Full wwPDB X-ray Structure Validation Report (i)

Sep 10, 2023 – 07:26 AM EDT

PDB ID	:	4IN3
Title	:	Crystal Structure of the Chs5-Bch1 Exomer Cargo Adaptor Complex
Authors	:	Richardson, B.C.; Fromme, J.C.
Deposited on	:	2013-01-03
Resolution	:	2.94 Å(reported)

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

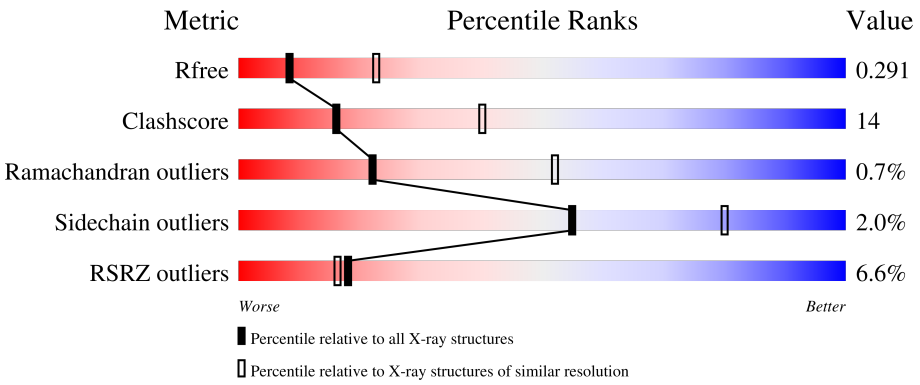
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.94 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	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	82	% 76% 21% • •
1	C	82	78% 13% 9%
2	B	739	7% 59% 20% • 20%
2	D	739	6% 62% 22% • 14%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11087 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 Chitin biosynthesis protein CHS5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	80	631	402	105	122	2	0	0	0
1	C	75	588	374	100	113	1	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	MET	-	expression tag	UNP Q12114
A	-3	ASP	-	expression tag	UNP Q12114
A	-2	PRO	-	expression tag	UNP Q12114
A	-1	GLU	-	expression tag	UNP Q12114
A	0	PHE	-	expression tag	UNP Q12114
C	-4	MET	-	expression tag	UNP Q12114
C	-3	ASP	-	expression tag	UNP Q12114
C	-2	PRO	-	expression tag	UNP Q12114
C	-1	GLU	-	expression tag	UNP Q12114
C	0	PHE	-	expression tag	UNP Q12114

- Molecule 2 is a protein called Protein BCH1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	589	4758	3065	781	890	22	0	0	0
2	D	632	5092	3276	836	956	24	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	725	GLY	-	expression tag	UNP Q05029
B	726	THR	-	expression tag	UNP Q05029

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Chain	Residue	Modelled	Actual	Comment	Reference
B	727	GLU	-	expression tag	UNP Q05029
B	728	ASN	-	expression tag	UNP Q05029
B	729	LEU	-	expression tag	UNP Q05029
B	730	TYR	-	expression tag	UNP Q05029
B	731	PHE	-	expression tag	UNP Q05029
B	732	GLN	-	expression tag	UNP Q05029
B	733	GLY	-	expression tag	UNP Q05029
B	734	HIS	-	expression tag	UNP Q05029
B	735	HIS	-	expression tag	UNP Q05029
B	736	HIS	-	expression tag	UNP Q05029
B	737	HIS	-	expression tag	UNP Q05029
B	738	HIS	-	expression tag	UNP Q05029
B	739	HIS	-	expression tag	UNP Q05029
D	725	GLY	-	expression tag	UNP Q05029
D	726	THR	-	expression tag	UNP Q05029
D	727	GLU	-	expression tag	UNP Q05029
D	728	ASN	-	expression tag	UNP Q05029
D	729	LEU	-	expression tag	UNP Q05029
D	730	TYR	-	expression tag	UNP Q05029
D	731	PHE	-	expression tag	UNP Q05029
D	732	GLN	-	expression tag	UNP Q05029
D	733	GLY	-	expression tag	UNP Q05029
D	734	HIS	-	expression tag	UNP Q05029
D	735	HIS	-	expression tag	UNP Q05029
D	736	HIS	-	expression tag	UNP Q05029
D	737	HIS	-	expression tag	UNP Q05029
D	738	HIS	-	expression tag	UNP Q05029
D	739	HIS	-	expression tag	UNP Q05029

- Molecule 3 is water.

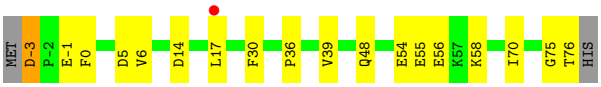
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	2	2	2	0	0
			Total	O		
3	B	9	9	9	0	0
			Total	O		
3	C	1	1	1	0	0
			Total	O		
3	D	6	6	6	0	0

3 Residue-property plots (i)

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

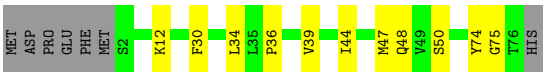
• Molecule 1: Chitin biosynthesis protein CHS5

Chain A:



