:185:LEU:HB2	1:C:234:VAL:HG13	1.89	0.55
1:D:200:LEU:O	1:D:214:LEU:HB3	2.06	0.55
1:A:364:ARG:HA	1:A:367:ARG:NH2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:VAL:HG13	1:C:120:LEU:HG	1.88	0.55
1:D:48:PHE:CD1	1:D:53:LEU:HD22	2.41	0.55
1:A:86:SER:HB2	1:A:210:ALA:HB3	1.89	0.55
1:B:381:VAL:HG12	1:D:279:ARG:HG2	1.87	0.55
1:C:159:VAL:HG23	1:C:160:LEU:HD23	1.88	0.55
1:D:357:THR:CG2	1:D:360:HIS:HB2	2.35	0.55
1:C:187:VAL:O	1:C:187:VAL:HG23	2.05	0.55
1:C:73:VAL:O	1:C:77:LEU:HD13	2.05	0.55
1:D:376:GLN:HE22	1:D:379:SER:CB	2.02	0.55
1:D:80:LEU:HD23	1:D:91:TRP:CE3	2.41	0.55
1:A:5:LEU:HD23	1:A:71:TYR:CE1	2.42	0.55
1:A:331:TYR:CE1	1:B:290:ASP:HB3	2.41	0.55
1:C:311:SER:HA	1:C:321:ARG:NH1	2.22	0.55
1:D:197:LEU:HD12	1:D:198:THR:N	2.21	0.55
1:D:386:TYR:CD2	1:D:387:LEU:HD12	2.40	0.55
1:D:41:PRO:HG3	1:D:87:THR:HG22	1.88	0.55
1:A:292:ARG:HH21	1:A:292:ARG:HG2	1.72	0.55
1:C:192:ARG:HH21	1:C:199:VAL:HG11	1.71	0.55
1:A:238:ARG:O	1:A:241:VAL:HG12	2.07	0.55
1:B:194:ALA:HB3	1:B:197:LEU:CB	2.37	0.55
1:C:274:ARG:HE	1:C:274:ARG:CA	2.20	0.55
1:D:110:PRO:N	1:D:111:PRO:HD2	2.22	0.55
1:C:128:ALA:HB1	1:C:169:HIS:HD2	1.72	0.54
1:D:263:ALA:HB2	1:D:344:VAL:HG12	1.89	0.54
1:B:321:ARG:C	1:B:321:ARG:HD3	2.28	0.54
1:C:188:PRO:HG3	1:C:228:LEU:HG	1.89	0.54
1:D:344:VAL:HG21	1:D:369:VAL:HG11	1.89	0.54
1:B:250:ILE:HA	1:B:329:PHE:HE2	1.73	0.54
1:C:70:LEU:HD11	1:C:247:VAL:HG23	1.89	0.54
1:C:53:LEU:H	1:C:53:LEU:HD12	1.72	0.54
1:A:394:LEU:HD12	1:A:394:LEU:N	2.23	0.54
1:B:110:PRO:N	1:B:111:PRO:HD2	2.22	0.54
1:D:70:LEU:HB2	1:D:308:ASP:OD2	2.07	0.54
1:A:333:LYS:HZ2	1:A:337:ASN:HD21	1.54	0.54
1:B:152:TRP:O	1:B:153:LEU:HB2	2.07	0.54
1:D:14:ARG:NH1	1:D:14:ARG:HG3	2.21	0.54
1:D:20:LEU:HD21	1:D:80:LEU:HB2	1.89	0.53
1:A:161:VAL:HG21	1:A:216:VAL:HG12	1.91	0.53
1:A:61:GLU:HG3	1:A:62:LEU:HD22	1.91	0.53
1:B:168:THR:O	1:B:192:ARG:N	2.42	0.53
1:C:77:LEU:HD11	1:C:95:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:MET:C	1:A:115:MET:SD	2.87	0.53
1:D:80:LEU:HD23	1:D:91:TRP:HE3	1.72	0.53
1:C:252:MET:O	1:C:255:ILE:HG13	2.08	0.53
1:D:147:ASP:HB3	1:D:153:LEU:CD1	2.39	0.53
1:B:394:LEU:HD12	1:B:394:LEU:N	2.23	0.53
1:B:70:LEU:HD21	1:B:247:VAL:HG23	1.91	0.53
1:D:329:PHE:C	1:D:329:PHE:CD2	2.80	0.53
1:B:58:VAL:HG22	1:B:120:LEU:CD1	2.39	0.53
1:D:155:SER:HA	1:D:218:PHE:O	2.09	0.53
1:A:153:LEU:CD1	1:A:153:LEU:N	2.71	0.53
1:D:8:PRO:HG2	1:D:14:ARG:HD2	1.91	0.53
1:C:109:THR:OG1	1:C:112:VAL:HG22	2.09	0.52
1:C:20:LEU:HD13	1:C:53:LEU:HD23	1.91	0.52
1:B:104:GLU:HA	1:B:104:GLU:OE1	2.10	0.52
1:A:164:ALA:N	1:A:165:PRO:HD2	2.25	0.52
1:A:201:ASP:HA	1:A:214:LEU:HD22	1.91	0.52
1:C:334:MET:HB3	1:D:291:THR:HG21	1.91	0.52
1:D:24:ILE:N	1:D:25:PRO:HD2	2.24	0.52
1:D:264:ARG:HD3	1:D:293:LEU:HD22	1.91	0.52
