



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:59 AM UTC

PDB ID : 6HZO / pdb_00006hzo
Title : Apo structure of TP domain from Haemophilus influenzae Penicillin-Binding Protein 3
Authors : Bellini, D.; Koekemoer, L.; Newman, H.; Dowson, C.G.
Deposited on : 2018-10-23
Resolution : 2.44 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

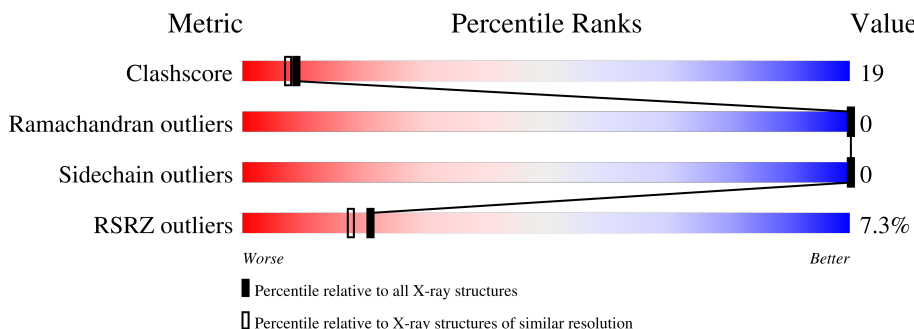
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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))
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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

Mol	Chain	Length	Quality of chain
1	A	325	5% 64% 23% • 12%
1	B	325	5% 54% 32% • 13%
1	C	325	7% 67% 20% • 13%
1	D	325	10% 56% 31% 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8727 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 FtsI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2182	1383	383	409	7			
1	B	283	Total	C	N	O	S	0	0	0
			2165	1371	380	407	7			
1	C	284	Total	C	N	O	S	0	0	0
			2176	1379	383	407	7			
1	D	285	Total	C	N	O	S	0	0	0
			2182	1383	383	409	7			

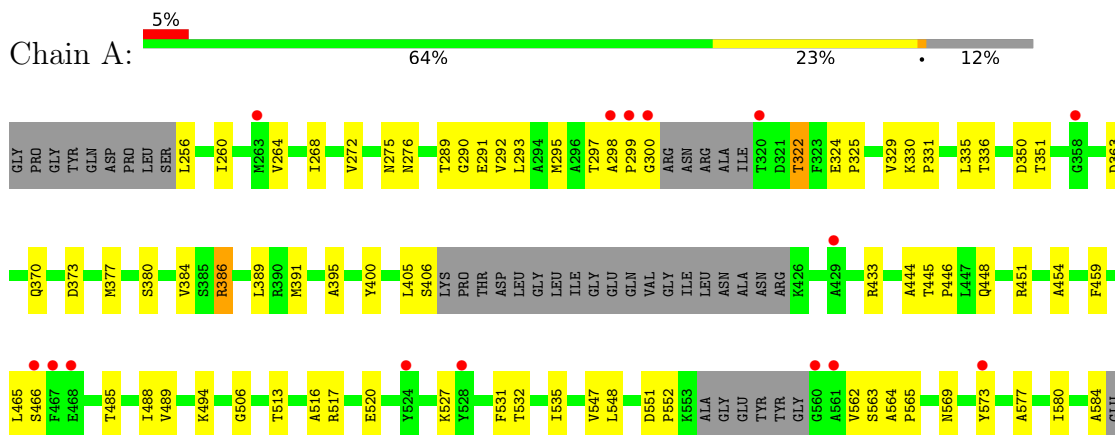
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	6	Total	O	0	0
			6	6		
2	B	5	Total	O	0	0
			5	5		
2	C	5	Total	O	0	0
			5	5		
2	D	6	Total	O	0	0
			6	6		