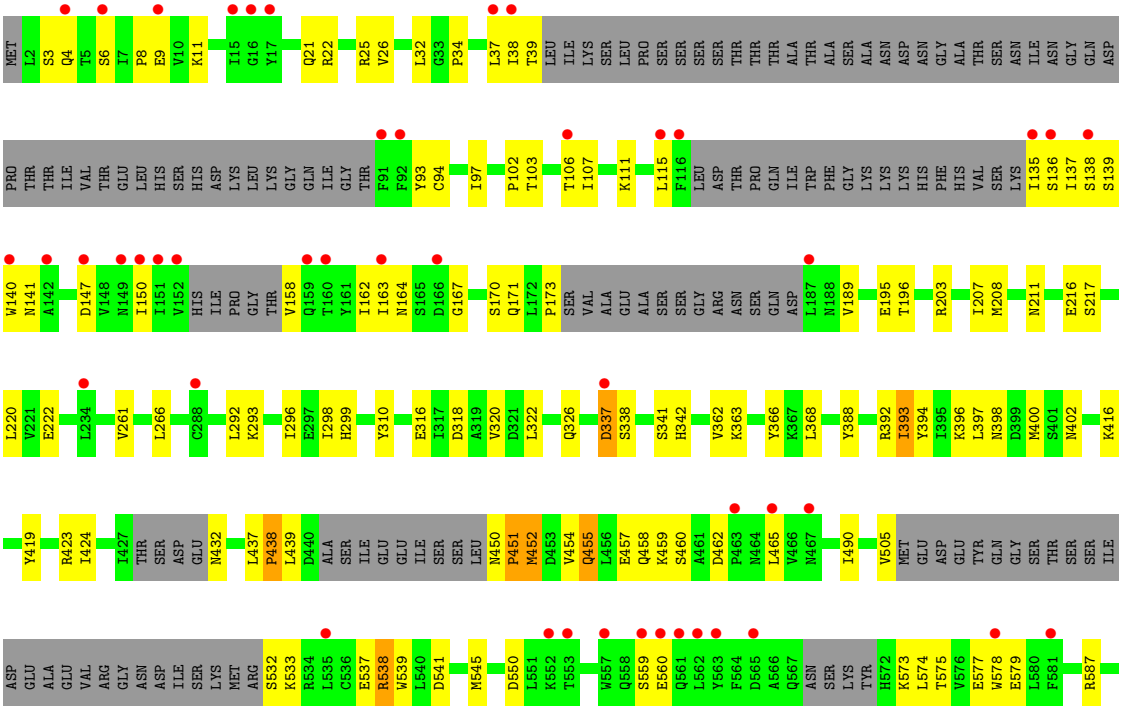
• Molecule 1: Chitin biosynthesis protein CHS5

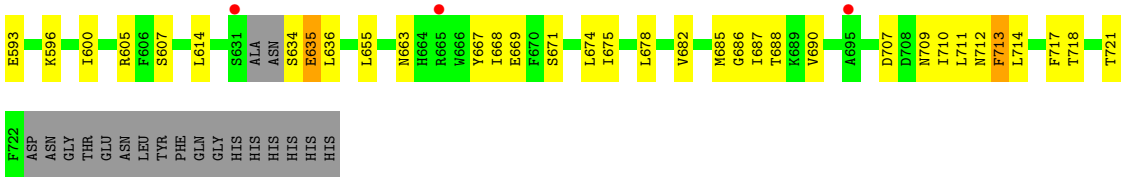
Chain C:



• Molecule 2: Protein BCH1

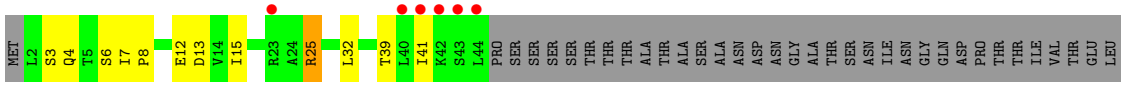
Chain B:

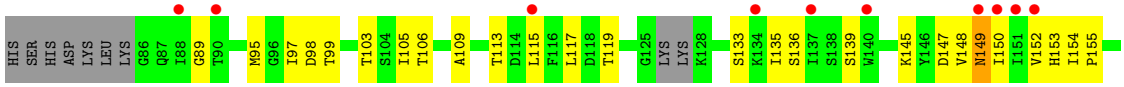


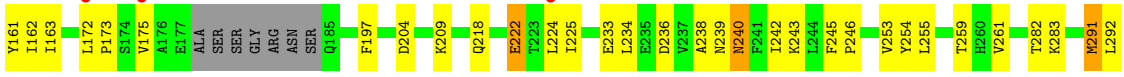


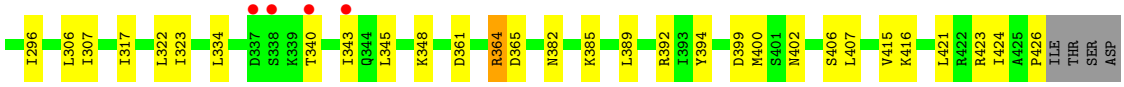
• Molecule 2: Protein BCH1

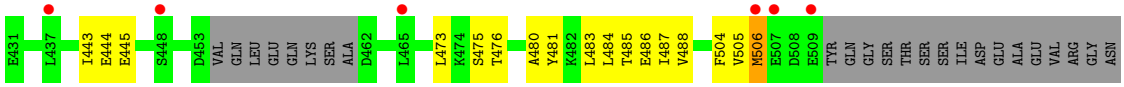
Chain D:

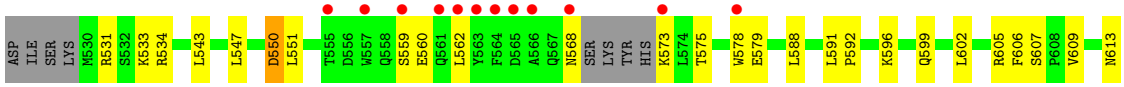


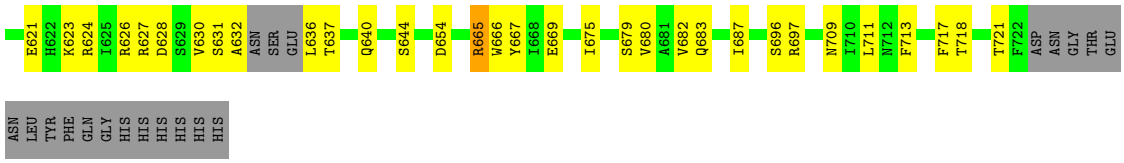












4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	141.39Å 155.69Å 99.05Å 90.00° 95.34° 90.00°	Depositor
Resolution (Å)	38.73 – 2.94 49.31 – 2.94	Depositor EDS
% Data completeness (in resolution range)	95.9 (38.73-2.94) 90.0 (49.31-2.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.93 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.237 , 0.289 0.238 , 0.291	Depositor DCC
R_{free} test set	2309 reflections (5.28%)	wwPDB-VP
Wilson B-factor (Å^2)	65.7	Xtriage
Anisotropy	0.618	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 71.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11087	wwPDB-VP
Average B, all atoms (Å^2)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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	0.26	0/640	0.49	0/863
1	C	0.26	0/595	0.47	0/802
2	B	0.29	0/4845	0.48	0/6560
2	D	0.27	0/5188	0.47	0/7026
All	All	0.27	0/11268	0.48	0/15251

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	631	0	653	14	0
1	C	588	0	615	9	0
2	B	4758	0	4801	153	0
2	D	5092	0	5125	155	0
3	A	2	0	0	0	0
3	B	9	0	0	0	0
3	C	1	0	0	0	0
3	D	6	0	0	0	0
All	All	11087	0	11194	322	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 14.