1:D:317:ASP:OD2	1:D:318:PRO:HD2	2.09	0.52
1:A:244:GLY:O	1:A:247:VAL:HG12	2.10	0.52
1:A:23:VAL:HG22	1:A:47:GLN:NE2	2.25	0.52
1:C:191:HIS:ND1	1:C:192:ARG:N	2.58	0.52
1:B:165:PRO:HD3	1:B:214:LEU:HD11	1.92	0.52
1:B:264:ARG:HD2	1:B:290:ASP:OD2	2.10	0.52
1:D:338:GLU:O	1:D:342:ALA:HB2	2.10	0.52
1:B:134:LEU:HD13	1:B:173:HIS:CD2	2.45	0.52
1:B:333:LYS:HZ3	1:B:337:ASN:HD21	1.58	0.52
1:C:274:ARG:HA	1:C:274:ARG:NE	2.24	0.52
1:D:154:LEU:HD22	1:D:218:PHE:HB3	1.92	0.52
1:D:341:PRO:HA	1:D:344:VAL:HG22	1.92	0.52
1:B:333:LYS:NZ	1:B:337:ASN:HD21	2.07	0.52
1:D:293:LEU:O	1:D:297:ARG:HG3	2.09	0.52
1:A:192:ARG:HH21	1:A:199:VAL:HG11	1.74	0.51
1:B:192:ARG:NH2	1:B:199:VAL:HG11	2.24	0.51
1:C:125:GLU:HA	1:C:125:GLU:OE2	2.09	0.51
1:A:264:ARG:NH1	1:A:268:VAL:HG21	2.24	0.51
1:B:357:THR:HG23	1:B:360:HIS:H	1.76	0.51
1:A:370:ARG:HG3	1:C:366:TYR:OH	2.11	0.51
1:C:2:ALA:O	1:C:3:ALA:HB3	2.09	0.51
1:A:357:THR:HG23	1:A:360:HIS:N	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:ARG:HG3	1:B:280:ALA:N	2.26	0.51
1:D:171:PHE:CE1	1:D:189:VAL:HG22	2.45	0.51
1:A:197:LEU:HD13	1:A:218:PHE:CE1	2.45	0.51
1:A:259:ILE:HG23	1:A:365:LEU:HD22	1.92	0.51
1:B:142:THR:HG22	1:B:142:THR:O	2.09	0.51
1:B:394:LEU:HD12	1:B:394:LEU:H	1.74	0.51
1:B:261:GLN:OE1	1:B:293:LEU:HD21	2.10	0.51
1:A:282:ALA:O	1:A:286:VAL:HG12	2.10	0.51
1:B:360:HIS:ND1	1:B:361:PRO:HD2	2.26	0.51
1:D:77:LEU:HB3	1:D:255:ILE:HG22	1.92	0.51
1:A:140:VAL:HG12	1:A:141:VAL:N	2.25	0.51
1:A:392:LEU:HB2	1:A:394:LEU:HD13	1.92	0.51
1:C:256:TYR:HE1	1:C:375:MET:HE1	1.76	0.51
1:D:244:GLY:O	1:D:247:VAL:HG12	2.10	0.51
1:D:8:PRO:HG3	1:D:17:VAL:CG2	2.34	0.51
1:D:77:LEU:HD11	1:D:95:LEU:CD1	2.41	0.50
1:A:110:PRO:N	1:A:111:PRO:HD2	2.26	0.50
1:B:172:VAL:HG22	1:B:173:HIS:N	2.26	0.50
1:C:330:GLN:OE1	1:C:378:TYR:HB2	2.11	0.50
1:D:253:LEU:HG	1:D:336:VAL:HG11	1.93	0.50
1:C:195:PRO:HG2	1:C:222:PRO:HD2	1.94	0.50
1:D:77:LEU:HD21	1:D:92:HIS:HB2	1.94	0.50
1:C:94:GLN:HE22	1:C:123:MET:HB2	1.76	0.50
1:C:302:ALA:HB2	1:D:298:THR:HG23	1.93	0.50
1:C:333:LYS:HG2	1:C:337:ASN:ND2	2.23	0.50
1:C:344:VAL:HG21	1:C:369:VAL:HG11	1.93	0.50
1:D:142:THR:OG1	1:D:158:LYS:HE2	2.11	0.50
1:D:255:ILE:HD12	1:D:255:ILE:C	2.32	0.50
1:D:339:LEU:O	1:D:343:VAL:HG13	2.10	0.50
1:D:384:VAL:HG13	1:D:385:ASP:N	2.26	0.50
1:B:186:ALA:CB	1:B:228:LEU:HD11	2.40	0.50
1:B:379:SER:HB3	1:B:382:ASP:OD2	2.12	0.50
1:D:157:ARG:HB3	1:D:217:VAL:HG12	1.94	0.50
1:D:238:ARG:O	1:D:241:VAL:HG12	2.11	0.50
1:B:206:LEU:HD13	1:D:363:SER:OG	2.11	0.50
1:A:298:THR:CG2	1:B:298:THR:HG22	2.30	0.50
1:C:166:ILE:HG12	1:C:166:ILE:O	2.12	0.50
1:C:224:ARG:CD	1:C:224:ARG:H	2.18	0.50
1:C:292:ARG:CG	1:C:292:ARG:HH21	2.22	0.50
1:B:224:ARG:HD3	1:B:224:ARG:H	1.76	0.49