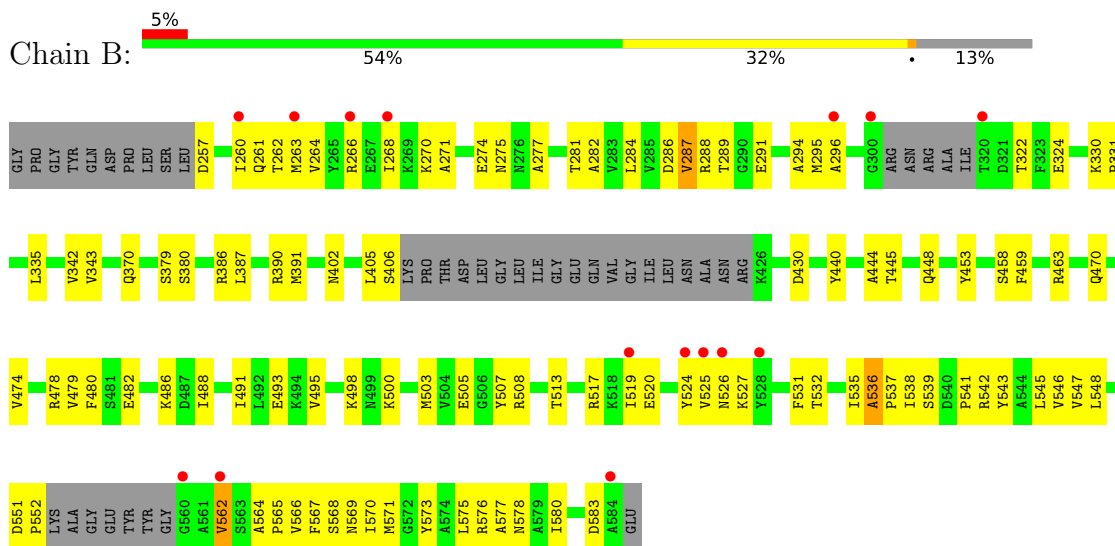
3 Residue-property plots

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.