All (322) 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)
2:D:154:ILE:CG2	2:D:155:PRO:HD3	1.68	1.22
2:D:245:PHE:HB3	2:D:291:MET:HE1	1.24	1.13
2:B:450:ASN:CB	2:B:451:PRO:HD3	1.80	1.11
2:B:450:ASN:HB3	2:B:451:PRO:HD3	1.28	1.10
2:B:450:ASN:CB	2:B:451:PRO:CD	2.30	1.09
2:D:154:ILE:HG22	2:D:155:PRO:HD3	1.16	1.09
2:B:538:ARG:HH11	2:B:538:ARG:HA	1.14	1.09
2:D:665:ARG:HG3	2:D:665:ARG:HH11	1.18	1.07
2:D:443:ILE:HG22	2:D:444:GLU:H	1.25	1.01
2:B:450:ASN:HB2	2:B:451:PRO:CD	1.90	1.00
2:D:153:HIS:HB3	2:D:155:PRO:HD2	1.45	0.96
2:B:678:LEU:HD23	2:B:710:ILE:HG22	1.48	0.96
2:B:682:VAL:HG13	2:B:687:ILE:HG22	1.45	0.96
2:B:450:ASN:HB2	2:B:451:PRO:HD2	1.46	0.94
2:B:362:VAL:HG23	2:B:363:LYS:HG2	1.49	0.94
2:D:682:VAL:CG1	2:D:687:ILE:HG12	1.98	0.94
2:B:538:ARG:HA	2:B:538:ARG:NH1	1.83	0.93
2:B:457:GLU:HG2	2:B:458:GLN:H	1.31	0.93
2:B:366:TYR:CE1	2:B:396:LYS:HG2	2.04	0.93
2:B:298:ILE:HG23	2:B:299:HIS:ND1	1.86	0.90
2:D:443:ILE:HG22	2:D:444:GLU:N	1.82	0.89
2:D:682:VAL:CG1	2:D:687:ILE:CG1	2.50	0.89
2:D:443:ILE:CG2	2:D:444:GLU:H	1.86	0.88
2:D:154:ILE:CG2	2:D:155:PRO:CD	2.51	0.88
2:B:451:PRO:N	2:B:452:MET:HE1	1.91	0.86
2:D:245:PHE:HB3	2:D:291:MET:CE	2.05	0.86
2:B:686:GLY:O	2:B:690:VAL:HG23	1.75	0.85
2:D:505:VAL:O	2:D:506:MET:HG2	1.75	0.85
2:D:682:VAL:HG13	2:D:687:ILE:CG1	2.06	0.85
2:B:678:LEU:HD23	2:B:710:ILE:CG2	2.06	0.85
2:D:245:PHE:CB	2:D:291:MET:HE1	2.07	0.85
2:D:682:VAL:HG11	2:D:687:ILE:HG12	1.59	0.84
2:D:399:ASP:HB3	2:D:402:ASN:HB2	1.61	0.82
2:B:682:VAL:CG1	2:B:687:ILE:HG22	2.08	0.82
2:B:682:VAL:HG13	2:B:687:ILE:CG2	2.09	0.82
2:B:94:CYS:SG	2:B:97:ILE:HD11	2.20	0.82
2:D:154:ILE:HG23	2:D:155:PRO:HD3	1.61	0.81
2:D:148:VAL:HG22	2:D:162:ILE:HG12	1.62	0.81
2:D:665:ARG:HG3	2:D:665:ARG:NH1	1.87	0.81
2:B:459:LYS:NZ	2:B:605:ARG:NH1	2.29	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:LEU:HD12	2:B:93:TYR:HE2	1.45	0.80
2:B:457:GLU:HG2	2:B:458:GLN:N	1.97	0.80
2:B:437:LEU:HD12	2:B:438:PRO:HD2	1.63	0.80
2:D:6:SER:O	2:D:224:LEU:HD13	1.82	0.79
2:B:634:SER:O	2:B:635:GLU:HB2	1.83	0.79
2:D:39:THR:HB	2:D:136:SER:OG	1.82	0.79
2:D:506:MET:HE1	2:D:533:LYS:HE2	1.65	0.79
2:B:397:LEU:O	2:B:398:ASN:HB3	1.81	0.78
2:D:573:LYS:HB2	2:D:578:TRP:HE1	1.48	0.77
2:D:99:THR:OG1	2:D:197:PHE:HA	1.84	0.76
2:D:506:MET:CE	2:D:533:LYS:HE2	2.16	0.76
1:A:36:PRO:HD2	1:A:39:VAL:HG21	1.67	0.76
2:B:459:LYS:HZ1	2:B:605:ARG:HH12	1.32	0.76
2:D:631:SER:O	2:D:632:ALA:HB3	1.87	0.74
2:D:626:ARG:O	2:D:630:VAL:HG23	1.88	0.73
2:D:154:ILE:HG22	2:D:155:PRO:CD	2.07	0.73
2:D:443:ILE:CG2	2:D:444:GLU:N	2.48	0.73
2:B:439:LEU:O	2:B:439:LEU:HG	1.89	0.72
2:D:113:THR:O	2:D:117:LEU:HD23	1.90	0.71
2:B:394:TYR:HA	2:B:397:LEU:HD12	1.73	0.71
2:D:245:PHE:CD2	2:D:291:MET:CE	2.74	0.71
2:D:682:VAL:CG1	2:D:687:ILE:HG13	2.19	0.71
2:B:685:MET:HE2	2:B:690:VAL:HA	1.71	0.70
2:B:393:ILE:O	2:B:397:LEU:HG	1.91	0.70
2:B:292:LEU:O	2:B:296:ILE:HG13	1.91	0.70
2:D:224:LEU:HD12	2:D:667:TYR:O	1.92	0.69
2:B:707:ASP:O	2:B:712:ASN:N	2.24	0.69
2:B:32:LEU:O	2:B:203:ARG:NH1	2.26	0.69
2:D:682:VAL:HG13	2:D:687:ILE:HG13	1.71	0.69
2:D:154:ILE:N	2:D:155:PRO:CD	2.56	0.69
1:A:56:GLU:HG3	1:C:44:ILE:HG12	1.73	0.69
2:D:245:PHE:CD2	2:D:291:MET:HE1	2.28	0.68
2:D:233:GLU:O	2:D:234:LEU:HG	1.94	0.68
2:D:154:ILE:HG23	2:D:155:PRO:CD	2.22	0.67
2:B:137:ILE:HG13	2:B:150:ILE:HG22	1.77	0.67
2:B:459:LYS:HZ3	2:B:605:ARG:NH1	1.92	0.66
2:D:475:SER:OG	2:D:476:THR:N	2.28	0.66
2:B:37:LEU:HD12	2:B:93:TYR:CE2	2.28	0.66
2:B:162:ILE:HB	2:B:170:SER:HB3	1.78	0.65
2:D:3:SER:HA	2:D:115:LEU:HD13	1.78	0.65