1:B:224:ARG:HD3	1:B:224:ARG:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:ARG:HG3	1:B:280:ALA:H	1.76	0.49
1:A:260:ALA:HB1	1:A:343:VAL:HG21	1.94	0.49
1:C:91:TRP:CE2	1:C:95:LEU:HD11	2.47	0.49
1:D:95:LEU:O	1:D:99:LEU:HD23	2.12	0.49
1:C:34:ARG:HG2	1:C:34:ARG:HH21	1.75	0.49
1:D:164:ALA:H	1:D:165:PRO:HD2	1.77	0.49
1:A:16:VAL:HG21	1:A:67:LEU:HD22	1.93	0.49
1:A:250:ILE:HG13	1:A:329:PHE:CD2	2.48	0.49
1:C:110:PRO:N	1:C:111:PRO:HD2	2.27	0.49
1:C:41:PRO:HG3	1:C:87:THR:CG2	2.37	0.49
1:C:41:PRO:O	1:C:45:PHE:HB2	2.13	0.49
1:D:73:VAL:O	1:D:77:LEU:HD13	2.12	0.49
1:A:379:SER:HB3	1:A:382:ASP:OD2	2.13	0.49
1:A:302:ALA:HB2	1:B:298:THR:HG23	1.94	0.49
1:D:333:LYS:HG2	1:D:337:ASN:ND2	2.28	0.49
1:A:171:PHE:CD1	1:A:189:VAL:HG22	2.47	0.49
1:A:384:VAL:HG11	1:C:281:GLY:CA	2.43	0.49
1:C:296:LEU:HD13	1:C:336:VAL:HA	1.95	0.49
1:D:267:ALA:HB2	1:D:347:CYS:HB3	1.94	0.49
1:B:58:VAL:HG22	1:B:120:LEU:HD11	1.95	0.48
1:C:59:PRO:HD2	1:C:120:LEU:HD21	1.95	0.48
1:D:154:LEU:C	1:D:154:LEU:HD23	2.34	0.48
1:B:109:THR:HB	1:B:111:PRO:HD2	1.93	0.48
1:D:172:VAL:O	1:D:188:PRO:HD2	2.14	0.48
1:B:370:ARG:NH2	1:D:348:LEU:HB3	2.27	0.48
1:A:41:PRO:HG3	1:A:87:THR:CG2	2.42	0.48
1:C:360:HIS:CG	1:C:361:PRO:HD2	2.47	0.48
1:B:165:PRO:HD3	1:B:214:LEU:CD1	2.43	0.48
1:B:250:ILE:HG13	1:B:329:PHE:CD2	2.48	0.48
1:B:78:MET:HE3	1:B:257:ALA:C	2.33	0.48
1:B:5:LEU:HD11	1:B:300:VAL:HG23	1.95	0.48
1:B:339:LEU:O	1:B:343:VAL:HG13	2.14	0.48
1:D:131:CYS:SG	1:D:163:MET:O	2.71	0.48
1:D:99:LEU:HD22	1:D:99:LEU:N	2.29	0.48
1:C:8:PRO:HG3	1:C:17:VAL:HG21	1.95	0.48
1:D:2:ALA:O	1:D:3:ALA:HB3	2.14	0.48
1:A:154:LEU:HD23	1:A:154:LEU:C	2.34	0.48
1:B:24:ILE:N	1:B:25:PRO:HD2	2.29	0.48
1:B:377:PRO:HA	1:B:378:TYR:HA	1.66	0.48
1:D:197:LEU:HD13	1:D:218:PHE:CE1	2.49	0.48
1:D:34:ARG:HH21	1:D:34:ARG:HG2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:THR:HA	1:B:192:ARG:HB2	1.95	0.48
1:C:140:VAL:HG11	1:C:157:ARG:HG2	1.96	0.48
1:A:381:VAL:HG12	1:C:279:ARG:HG2	1.95	0.48
1:D:197:LEU:CD1	1:D:216:VAL:HG23	2.41	0.48
1:A:341:PRO:HA	1:A:344:VAL:HG22	1.96	0.48
1:B:310:ALA:O	1:B:321:ARG:NH2	2.41	0.48
1:B:386:TYR:CD2	1:B:387:LEU:HD12	2.49	0.48
1:C:334:MET:HA	1:C:334:MET:CE	2.44	0.48
1:A:20:LEU:HG	1:A:24:ILE:HD11	1.95	0.48
1:D:142:THR:HG22	1:D:174:ALA:HB2	1.96	0.48
1:A:338:GLU:O	1:A:342:ALA:HB2	2.13	0.47
1:A:348:LEU:HD12	1:A:362:LEU:HG	1.96	0.47
1:B:137:ALA:HB3	1:B:157:ARG:HG3	1.96	0.47
1:D:43:GLU:HA	1:D:46:GLU:HG2	1.96	0.47
1:C:53:LEU:HD12	1:C:53:LEU:N	2.30	0.47
1:D:61:GLU:HG3	1:D:62:LEU:HD22	1.95	0.47
1:A:227:GLU:C	1:A:228:LEU:HD12	2.35	0.47
1:C:279:ARG:HG3	1:C:280:ALA:N	2.30	0.47
1:C:43:GLU:H	1:C:43:GLU:CD	2.16	0.47
1:B:262:ALA:O	1:B:266:ILE:HG12	2.15	0.47
1:C:238:ARG:O	1:C:241:VAL:HG12	2.14	0.47
1:C:302:ALA:CB	1:D:298:THR:HG23	2.45	0.47