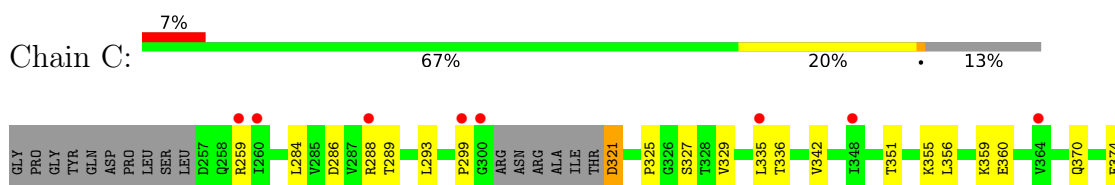
• Molecule 1: FtsI

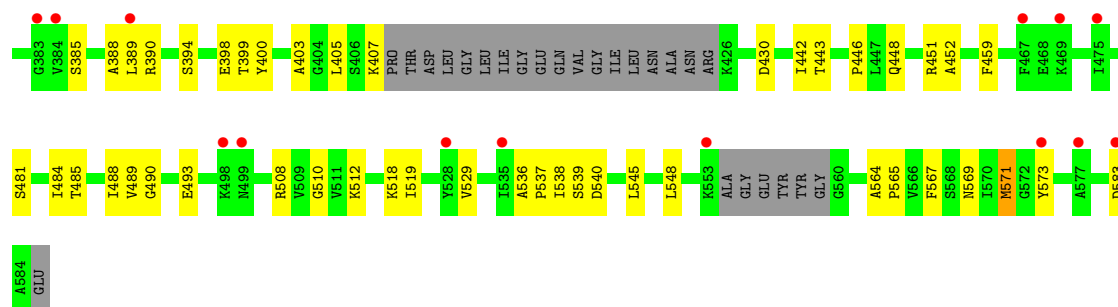


• Molecule 1: FtsI

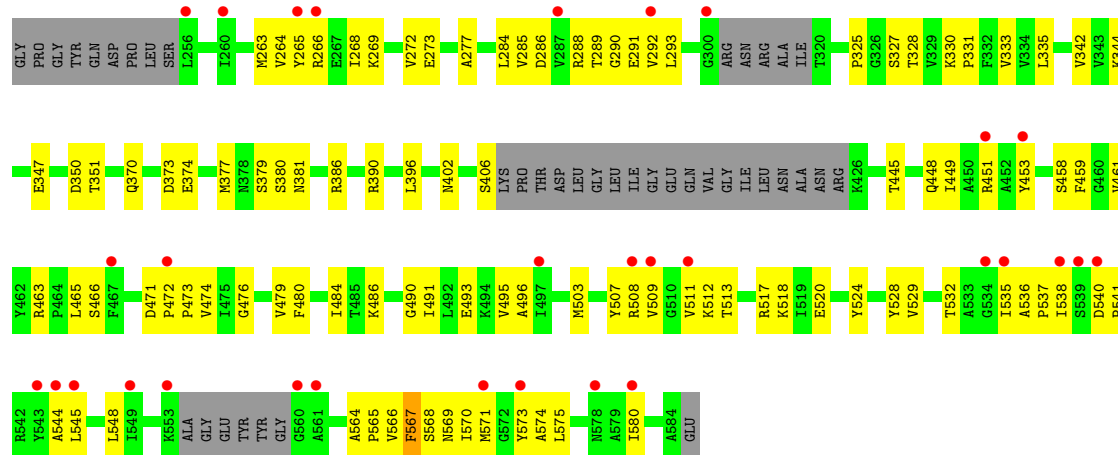


• Molecule 1: FtsI





● Molecule 1: FtsI



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.01Å 93.63Å 95.83Å 90.00° 95.46° 90.00°	Depositor
Resolution (Å)	95.40 – 2.44 95.39 – 2.44	Depositor EDS
% Data completeness (in resolution range)	67.8 (95.40-2.44) 67.8 (95.39-2.44)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.224 , (Not available) 0.229 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	59.7	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 30.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8727	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

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	1.07	1/2215 (0.0%)	1.53	3/2998 (0.1%)
1	B	1.04	0/2198	1.56	8/2976 (0.3%)
1	C	1.06	0/2209	1.57	6/2988 (0.2%)
1	D	1.05	0/2215	1.50	3/2998 (0.1%)
All	All	1.05	1/8837 (0.0%)	1.54	20/11960 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	386	ARG	C-O	5.16	1.30	1.24

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	299	PRO	N-CA-C	-8.34	101.55	113.47
1	D	472	PRO	N-CA-C	7.27	119.56	110.70
1	C	321	ASP	CA-CB-CG	6.74	119.33	112.60
1	B	294	ALA	CA-C-N	6.46	130.37	121.33
1	B	294	ALA	C-N-CA	6.46	130.37	121.33
1	C	259	ARG	CA-C-N	6.10	128.33	120.70
1	C	259	ARG	C-N-CA	6.10	128.33	120.70
1	B	287	VAL	CA-C-O	-6.05	114.75	121.05
1	C	571	MET	CA-C-N	5.93	126.56	119.98
1	C	571	MET	C-N-CA	5.93	126.56	119.98
1	B	295	MET	CB-CA-C	-5.82	104.21	111.43
1	A	322	THR	CA-CB-OG1	-5.69	101.06	109.60
1	A	400	TYR	N-CA-C	-5.36	105.35	111.14
1	A	580	ILE	CA-C-O	5.27	122.07	119.12
1	B	536	ALA	N-CA-C	5.24	112.93	108.22
1	B	562	VAL	N-CA-C	-5.22	107.39	112.29
1	D	567	PHE	CA-C-N	5.09	128.82	120.63
1	D	567	PHE	C-N-CA	5.09	128.82	120.63
1	B	458	SER	CA-C-N	5.06	129.30	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	458	SER	C-N-CA	5.06	129.30	122.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2182	0	2247	60	1
1	B	2165	0	2223	108	3
1	C	2176	0	2242	60	1
1	D	2182	0	2247	102	3
2	A	6	0	0	1	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	6	0	0	0	0
All	All	8727	0	8959	329	4

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 19.