2:B:459:LYS:NZ	2:B:605:ARG:HH12	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:149:ASN:OD1	2:D:149:ASN:N	2.30	0.64
2:B:164:ASN:OD1	2:B:167:GLY:N	2.30	0.64
2:D:682:VAL:HG13	2:D:687:ILE:HG12	1.66	0.64
2:B:459:LYS:HZ3	2:B:605:ARG:HH11	1.42	0.64
2:B:462:ASP:HB3	2:B:465:LEU:HB2	1.79	0.64
2:D:573:LYS:HB2	2:D:578:TRP:NE1	2.12	0.64
1:A:-3:ASP:OD2	1:A:-3:ASP:N	2.30	0.63
2:B:721:THR:O	2:B:721:THR:HG22	1.96	0.63
2:D:340:THR:O	2:D:343:ILE:HG22	1.97	0.63
1:A:48:GLN:HB2	1:C:48:GLN:HB3	1.81	0.62
2:B:537:GLU:O	2:B:538:ARG:HB2	1.98	0.62
2:B:459:LYS:HD2	2:B:574:LEU:HD22	1.82	0.62
2:B:38:ILE:HG12	2:B:137:ILE:HG22	1.81	0.61
1:C:75:GLY:HA2	2:D:317:ILE:HG23	1.82	0.61
2:D:154:ILE:N	2:D:155:PRO:HD2	2.15	0.61
2:D:682:VAL:HG11	2:D:687:ILE:CG1	2.25	0.61
2:B:634:SER:O	2:B:635:GLU:CB	2.48	0.61
2:B:38:ILE:HG23	2:B:137:ILE:HG22	1.83	0.60
2:B:538:ARG:O	2:B:541:ASP:N	2.34	0.60
2:D:631:SER:O	2:D:632:ALA:CB	2.50	0.60
2:D:245:PHE:CD2	2:D:291:MET:HE3	2.37	0.60
1:A:14:ASP:HB3	1:A:17:LEU:H	1.67	0.60
2:D:550:ASP:HB3	2:D:588:LEU:HD21	1.84	0.59
2:B:452:MET:SD	2:B:452:MET:N	2.76	0.59
2:D:443:ILE:HG22	2:D:444:GLU:CD	2.23	0.59
2:B:137:ILE:CG1	2:B:150:ILE:CG2	2.81	0.59
2:D:445:GLU:HG3	2:D:606:PHE:HB2	1.85	0.59
2:B:102:PRO:O	2:B:106:THR:HG23	2.02	0.59
2:B:316:GLU:O	2:B:320:VAL:HG23	2.03	0.59
2:B:636:LEU:N	2:B:636:LEU:HD12	2.18	0.59
2:B:537:GLU:O	2:B:538:ARG:CB	2.50	0.58
2:D:627:ARG:O	2:D:630:VAL:HB	2.03	0.58
1:C:36:PRO:O	2:D:531:ARG:NH2	2.35	0.58
2:D:6:SER:O	2:D:224:LEU:CD1	2.51	0.58
2:D:139:SER:O	2:D:147:ASP:OD1	2.22	0.58
2:D:282:THR:HA	2:D:718:THR:HG22	1.83	0.58
2:D:361:ASP:OD1	2:D:392:ARG:NH2	2.35	0.58
2:B:135:ILE:HG13	2:B:135:ILE:O	2.03	0.58
2:D:95:MET:HE1	2:D:421:LEU:HD11	1.85	0.58
2:D:172:LEU:HD12	2:D:173:PRO:HD2	1.86	0.57
2:D:240:ASN:HA	2:D:243:LYS:HE2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:SER:O	2:B:4:GLN:HB2	2.04	0.57
2:D:245:PHE:HD2	2:D:291:MET:CE	2.17	0.57
2:B:541:ASP:O	2:B:545:MET:HG2	2.05	0.57
2:D:505:VAL:HG13	2:D:534:ARG:O	2.05	0.57
2:B:366:TYR:CZ	2:B:396:LYS:HG2	2.41	0.56
2:B:459:LYS:HZ1	2:B:605:ARG:NH1	1.93	0.56
2:D:340:THR:OG1	2:D:343:ILE:HG22	2.05	0.56
2:D:665:ARG:HH11	2:D:665:ARG:CG	2.02	0.56
2:B:158:VAL:HG23	2:B:158:VAL:O	2.05	0.56
2:B:293:LYS:HA	2:B:296:ILE:HD12	1.86	0.56
2:D:400:MET:SD	2:D:487:ILE:HG22	2.45	0.56
1:C:74:TYR:OH	2:D:365:ASP:OD1	2.23	0.56
2:D:696:SER:OG	2:D:697:ARG:N	2.39	0.56
2:B:173:PRO:HG2	2:B:189:VAL:HG21	1.87	0.56
2:B:173:PRO:HG2	2:B:189:VAL:CG2	2.35	0.55
2:B:713:PHE:O	2:B:717:PHE:N	2.39	0.55
2:B:397:LEU:O	2:B:398:ASN:CB	2.54	0.55
2:B:538:ARG:HH12	2:B:541:ASP:HB3	1.71	0.55
2:D:259:THR:HA	2:D:416:LYS:HE2	1.88	0.55
2:D:4:GLN:NE2	2:D:119:THR:O	2.40	0.55
2:D:25:ARG:HH22	2:D:426:PRO:HD3	1.72	0.55
1:A:5:ASP:OD1	1:A:48:GLN:HG2	2.07	0.54
2:B:682:VAL:CG1	2:B:687:ILE:CG2	2.76	0.54
2:B:207:ILE:O	2:B:211:ASN:ND2	2.35	0.54
2:D:443:ILE:CG2	2:D:444:GLU:OE1	2.56	0.54
2:D:6:SER:HA	2:D:667:TYR:HD1	1.71	0.54
2:B:111:LYS:O	2:B:115:LEU:HG	2.07	0.54
2:B:8:PRO:O	2:B:9:GLU:HG3	2.07	0.54
2:B:203:ARG:HG2	2:B:419:TYR:OH	2.08	0.54
1:A:-3:ASP:O	1:A:0:PHE:N	2.33	0.53
1:A:6:VAL:HG21	1:C:34:LEU:HG	1.90	0.53
2:D:13:ASP:OD1	2:D:13:ASP:N	2.39	0.53
2:B:94:CYS:SG	2:B:97:ILE:CD1	2.95	0.53
2:D:609:VAL:O	2:D:613:ASN:ND2	2.34	0.53
2:B:678:LEU:CD2	2:B:710:ILE:CG2	2.84	0.53
2:D:97:ILE:HG22	2:D:98:ASP:N	2.23	0.53
2:B:458:GLN:O	2:B:458:GLN:HG3	2.09	0.53
2:B:678:LEU:O	2:B:682:VAL:HG23	2.09	0.53
2:D:636:LEU:CD1	2:D:636:LEU:N	2.72	0.52
2:D:636:LEU:N	2:D:636:LEU:HD12	2.24	0.52
2:B:400:MET:CE	2:B:490:ILE:HG21	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:675:ILE:O	2:D:679:SER:OG	2.21	0.52