1:A:224:ARG:H	1:A:224:ARG:HD3	1.80	0.47
1:B:133:ALA:HB3	1:B:172:VAL:HA	1.97	0.47
1:B:244:GLY:O	1:B:247:VAL:HG12	2.14	0.47
1:B:77:LEU:HB3	1:B:255:ILE:HG22	1.96	0.47
1:B:80:LEU:HD23	1:B:88:ALA:HA	1.97	0.47
1:D:133:ALA:HB1	1:D:158:LYS:CG	2.40	0.47
1:A:133:ALA:CB	1:A:158:LYS:HG3	2.30	0.47
1:A:250:ILE:HG12	1:A:250:ILE:O	2.14	0.47
1:B:264:ARG:NH1	1:B:268:VAL:HG21	2.29	0.47
1:C:164:ALA:N	1:C:165:PRO:CD	2.78	0.47
1:D:154:LEU:HD11	1:D:172:VAL:HG11	1.97	0.47
1:D:187:VAL:O	1:D:187:VAL:HG23	2.15	0.47
1:D:348:LEU:HD22	1:D:366:TYR:CD2	2.49	0.47
1:B:134:LEU:HA	1:B:173:HIS:HD2	1.79	0.47
1:B:115:MET:HE2	1:B:189:VAL:HG21	1.96	0.47
1:A:62:LEU:HD21	1:A:105:TRP:CZ2	2.50	0.47
1:B:338:GLU:O	1:B:342:ALA:HB2	2.14	0.47
1:B:62:LEU:HG	1:B:120:LEU:HD23	1.97	0.47
1:D:259:ILE:HG23	1:D:365:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:LEU:O	1:D:80:LEU:HD12	2.14	0.47
1:A:348:LEU:CD1	1:A:362:LEU:HG	2.45	0.47
1:B:48:PHE:CD1	1:B:53:LEU:HD22	2.50	0.47
1:C:134:LEU:HD13	1:C:173:HIS:CE1	2.50	0.47
1:C:383:ALA:O	1:C:387:LEU:HD13	2.14	0.47
1:B:300:VAL:O	1:B:304:LEU:HG	2.15	0.46
1:B:333:LYS:HG2	1:B:337:ASN:ND2	2.30	0.46
1:A:197:LEU:HD13	1:A:218:PHE:CD1	2.51	0.46
1:A:333:LYS:HZ3	1:A:337:ASN:HD21	1.62	0.46
1:C:338:GLU:O	1:C:342:ALA:HB2	2.16	0.46
1:D:357:THR:HG22	1:D:360:HIS:HB2	1.96	0.46
1:A:185:LEU:HD13	1:A:185:LEU:C	2.36	0.46
1:A:195:PRO:HG2	1:A:222:PRO:CD	2.45	0.46
1:C:270:PHE:C	1:C:270:PHE:CD1	2.89	0.46
1:C:57:THR:HG23	1:C:95:LEU:HD22	1.98	0.46
1:B:23:VAL:O	1:B:27:ILE:HG22	2.15	0.46
1:D:264:ARG:HG3	1:D:289:LEU:CD1	2.45	0.46
1:B:366:TYR:OH	1:D:370:ARG:HG3	2.15	0.46
1:D:79:ARG:NH2	1:D:82:GLU:OE2	2.47	0.46
1:A:263:ALA:CB	1:A:344:VAL:HG12	2.46	0.46
1:A:25:PRO:HG2	1:A:26:ARG:H	1.80	0.46
1:A:4:ASP:O	1:A:5:LEU:HB2	2.16	0.46
1:B:159:VAL:HG23	1:B:160:LEU:HD23	1.98	0.46
1:B:77:LEU:HD11	1:B:95:LEU:HD12	1.98	0.46
1:C:277:GLU:N	1:C:277:GLU:OE1	2.44	0.46
1:A:79:ARG:NE	1:A:79:ARG:HA	2.30	0.46
1:B:267:ALA:HB2	1:B:347:CYS:HB3	1.98	0.46
1:A:154:LEU:HD11	1:A:172:VAL:HG21	1.98	0.46
1:B:9:LEU:HD13	1:B:71:TYR:CE2	2.51	0.45
1:C:333:LYS:HA	1:C:336:VAL:HG12	1.98	0.45
1:B:292:ARG:HG2	1:B:292:ARG:NH2	2.31	0.45
1:D:147:ASP:HB3	1:D:153:LEU:HD13	1.98	0.45
1:D:6:ARG:HD3	1:D:297:ARG:HH22	1.80	0.45
1:A:173:HIS:HA	1:A:187:VAL:HG12	1.99	0.45
1:B:20:LEU:O	1:B:24:ILE:HG12	2.17	0.45
1:B:335:THR:HG23	1:B:339:LEU:HD22	1.97	0.45
1:D:228:LEU:CD1	1:D:228:LEU:N	2.78	0.45
1:D:333:LYS:HG2	1:D:337:ASN:HD21	1.80	0.45
1:A:57:THR:HA	1:A:67:LEU:O	2.17	0.45
1:C:99:LEU:HD22	1:C:99:LEU:N	2.32	0.45
1:C:9:LEU:N	1:C:72:ASP:OD1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:GLY:O	1:A:247:VAL:CG1	2.64	0.45
1:A:256:TYR:CE1	1:A:375:MET:HE1	2.51	0.45