All (329) 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:291:GLU:HA	1:D:466:SER:OG	1.26	1.27
1:B:536:ALA:HB3	1:B:571:MET:HE2	1.24	1.12
1:D:513:THR:HG22	1:D:532:THR:OG1	1.50	1.11
1:B:536:ALA:HB3	1:B:571:MET:CE	1.96	0.95
1:A:351:THR:HG21	1:A:370:GLN:HE21	1.31	0.95
1:D:536:ALA:HB3	1:D:571:MET:HE2	1.47	0.94
1:C:481:SER:OG	1:C:484:ILE:HD12	1.71	0.90
1:B:513:THR:HG22	1:B:532:THR:HG22	1.53	0.90
1:B:288:ARG:HA	1:B:463:ARG:NH2	1.85	0.90
1:D:292:VAL:HG23	1:D:466:SER:O	1.72	0.90
1:B:505:GLU:O	1:B:576:ARG:NH2	2.05	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:GLU:CA	1:D:466:SER:OG	2.19	0.88
1:B:287:VAL:O	1:B:463:ARG:NH2	2.08	0.86
1:B:520:GLU:HB2	1:B:525:VAL:HG21	1.55	0.85
1:C:329:VAL:HG11	1:C:400:TYR:OH	1.78	0.83
1:B:513:THR:CG2	1:B:532:THR:HG22	2.09	0.83
1:B:513:THR:HG22	1:B:532:THR:CG2	2.09	0.82
1:D:529:VAL:CG1	1:D:548:LEU:HD11	2.10	0.81
1:C:329:VAL:CG1	1:C:400:TYR:OH	2.30	0.80
1:D:536:ALA:HB3	1:D:571:MET:CE	2.12	0.79
1:D:529:VAL:HG13	1:D:548:LEU:HD11	1.64	0.79
1:A:335:LEU:HA	1:A:488:ILE:HD11	1.65	0.78
1:B:287:VAL:C	1:B:463:ARG:HH21	1.91	0.78
1:B:517:ARG:HE	1:B:524:TYR:HB3	1.48	0.78
1:C:443:THR:HG22	1:C:519:ILE:HD13	1.63	0.78
1:A:373:ASP:O	1:A:377:MET:HG3	1.81	0.78
1:D:402:ASN:HB3	1:D:479:VAL:HG11	1.66	0.77
1:B:459:PHE:CD1	1:B:486:LYS:HG2	2.19	0.77
1:C:407:LYS:HG3	1:C:448:GLN:HE21	1.49	0.77
1:B:517:ARG:HE	1:B:524:TYR:CB	1.97	0.76
1:C:529:VAL:CG1	1:C:548:LEU:HD11	2.15	0.76
1:C:321:ASP:HB3	1:C:518:LYS:NZ	1.98	0.76
1:D:286:ASP:HB3	1:D:289:THR:OG1	1.84	0.76
1:D:459:PHE:CE1	1:D:486:LYS:HG2	2.21	0.74
1:B:517:ARG:CD	1:B:524:TYR:HB2	2.16	0.74
1:B:343:VAL:HG21	1:B:387:LEU:CD2	2.18	0.73
1:C:536:ALA:HB3	1:C:571:MET:CE	2.19	0.72
1:B:493:GLU:HB2	1:B:538:ILE:HD13	1.71	0.72
1:D:342:VAL:CG1	1:D:390:ARG:HB3	2.19	0.72
1:B:564:ALA:HB3	1:B:565:PRO:HD3	1.72	0.72
1:D:493:GLU:HB2	1:D:538:ILE:HD13	1.72	0.71
1:B:539:SER:OG	1:B:583:ASP:OD1	2.08	0.70
1:C:485:THR:O	1:C:489:VAL:HG23	1.90	0.70
1:B:288:ARG:CA	1:B:463:ARG:NH2	2.54	0.70
1:C:481:SER:OG	1:C:484:ILE:CD1	2.39	0.70
1:D:507:TYR:CD2	1:D:575:LEU:HD13	2.27	0.70
1:B:520:GLU:HB2	1:B:525:VAL:CG2	2.22	0.70
1:B:517:ARG:HD2	1:B:524:TYR:HB2	1.73	0.69
1:D:493:GLU:OE2	1:D:508:ARG:HD3	1.91	0.69