1:A:36:PRO:CD	1:A:39:VAL:HG21	2.40	0.52
2:B:687:ILE:HG13	2:B:688:THR:N	2.25	0.52
2:D:25:ARG:NE	2:D:424:ILE:O	2.42	0.51
2:D:245:PHE:CG	2:D:291:MET:HE1	2.45	0.51
2:B:220:LEU:HD11	2:B:423:ARG:HB3	1.92	0.51
2:B:457:GLU:CG	2:B:458:GLN:N	2.66	0.51
2:B:678:LEU:HD23	2:B:710:ILE:HG21	1.91	0.51
2:B:137:ILE:HG13	2:B:150:ILE:CG2	2.38	0.51
2:B:550:ASP:OD2	2:B:587:ARG:NH1	2.42	0.51
2:D:334:LEU:HD13	2:D:348:LYS:HG3	1.93	0.51
2:D:628:ASP:O	2:D:631:SER:HB2	2.10	0.51
2:B:636:LEU:N	2:B:636:LEU:CD1	2.73	0.51
2:B:137:ILE:HG12	2:B:150:ILE:HG23	1.93	0.51
2:D:291:MET:HG3	2:D:292:LEU:N	2.25	0.51
2:D:665:ARG:NH1	2:D:665:ARG:CG	2.64	0.51
2:D:575:THR:HG21	2:D:605:ARG:HB2	1.93	0.50
2:D:135:ILE:CG2	2:D:152:VAL:HB	2.42	0.50
2:B:11:LYS:HZ2	2:B:432:ASN:CG	2.15	0.50
2:B:310:TYR:CE2	2:B:318:ASP:HB3	2.46	0.50
2:D:481:TYR:HD1	2:D:543:LEU:HD22	1.76	0.50
2:B:575:THR:HG21	2:B:605:ARG:HB2	1.94	0.50
2:B:6:SER:HA	2:B:667:TYR:HD1	1.76	0.50
2:D:261:VAL:O	2:D:416:LYS:NZ	2.44	0.50
2:B:362:VAL:HG23	2:B:363:LYS:CG	2.32	0.49
2:D:623:LYS:HG2	2:D:627:ARG:HH21	1.76	0.49
2:D:307:ILE:HD13	2:D:323:ILE:HG12	1.94	0.49
2:B:398:ASN:OD1	2:B:398:ASN:O	2.30	0.49
2:B:682:VAL:O	2:B:685:MET:O	2.30	0.49
2:D:245:PHE:HD2	2:D:291:MET:HE1	1.73	0.49
2:B:685:MET:HG3	2:B:690:VAL:HG22	1.95	0.49
2:D:407:LEU:HD11	2:D:480:ALA:HB1	1.95	0.49
2:B:707:ASP:HA	2:B:711:LEU:HB3	1.94	0.49
2:B:21:GLN:OE1	2:B:25:ARG:NH2	2.34	0.49
2:D:97:ILE:CG2	2:D:98:ASP:N	2.77	0.48
2:D:505:VAL:O	2:D:506:MET:CG	2.55	0.48
2:B:439:LEU:O	2:B:439:LEU:CG	2.61	0.48
2:B:675:ILE:HG23	2:B:714:LEU:HD21	1.95	0.48
2:B:559:SER:OG	2:B:560:GLU:N	2.46	0.48
2:D:148:VAL:CG2	2:D:162:ILE:HG12	2.39	0.48
2:B:141:ASN:HB3	2:B:196:THR:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:SER:OG	2:B:171:GLN:N	2.47	0.48
2:B:669:GLU:OE1	2:B:709:ASN:ND2	2.42	0.48
2:B:721:THR:O	2:B:721:THR:CG2	2.61	0.48
1:A:75:GLY:O	1:A:76:THR:OG1	2.26	0.48
2:D:218:GLN:HE22	2:D:225:ILE:HD11	1.79	0.48
2:B:388:TYR:O	2:B:392:ARG:HG3	2.13	0.47
2:D:3:SER:HA	2:D:115:LEU:HD22	1.96	0.47
2:D:713:PHE:HA	2:D:717:PHE:HB2	1.96	0.47
2:D:153:HIS:HB3	2:D:155:PRO:CD	2.30	0.47
2:D:233:GLU:C	2:D:234:LEU:HG	2.34	0.47
2:D:95:MET:HG3	2:D:204:ASP:OD1	2.14	0.47
2:D:484:LEU:HD12	2:D:487:ILE:HD11	1.96	0.47
2:D:385:LYS:HE2	2:D:389:LEU:HD11	1.95	0.47
2:D:364:ARG:H	2:D:364:ARG:HG2	1.47	0.47
2:B:714:LEU:O	2:B:718:THR:OG1	2.33	0.47
2:B:107:ILE:O	2:B:111:LYS:HG2	2.14	0.46
2:B:575:THR:OG1	2:B:605:ARG:NH1	2.48	0.46
2:B:538:ARG:O	2:B:539:TRP:C	2.54	0.46
2:B:671:SER:HB3	2:B:674:LEU:HB2	1.98	0.46
2:D:12:GLU:HG2	2:D:89:GLY:O	2.15	0.46
2:D:283:LYS:HG3	2:D:721:THR:HG21	1.97	0.46
2:D:32:LEU:HD23	2:D:32:LEU:HA	1.78	0.46
2:B:141:ASN:HD22	2:B:195:GLU:HB3	1.81	0.46
2:B:579:GLU:OE2	2:B:607:SER:OG	2.20	0.46
2:D:236:ASP:HB3	2:D:239:ASN:HB2	1.97	0.46
2:B:394:TYR:CD1	2:B:397:LEU:HD12	2.51	0.46
2:B:11:LYS:NZ	2:B:432:ASN:CG	2.69	0.46
2:B:22:ARG:NH2	2:B:138:SER:O	2.49	0.46
2:D:306:LEU:HD23	2:D:322:LEU:HD21	1.97	0.46
2:B:457:GLU:CG	2:B:458:GLN:H	2.03	0.46
1:C:39:VAL:HG12	2:D:531:ARG:HH12	1.81	0.46
2:D:665:ARG:HG2	2:D:666:TRP:CD1	2.51	0.46
2:B:538:ARG:NH1	2:B:538:ARG:CA	2.69	0.46
2:B:322:LEU:O	2:B:326:GLN:HG2	2.16	0.45
2:D:292:LEU:O	2:D:296:ILE:HG12	2.16	0.45
2:B:678:LEU:CD2	2:B:710:ILE:HG21	2.45	0.45
2:D:209:LYS:HD2	2:D:209:LYS:HA	1.66	0.45
2:D:637:THR:O	2:D:640:GLN:N	2.49	0.45
2:B:337:ASP:OD1	2:B:338:SER:N	2.49	0.45
2:B:394:TYR:HD1	2:B:397:LEU:HD12	1.81	0.45
2:B:538:ARG:NH1	2:B:541:ASP:HB3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:614:LEU:HD23	2:B:655:LEU:HD11	1.99	0.45