1:A:91:TRP:O	1:A:95:LEU:HG	2.16	0.45
1:B:20:LEU:HD13	1:B:53:LEU:HD23	1.98	0.45
1:C:57:THR:HA	1:C:67:LEU:O	2.17	0.45
1:C:291:THR:HG21	1:D:334:MET:HG2	1.98	0.45
1:A:14:ARG:O	1:A:18:ASP:OD2	2.35	0.45
1:A:99:LEU:HD22	1:A:99:LEU:N	2.32	0.45
1:B:384:VAL:CG1	1:B:385:ASP:N	2.79	0.45
1:A:302:ALA:CB	1:B:298:THR:HG23	2.46	0.45
1:B:34:ARG:HG2	1:B:34:ARG:HH21	1.80	0.45
1:B:289:LEU:HD12	1:B:290:ASP:N	2.31	0.45
1:C:201:ASP:CA	1:C:214:LEU:HD22	2.37	0.45
1:D:48:PHE:CE1	1:D:53:LEU:HD22	2.52	0.45
1:B:250:ILE:HG13	1:B:329:PHE:HD2	1.80	0.45
1:B:57:THR:HA	1:B:67:LEU:O	2.17	0.45
1:D:57:THR:HA	1:D:67:LEU:O	2.17	0.45
1:A:19:LEU:HG	1:A:53:LEU:HD11	1.99	0.45
1:C:172:VAL:HG22	1:C:173:HIS:N	2.32	0.45
1:C:213:THR:HG22	1:C:213:THR:O	2.17	0.45
1:D:84:ASP:HB3	1:D:87:THR:OG1	2.17	0.45
1:C:377:PRO:HA	1:C:378:TYR:HA	1.66	0.44
1:D:154:LEU:HB3	1:D:221:CYS:HB2	1.99	0.44
1:D:255:ILE:O	1:D:259:ILE:HG13	2.17	0.44
1:C:291:THR:HA	1:D:331:TYR:CD1	2.52	0.44
1:B:307:ALA:O	1:B:311:SER:HB2	2.17	0.44
1:C:335:THR:O	1:C:339:LEU:HB2	2.17	0.44
1:B:370:ARG:HG3	1:D:366:TYR:CZ	2.52	0.44
1:A:154:LEU:HD11	1:A:172:VAL:CG1	2.46	0.44
1:A:23:VAL:HG12	1:A:23:VAL:O	2.17	0.44
1:A:277:GLU:OE1	1:A:277:GLU:N	2.41	0.44
1:B:264:ARG:HD3	1:B:293:LEU:HD22	1.98	0.44
1:C:133:ALA:HB1	1:C:158:LYS:CG	2.36	0.44
1:C:296:LEU:O	1:C:300:VAL:HG22	2.16	0.44
1:D:198:THR:HB	1:D:217:VAL:HG22	1.99	0.44
1:D:154:LEU:HD22	1:D:218:PHE:CB	2.48	0.44
1:A:224:ARG:N	1:A:224:ARG:HD3	2.32	0.44
1:B:172:VAL:CG2	1:B:173:HIS:N	2.81	0.44
1:B:260:ALA:HB1	1:B:343:VAL:HG21	1.99	0.44
1:C:109:THR:HB	1:C:111:PRO:HD2	1.99	0.44
1:B:97:ARG:HH21	1:B:171:PHE:HB2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:LEU:HD13	1:C:185:LEU:C	2.37	0.44
1:C:296:LEU:CD1	1:C:336:VAL:HA	2.48	0.44
1:A:250:ILE:HA	1:A:329:PHE:CE2	2.53	0.44
1:A:279:ARG:O	1:A:283:ARG:HG3	2.17	0.44
1:C:173:HIS:HA	1:C:187:VAL:HG12	2.00	0.44
1:A:360:HIS:ND1	1:A:361:PRO:CD	2.80	0.44
1:B:384:VAL:HG13	1:B:385:ASP:N	2.33	0.44
1:C:250:ILE:CA	1:C:329:PHE:CE2	2.91	0.44
1:D:97:ARG:HG2	1:D:130:VAL:HG21	2.00	0.44
1:A:119:LEU:HD11	1:A:189:VAL:HG11	1.99	0.43
1:A:225:ALA:O	1:A:228:LEU:HD13	2.18	0.43
1:B:192:ARG:HH11	1:B:192:ARG:HG2	1.83	0.43
1:A:204:ASP:OD2	1:C:358:ALA:HB3	2.18	0.43
1:D:115:MET:C	1:D:115:MET:SD	2.97	0.43
1:D:377:PRO:HA	1:D:378:TYR:HA	1.68	0.43
1:A:264:ARG:HA	1:A:347:CYS:SG	2.58	0.43
1:A:41:PRO:O	1:A:45:PHE:HB2	2.17	0.43
1:A:61:GLU:HG3	1:A:62:LEU:CD2	2.48	0.43
1:B:264:ARG:HG3	1:B:289:LEU:HD13	2.00	0.43
1:C:86:SER:OG	1:C:208:MET:HA	2.18	0.43
1:C:215:GLU:HG2	1:C:216:VAL:N	2.33	0.43
1:D:223:VAL:HG22	1:D:228:LEU:HD11	1.98	0.43
1:D:357:THR:HG23	1:D:360:HIS:N	2.28	0.43
1:D:41:PRO:O	1:D:45:PHE:HB2	2.18	0.43
1:B:160:LEU:HA	1:B:213:THR:HG23	2.00	0.43
1:D:207:GLY:O	1:D:208:MET:HB2	2.17	0.43