1:D:463:ARG:HG2	1:D:476:GLY:HA2	1.73	0.69
1:B:507:TYR:OH	1:B:580:ILE:O	2.09	0.69
1:B:536:ALA:CB	1:B:571:MET:HE2	2.14	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:451:ARG:HE	1:D:465:LEU:HD12	1.59	0.68
1:A:350:ASP:O	1:A:386:ARG:NE	2.26	0.68
1:A:532:THR:HG23	1:A:563:SER:OG	1.94	0.67
1:D:327:SER:HB3	1:D:512:LYS:HE3	1.77	0.66
1:D:330:LYS:HE3	1:D:379:SER:OG	1.95	0.66
1:B:545:LEU:HD23	1:B:567:PHE:CD2	2.31	0.66
1:D:459:PHE:CD1	1:D:486:LYS:HG2	2.32	0.65
1:B:291:GLU:OE2	1:B:470:GLN:O	2.15	0.65
1:D:330:LYS:NZ	1:D:381:ASN:OD1	2.29	0.65
1:A:299:PRO:O	1:A:300:GLY:C	2.39	0.65
1:B:257:ASP:O	1:B:261:GLN:N	2.21	0.65
1:B:459:PHE:CE1	1:B:486:LYS:HG2	2.32	0.64
1:A:256:LEU:HD12	1:A:293:LEU:O	1.98	0.64
1:A:513:THR:OG1	1:A:532:THR:HG22	1.98	0.64
1:B:537:PRO:HB2	1:B:583:ASP:OD2	1.96	0.64
1:C:394:SER:HB2	1:C:398:GLU:OE2	1.99	0.63
1:D:513:THR:CG2	1:D:532:THR:OG1	2.39	0.63
1:C:336:THR:OG1	1:C:399:THR:HG21	1.99	0.62
1:D:402:ASN:CB	1:D:479:VAL:HG11	2.30	0.62
1:A:291:GLU:HA	1:A:466:SER:O	2.00	0.62
1:B:531:PHE:HB3	1:B:548:LEU:HD12	1.80	0.62
1:A:389:LEU:HD23	1:A:433:ARG:HE	1.65	0.61
1:B:531:PHE:HA	1:B:547:VAL:O	2.00	0.61
1:C:536:ALA:HB3	1:C:571:MET:HE3	1.82	0.61
1:B:402:ASN:HB3	1:B:479:VAL:CG1	2.31	0.61
1:A:506:GLY:O	1:A:584:ALA:HB3	1.99	0.61
1:C:329:VAL:HG13	1:C:400:TYR:CZ	2.36	0.60
1:D:328:THR:O	1:D:453:TYR:OH	2.15	0.60
1:D:529:VAL:HG13	1:D:548:LEU:CD1	2.31	0.60
1:D:402:ASN:HB3	1:D:479:VAL:CG1	2.31	0.60
1:D:265:TYR:HA	1:D:268:ILE:HG22	1.83	0.60
1:B:268:ILE:HD11	1:B:282:ALA:HB2	1.84	0.60
1:B:517:ARG:NE	1:B:524:TYR:CB	2.64	0.60
1:C:321:ASP:HB3	1:C:518:LYS:HZ1	1.65	0.59
1:C:321:ASP:HB3	1:C:518:LYS:HZ2	1.63	0.59
1:D:377:MET:HA	1:D:495:VAL:HG22	1.85	0.59
1:B:266:ARG:CZ	1:D:288:ARG:NH1	2.66	0.59
1:D:291:GLU:HA	1:D:466:SER:HG	1.63	0.59
1:B:286:ASP:OD2	1:B:289:THR:OG1	2.16	0.59
1:A:335:LEU:CA	1:A:488:ILE:HD11	2.32	0.59
1:B:330:LYS:NZ	1:B:379:SER:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:GLU:OE2	1:A:517:ARG:NH2	2.35	0.59
1:C:329:VAL:HG13	1:C:400:TYR:CE1	2.37	0.59
1:D:370:GLN:HA	1:D:374:GLU:OE1	2.02	0.59
1:A:351:THR:HG21	1:A:370:GLN:NE2	2.09	0.58
1:B:275:ASN:OD1	1:B:562:VAL:HG11	2.03	0.58
1:B:525:VAL:HG12	1:B:527:LYS:H	1.67	0.58