2:D:559:SER:OG	2:D:560:GLU:N	2.50	0.45
2:B:663:ASN:O	2:B:668:ILE:N	2.44	0.45
2:B:398:ASN:O	2:B:398:ASN:CG	2.55	0.45
2:D:485:THR:HA	2:D:488:VAL:HG12	1.99	0.45
2:B:341:SER:OG	2:B:342:HIS:N	2.50	0.45
2:B:505:VAL:HG12	2:B:533:LYS:HE3	1.98	0.45
2:D:596:LYS:HA	2:D:599:GLN:HB2	1.99	0.45
2:D:602:LEU:HD12	2:D:602:LEU:HA	1.73	0.45
2:B:400:MET:HE2	2:B:490:ILE:CG2	2.47	0.45
2:D:105:ILE:CD1	2:D:150:ILE:HD13	2.47	0.45
1:A:55:GLU:HA	1:A:58:LYS:HB2	1.98	0.44
2:B:573:LYS:HB2	2:B:578:TRP:CZ2	2.52	0.44
2:D:103:THR:O	2:D:106:THR:OG1	2.30	0.44
2:D:109:ALA:HB1	2:D:135:ILE:HD13	1.99	0.44
2:B:39:THR:O	2:B:136:SER:N	2.50	0.44
2:D:222:GLU:OE1	2:D:423:ARG:NH2	2.44	0.44
2:D:579:GLU:OE2	2:D:607:SER:OG	2.28	0.44
2:D:39:THR:HB	2:D:136:SER:HG	1.78	0.44
2:D:154:ILE:HG23	2:D:155:PRO:N	2.32	0.44
2:B:452:MET:O	2:B:452:MET:HG2	2.18	0.44
2:B:266:LEU:HD23	2:B:266:LEU:HA	1.86	0.44
2:B:685:MET:CE	2:B:690:VAL:HA	2.43	0.44
2:D:6:SER:HA	2:D:667:TYR:CD1	2.51	0.43
2:D:637:THR:OG1	2:D:640:GLN:HB2	2.18	0.43
2:D:669:GLU:HG3	2:D:709:ASN:HD21	1.82	0.43
2:B:574:LEU:HB2	2:B:577:GLU:HG3	1.99	0.43
2:D:562:LEU:HD12	2:D:562:LEU:HA	1.88	0.43
2:B:310:TYR:HE2	2:B:318:ASP:HB3	1.82	0.43
2:D:711:LEU:HD12	2:D:711:LEU:HA	1.80	0.43
2:B:261:VAL:O	2:B:416:LYS:NZ	2.35	0.43
2:D:654:ASP:HB2	2:D:697:ARG:NH1	2.34	0.43
1:C:12:LYS:HB3	1:C:12:LYS:HE3	1.81	0.42
2:B:222:GLU:OE2	2:B:423:ARG:NH1	2.43	0.42
2:D:680:VAL:HA	2:D:683:GLN:HB2	2.02	0.42
2:D:504:PHE:O	2:D:533:LYS:HD2	2.20	0.42
1:A:-3:ASP:O	1:A:-1:GLU:N	2.53	0.42
2:D:154:ILE:H	2:D:155:PRO:CD	2.30	0.42
2:D:345:LEU:HD23	2:D:345:LEU:HA	1.84	0.42
2:D:444:GLU:HG2	2:D:445:GLU:HG2	2.02	0.42
2:D:483:LEU:HA	2:D:486:GLU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:394:TYR:CE2	2:B:402:ASN:HB3	2.55	0.42
2:D:640:GLN:O	2:D:644:SER:OG	2.27	0.42
2:D:105:ILE:HD13	2:D:150:ILE:HD13	2.01	0.42
2:B:400:MET:HE2	2:B:490:ILE:HG21	2.01	0.41
2:B:322:LEU:HD12	2:B:322:LEU:HA	1.91	0.41
2:B:458:GLN:O	2:B:458:GLN:CG	2.68	0.41
2:D:551:LEU:HD23	2:D:588:LEU:HD13	2.02	0.41
2:B:394:TYR:O	2:B:397:LEU:HB2	2.20	0.41
2:B:424:ILE:H	2:B:424:ILE:HG12	1.66	0.41
2:D:41:ILE:O	2:D:133:SER:N	2.52	0.41
2:D:473:LEU:HD12	2:D:473:LEU:HA	1.83	0.41
2:B:147:ASP:HB3	2:B:163:ILE:HB	2.01	0.41
2:D:154:ILE:H	2:D:155:PRO:HD2	1.84	0.41
2:B:139:SER:OG	2:B:140:TRP:N	2.52	0.41
2:B:298:ILE:HG12	2:B:299:HIS:CE1	2.56	0.41
2:D:238:ALA:O	2:D:242:ILE:HG12	2.20	0.41
2:D:488:VAL:HG11	2:D:547:LEU:HD11	2.02	0.41
2:D:621:GLU:OE2	2:D:624:ARG:NH2	2.36	0.41
2:B:103:THR:O	2:B:106:THR:OG1	2.33	0.41
2:B:596:LYS:O	2:B:600:ILE:HG13	2.21	0.41
2:D:253:VAL:C	2:D:255:LEU:N	2.74	0.41
1:A:30:PHE:HE1	1:C:47:MET:HE1	1.85	0.41
2:D:161:TYR:HE1	2:D:163:ILE:HD11	1.84	0.41
2:D:505:VAL:C	2:D:506:MET:CG	2.89	0.41
2:B:26:VAL:HG13	2:B:140:TRP:HZ3	1.85	0.40
2:B:451:PRO:C	2:B:452:MET:CE	2.89	0.40
2:B:454:VAL:HG22	2:B:455:GLN:N	2.35	0.40
1:A:70:ILE:HG12	2:B:368:LEU:HD13	2.02	0.40
2:B:22:ARG:HH12	2:B:34:PRO:HB2	1.86	0.40
2:B:438:PRO:HB2	2:B:439:LEU:H	1.64	0.40
2:B:207:ILE:HG23	2:B:208:MET:HG2	2.03	0.40
2:B:532:SER:O	2:B:532:SER:OG	2.36	0.40
2:D:7:ILE:HA	2:D:8:PRO:HD2	1.90	0.40
2:D:246:PRO:HG3	2:D:291:MET:SD	2.61	0.40
2:D:443:ILE:HG22	2:D:444:GLU:OE1	2.21	0.40
2:D:591:LEU:HB2	2:D:592:PRO:HD3	2.03	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	78/82 (95%)	74 (95%)	4 (5%)	0	100	100
1	C	73/82 (89%)	70 (96%)	3 (4%)	0	100	100
2	B	569/739 (77%)	526 (92%)	37 (6%)	6 (1%)	14	40
2	D	614/739 (83%)	581 (95%)	29 (5%)	4 (1%)	22	52
All	All	1334/1642 (81%)	1251 (94%)	73 (6%)	10 (1%)	22	52