1:D:59:PRO:HD2	1:D:120:LEU:HD21	2.00	0.43
1:A:264:ARG:HG3	1:A:289:LEU:HD11	1.99	0.43
1:A:366:TYR:OH	1:C:370:ARG:HG3	2.19	0.43
1:A:386:TYR:HD2	1:A:387:LEU:HD13	1.82	0.43
1:B:186:ALA:C	1:B:188:PRO:HD3	2.38	0.43
1:B:255:ILE:HG13	1:B:256:TYR:N	2.33	0.43
1:A:358:ALA:HB3	1:C:204:ASP:OD2	2.18	0.43
1:C:70:LEU:HD22	1:C:251:THR:HG23	2.00	0.43
1:A:119:LEU:O	1:A:123:MET:HG2	2.18	0.43
1:A:327:THR:HG22	1:A:331:TYR:CE2	2.54	0.43
1:C:209:ARG:HG2	1:C:209:ARG:HH21	1.83	0.43
1:C:255:ILE:HD12	1:C:255:ILE:C	2.39	0.43
1:C:384:VAL:HG13	1:C:385:ASP:N	2.34	0.43
1:D:109:THR:HB	1:D:111:PRO:HD2	1.99	0.43
1:D:34:ARG:NH2	1:D:34:ARG:HG2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:ARG:HG2	1:A:292:ARG:NH2	2.32	0.43
1:C:283:ARG:NH2	1:D:394:LEU:CD2	2.81	0.43
1:D:187:VAL:HG23	1:D:229:LEU:HB3	2.00	0.43
1:D:296:LEU:O	1:D:300:VAL:HG13	2.19	0.43
1:A:320:GLU:OE2	1:A:323:ARG:NH1	2.51	0.43
1:A:8:PRO:HB2	1:A:72:ASP:OD1	2.19	0.43
1:D:147:ASP:HB3	1:D:153:LEU:HD11	2.01	0.43
1:D:164:ALA:O	1:D:167:ALA:HB3	2.19	0.43
1:D:131:CYS:HB2	1:D:170:PHE:CD1	2.54	0.43
1:D:48:PHE:HD1	1:D:53:LEU:HD22	1.83	0.43
1:A:62:LEU:HD21	1:A:105:TRP:CH2	2.53	0.43
1:B:128:ALA:HB1	1:B:169:HIS:CD2	2.54	0.43
1:C:57:THR:HB	1:C:99:LEU:HD22	1.99	0.43
1:A:23:VAL:O	1:A:27:ILE:HG22	2.18	0.43
1:B:62:LEU:HD21	1:B:105:TRP:CZ2	2.54	0.43
1:B:51:LEU:HD12	1:B:51:LEU:N	2.34	0.43
1:C:360:HIS:ND1	1:C:362:LEU:HB2	2.34	0.43
1:D:185:LEU:HD12	1:D:231:ARG:HD2	2.01	0.43
1:D:164:ALA:CB	1:D:214:LEU:HD12	2.45	0.43
1:A:296:LEU:CD1	1:A:336:VAL:HG23	2.28	0.42
1:A:370:ARG:NH2	1:C:345:ASP:OD1	2.52	0.42
1:A:89:LEU:HD12	1:A:252:MET:HE2	2.01	0.42
1:A:8:PRO:HG3	1:A:17:VAL:CG2	2.38	0.42
1:B:5:LEU:HD23	1:B:71:TYR:CE1	2.54	0.42
1:D:147:ASP:OD1	1:D:149:ALA:N	2.52	0.42
1:B:329:PHE:CE1	1:B:330:GLN:NE2	2.87	0.42
1:C:332:ALA:O	1:C:336:VAL:HG12	2.18	0.42
1:D:174:ALA:O	1:D:185:LEU:HD22	2.19	0.42
1:D:384:VAL:CG1	1:D:385:ASP:N	2.82	0.42
1:C:164:ALA:H	1:C:165:PRO:HD2	1.82	0.42
1:A:20:LEU:HD13	1:A:53:LEU:CD2	2.50	0.42
1:B:128:ALA:HB1	1:B:169:HIS:HD2	1.84	0.42
1:B:34:ARG:HG2	1:B:34:ARG:NH2	2.34	0.42
1:A:56:ALA:O	1:A:58:VAL:HG23	2.19	0.42
1:B:134:LEU:HA	1:B:173:HIS:CD2	2.54	0.42
1:B:334:MET:HA	1:B:334:MET:CE	2.49	0.42
1:C:194:ALA:HB3	1:C:197:LEU:HB2	2.01	0.42
1:B:41:PRO:O	1:B:45:PHE:HB2	2.20	0.42
1:B:306:ASN:ND2	1:B:328:PRO:HG3	2.34	0.42
1:C:141:VAL:O	1:C:142:THR:C	2.58	0.42
1:C:170:PHE:HB2	1:C:190:VAL:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:ASP:HB3	1:D:331:TYR:HE1	1.82	0.42
1:C:34:ARG:HG2	1:C:34:ARG:NH2	2.34	0.42
1:D:260:ALA:HB1	1:D:343:VAL:HG21	2.02	0.42
1:A:386:TYR:CD2	1:A:387:LEU:CD1	3.03	0.42
1:A:370:ARG:HD2	1:C:345:ASP:OD1	2.20	0.42
1:A:80:LEU:HD23	1:A:88:ALA:HA	2.01	0.42
1:B:242:LEU:HD22	1:B:326:MET:HE3	2.01	0.42
1:C:171:PHE:HE1	1:C:187:VAL:HG23	1.85	0.42
1:C:195:PRO:CG	1:C:222:PRO:HD2	2.50	0.42
1:D:199:VAL:HG13	1:D:199:VAL:O	2.20	0.42
1:D:62:LEU:HD21	1:D:105:TRP:CH2	2.55	0.42
1:B:91:TRP:O	1:B:95:LEU:HG	2.19	0.42
1:B:91:TRP:CZ2	1:B:95:LEU:HD11	2.55	0.42
1:C:80:LEU:HD23	1:C:88:ALA:CA	2.47	0.42
1:B:370:ARG:HD3	1:D:348:LEU:HD23	2.01	0.42
1:D:57:THR:HB	1:D:99:LEU:HD22	2.01	0.42
1:B:195:PRO:HG3	1:B:222:PRO:HG3	2.01	0.41
1:D:6:ARG:HA	1:D:6:ARG:HD2	1.77	0.41
1:A:192:ARG:O	1:A:197:LEU:HD23	2.20	0.41
1:A:256:TYR:HE1	1:A:375:MET:HE1	1.84	0.41
1:A:333:LYS:O	1:A:336:VAL:HG12	2.21	0.41
1:B:203:TRP:HB2	1:B:213:THR:O	2.20	0.41
1:A:307:ALA:O	1:A:311:SER:HB2	2.20	0.41
1:B:162:SER:HA	1:B:213:THR:HA	2.01	0.41
1:B:199:VAL:HG13	1:B:199:VAL:O	2.20	0.41
1:B:62:LEU:HD21	1:B:105:TRP:CH2	2.55	0.41
1:C:48:PHE:HD1	1:C:53:LEU:HD22	1.85	0.41
1:C:59:PRO:CD	1:C:120:LEU:HD21	2.50	0.41
1:B:10:THR:O	1:B:14:ARG:HG3	2.21	0.41
1:C:62:LEU:HD21	1:C:105:TRP:CZ2	2.54	0.41
1:D:306:ASN:ND2	1:D:328:PRO:HG3	2.36	0.41
1:B:366:TYR:CZ	1:D:370:ARG:HG3	2.55	0.41
1:D:372:GLY:HA2	1:D:375:MET:HE2	2.02	0.41
1:D:264:ARG:HD2	1:D:290:ASP:OD2	2.20	0.41
1:D:274:ARG:NE	1:D:274:ARG:HA	2.36	0.41
1:A:209:ARG:HH21	1:A:209:ARG:HG2	1.86	0.41
1:C:24:ILE:N	1:C:25:PRO:HD2	2.36	0.41
1:C:339:LEU:HA	1:C:339:LEU:HD12	1.89	0.41
1:C:97:ARG:HH11	1:C:97:ARG:HG3	1.84	0.41
1:A:86:SER:HB3	1:A:210:ALA:HB3	2.03	0.41
1:A:296:LEU:HD13	1:A:336:VAL:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:THR:HG22	1:C:72:ASP:OD1	2.21	0.41
1:B:274:ARG:NE	1:B:274:ARG:HA	2.35	0.41
1:B:327:THR:HB	1:B:328:PRO:CD	2.51	0.41
1:D:173:HIS:HA	1:D:187:VAL:HG12	2.03	0.41
1:B:356:TYR:CE1	1:D:206:LEU:HB3	2.56	0.41
1:A:255:ILE:O	1:A:259:ILE:HG13	2.21	0.41
1:A:377:PRO:HA	1:A:378:TYR:HA	1.67	0.41
1:C:330:GLN:HB3	1:C:387:LEU:HD11	2.03	0.41
1:A:384:VAL:HG13	1:A:385:ASP:N	2.36	0.41
1:C:292:ARG:CG	1:C:292:ARG:NH2	2.78	0.41
1:C:9:LEU:HD12	1:C:9:LEU:N	2.36	0.40
1:D:206:LEU:O	1:D:367:ARG:NH2	2.43	0.40
1:A:43:GLU:CD	1:A:43:GLU:H	2.24	0.40
1:B:133:ALA:HB1	1:B:158:LYS:CB	2.51	0.40
1:A:187:VAL:CG2	1:A:229:LEU:HD23	2.51	0.40
1:D:15:THR:O	1:D:19:LEU:HG	2.21	0.40
1:A:255:ILE:C	1:A:255:ILE:HD12	2.42	0.40
1:D:40:PHE:CD1	1:D:41:PRO:HD2	2.57	0.40
1:D:197:LEU:HD13	1:D:218:PHE:CD1	2.57	0.40
1:D:34:ARG:NH1	1:D:43:GLU:OE2	2.54	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	392/395 (99%)	353 (90%)	35 (9%)	4 (1%)	15	51
1	B	362/395 (92%)	331 (91%)	28 (8%)	3 (1%)	19	55
1	C	359/395 (91%)	327 (91%)	31 (9%)	1 (0%)	41	73
1	D	385/395 (98%)	354 (92%)	29 (8%)	2 (0%)	29	65
All	All	1498/1580 (95%)	1365 (91%)	123 (8%)	10 (1%)	22	59

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	VAL
1	A	313	ASP
1	B	2	ALA