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	438	PRO
2	D	415	VAL
2	B	451	PRO
2	B	538	ARG
2	B	635	GLU
2	B	460	SER
2	B	713	PHE
2	D	254	TYR
2	D	145	LYS
2	D	175	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	73/75 (97%)	71 (97%)	2 (3%)	44	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	68/75 (91%)	66 (97%)	2 (3%)	42	73
2	B	542/672 (81%)	535 (99%)	7 (1%)	69	88
2	D	579/672 (86%)	565 (98%)	14 (2%)	49	77
All	All	1262/1494 (84%)	1237 (98%)	25 (2%)	55	80

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-3	ASP
1	A	54	GLU
2	B	216	GLU
2	B	217	SER
2	B	337	ASP
2	B	393	ILE
2	B	452	MET
2	B	455	GLN
2	B	593	GLU
1	C	30	PHE
1	C	50	SER
2	D	15	ILE
2	D	25	ARG
2	D	149	ASN
2	D	222	GLU
2	D	240	ASN
2	D	291	MET
2	D	364	ARG
2	D	382	ASN
2	D	394	TYR
2	D	406	SER
2	D	506	MET
2	D	550	ASP
2	D	568	ASN
2	D	665	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	495	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 monosaccharides 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	80/82 (97%)	0.32	1 (1%) 77 78	62, 88, 126, 147	0
1	C	75/82 (91%)	0.19	0 100 100	54, 88, 117, 130	0
2	B	589/739 (79%)	0.67	49 (8%) 11 9	55, 104, 154, 177	0
2	D	632/739 (85%)	0.51	41 (6%) 18 17	56, 97, 146, 176	0
All	All	1376/1642 (83%)	0.55	91 (6%) 18 16	54, 98, 149, 177	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	152	VAL	6.0
2	D	566	ALA	5.5
2	B	563	TYR	5.4
2	B	150	ILE	5.2
2	B	151	ILE	5.0
2	D	448	SER	4.7
2	B	159	GLN	4.5
2	B	91	PHE	4.5
2	D	115	LEU	4.4
2	D	40	LEU	4.2
2	B	562	LEU	4.2
2	D	568	ASN	4.0
2	D	90	THR	3.7
2	D	559	SER	3.6
2	D	555	THR	3.4
2	D	88	ILE	3.4
2	B	92	PHE	3.4
2	B	37	LEU	3.4
2	B	115	LEU	3.3
2	B	559	SER	3.3
2	D	150	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
2	D	562	LEU	3.2
2	B	135	ILE	3.2
2	B	553	THR	3.1
2	D	557	TRP	3.1
2	B	138	SER	3.1
2	D	506	MET	3.1
2	B	160	THR	3.1
2	B	166	ASP	3.1
2	D	42	LYS	3.0
2	B	234	LEU	3.0
1	A	17	LEU	3.0
2	B	9	GLU	3.0
2	B	149	ASN	2.9
2	B	665	ARG	2.9
2	D	561	GLN	2.9
2	B	565	ASP	2.9
2	B	557	TRP	2.9
2	B	6	SER	2.9
2	B	106	THR	2.9
2	B	142	ALA	2.9
2	D	465	LEU	2.9
2	D	565	ASP	2.8
2	B	147	ASP	2.8
2	B	578	TRP	2.8
2	B	337	ASP	2.8
2	B	465	LEU	2.7
2	D	43	SER	2.6
2	B	631	SER	2.6
2	D	563	TYR	2.6
2	B	4	GLN	2.6
2	B	116	PHE	2.6
2	D	564	PHE	2.6
2	B	15	ILE	2.6
2	B	463	PRO	2.5
2	D	23	ARG	2.5
2	D	41	ILE	2.5
2	D	338	SER	2.5
2	D	578	TRP	2.5
2	D	507	GLU	2.5
2	D	509	GLU	2.4
2	B	581	PHE	2.4
2	B	140	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	140	TRP	2.4
2	D	137	ILE	2.4
2	B	561	GLN	2.3
2	D	224	LEU	2.3
2	D	134	LYS	2.3
2	B	163	ILE	2.3
2	B	467	ASN	2.3
2	B	16	GLY	2.3
2	B	288	CYS	2.2
2	D	151	ILE	2.2
2	D	175	VAL	2.2
2	B	17	TYR	2.2
2	D	343	ILE	2.2
2	D	172	LEU	2.2
2	D	337	ASP	2.2
2	D	437	LEU	2.2
2	D	149	ASN	2.2
2	B	136	SER	2.2
2	B	695	ALA	2.1
2	B	187	LEU	2.1
2	B	552	LYS	2.1
2	D	340	THR	2.1
2	B	535	LEU	2.0
2	D	44	LEU	2.0
2	D	152	VAL	2.0
2	B	38	ILE	2.0
2	B	560	GLU	2.0
2	D	573	LYS	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.