1	B	220	ARG
1	A	63	GLY
1	B	63	GLY
1	C	63	GLY
1	D	63	GLY
1	A	138	PRO
1	D	223	VAL

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	274/290 (94%)	260 (95%)	14 (5%)	24	56
1	B	259/290 (89%)	246 (95%)	13 (5%)	24	57
1	C	258/290 (89%)	247 (96%)	11 (4%)	29	62
1	D	275/290 (95%)	261 (95%)	14 (5%)	24	56
All	All	1066/1160 (92%)	1014 (95%)	52 (5%)	25	59

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	97	ARG
1	A	115	MET
1	A	153	LEU
1	A	201	ASP
1	A	216	VAL
1	A	255	ILE
1	A	277	GLU
1	A	305	THR
1	A	321	ARG

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Mol	Chain	Res	Type
1	A	329	PHE
1	A	334	MET
1	A	370	ARG
1	A	385	ASP
1	B	1	MET
1	B	45	PHE
1	B	97	ARG
1	B	115	MET
1	B	152	TRP
1	B	154	LEU
1	B	224	ARG
1	B	228	LEU
1	B	255	ILE
1	B	321	ARG
1	B	334	MET
1	B	370	ARG
1	B	385	ASP
1	C	14	ARG
1	C	33	ASP
1	C	54	MET
1	C	97	ARG
1	C	171	PHE
1	C	224	ARG
1	C	249	SER
1	C	264	ARG
1	C	321	ARG
1	C	334	MET
1	C	370	ARG
1	D	1	MET
1	D	43	GLU
1	D	45	PHE
1	D	69	ARG
1	D	72	ASP
1	D	87	THR
1	D	97	ARG
1	D	216	VAL
1	D	255	ILE
1	D	321	ARG
1	D	329	PHE
1	D	334	MET
1	D	370	ARG
1	D	385	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	169	HIS
1	A	175	GLN
1	A	245	GLN
1	A	337	ASN
1	A	376	GLN
1	B	169	HIS
1	B	173	HIS
1	B	306	ASN
1	B	337	ASN
1	B	376	GLN
1	B	390	GLN
1	C	92	HIS
1	C	169	HIS
1	C	175	GLN
1	C	306	ASN
1	C	337	ASN
1	C	376	GLN
1	C	390	GLN
1	D	169	HIS
1	D	175	GLN
1	D	245	GLN
1	D	306	ASN
1	D	337	ASN
1	D	376	GLN
1	D	390	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)

There are no chain breaks in this entry.

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	394/395 (99%)	0.02	4 (1%)	82	73	79, 105, 151, 164	0
1	B	370/395 (93%)	0.18	17 (4%)	32	18	77, 119, 158, 189	0
1	C	369/395 (93%)	0.17	8 (2%)	62	47	77, 120, 156, 177	0
1	D	391/395 (98%)	0.06	13 (3%)	46	29	74, 110, 149, 169	0
All	All	1524/1580 (96%)	0.11	42 (2%)	53	36	74, 114, 154, 189	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	235	GLY	4.2
1	C	183	VAL	4.1
1	B	222	PRO	4.0
1	D	236	ALA	3.9
1	B	140	VAL	3.9
1	B	175	GLN	3.7
1	B	313	ASP	3.5
1	B	394	LEU	3.4
1	D	150	GLY	3.3
1	D	183	VAL	3.3
1	B	227	GLU	3.2
1	B	218	PHE	3.2
1	C	216	VAL	3.1
1	D	123	MET	3.1
1	B	170	PHE	3.0
1	B	66	GLY	3.0
1	B	65	LEU	3.0
1	C	184	PHE	2.9
1	A	182	SER	2.8
1	B	312	VAL	2.7
1	D	276	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	200	LEU	2.6
1	D	149	ALA	2.5
1	C	215	GLU	2.5
1	D	182	SER	2.5
1	B	157	ARG	2.4
1	A	3	ALA	2.4
1	B	105	TRP	2.4
1	D	119	LEU	2.4
1	C	197	LEU	2.3
1	B	156	GLY	2.3
1	B	153	LEU	2.2
1	D	151	GLY	2.2
1	A	149	ALA	2.2
1	B	215	GLU	2.2
1	C	12	ALA	2.2
1	D	234	VAL	2.2
1	C	175	GLN	2.1
1	A	2	ALA	2.1
1	D	66	GLY	2.1
1	D	122	ALA	2.0
1	C	394	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.