1:D:288:ARG:HA	1:D:463:ARG:NH2	2.17	0.58
1:D:288:ARG:NH2	1:D:540:ASP:CG	2.61	0.58
1:D:451:ARG:HE	1:D:465:LEU:CD1	2.15	0.58
1:D:451:ARG:HG2	1:D:465:LEU:HG	1.85	0.58
1:B:507:TYR:CD1	1:B:575:LEU:HD13	2.38	0.58
1:D:451:ARG:CG	1:D:465:LEU:HG	2.34	0.58
1:B:543:TYR:OH	1:B:578:ASN:ND2	2.36	0.57
1:C:508:ARG:H	1:C:583:ASP:HB2	1.69	0.57
1:A:292:VAL:HG11	1:A:295:MET:HE3	1.86	0.57
1:D:286:ASP:CB	1:D:289:THR:OG1	2.52	0.57
1:D:449:ILE:O	1:D:453:TYR:HD1	1.87	0.57
1:D:328:THR:CA	1:D:453:TYR:OH	2.53	0.57
1:B:263:MET:HE1	1:B:573:TYR:HB2	1.87	0.56
1:C:529:VAL:HG11	1:C:548:LEU:HD11	1.85	0.56
1:B:537:PRO:HD2	1:B:542:ARG:HG2	1.87	0.56
1:D:545:LEU:HD23	1:D:567:PHE:CD1	2.41	0.56
1:A:377:MET:HE3	1:A:494:LYS:C	2.31	0.56
1:B:343:VAL:HG21	1:B:387:LEU:HD22	1.85	0.56
1:B:517:ARG:HD2	1:B:524:TYR:CD2	2.41	0.56
1:A:370:GLN:HE22	1:A:380:SER:CB	2.18	0.56
1:D:292:VAL:CG2	1:D:466:SER:O	2.50	0.56
1:B:513:THR:CB	1:B:532:THR:HG22	2.36	0.56
1:C:407:LYS:HG2	1:C:451:ARG:HH22	1.71	0.56
1:C:481:SER:OG	1:C:484:ILE:CG1	2.55	0.55
1:D:265:TYR:HA	1:D:268:ILE:CG2	2.36	0.55
1:D:328:THR:O	1:D:331:PRO:HD2	2.07	0.55
1:D:269:LYS:O	1:D:273:GLU:HG2	2.07	0.55
1:D:517:ARG:HG2	1:D:528:TYR:CE1	2.42	0.55
1:D:453:TYR:C	1:D:535:ILE:HD11	2.32	0.55
1:A:335:LEU:HB2	1:A:488:ILE:HD13	1.89	0.55
1:B:569:ASN:O	1:B:573:TYR:HD1	1.90	0.54
1:C:288:ARG:NH2	1:C:540:ASP:OD2	2.40	0.54
1:C:537:PRO:HB2	1:C:583:ASP:OD2	2.07	0.54
1:D:479:VAL:HG12	1:D:480:PHE:CE1	2.43	0.54
1:B:508:ARG:HB3	1:B:538:ILE:HB	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:SER:HB3	1:C:512:LYS:HE3	1.89	0.54
1:C:407:LYS:HG3	1:C:448:GLN:NE2	2.19	0.54
1:A:459:PHE:HA	1:A:485:THR:CG2	2.38	0.54
1:B:406:SER:O	1:B:448:GLN:NE2	2.41	0.54
1:D:536:ALA:CB	1:D:571:MET:HE2	2.31	0.54
1:D:335:LEU:HD12	1:D:484:ILE:HG22	1.90	0.53
1:D:463:ARG:HD2	1:D:474:VAL:CG1	2.38	0.53
1:A:569:ASN:O	1:A:573:TYR:CD2	2.60	0.53
1:D:459:PHE:CD1	1:D:486:LYS:CG	2.91	0.53
1:B:260:ILE:HA	1:B:263:MET:HG2	1.90	0.53
1:C:284:LEU:HD23	1:C:293:LEU:HB2	1.90	0.53
1:D:529:VAL:CG1	1:D:548:LEU:CD1	2.84	0.53
1:C:329:VAL:CG1	1:C:400:TYR:CZ	2.92	0.53
1:C:569:ASN:O	1:C:573:TYR:HD2	1.91	0.53
1:D:264:VAL:HA	1:D:570:ILE:HD12	1.91	0.53
1:A:506:GLY:C	1:A:584:ALA:HB3	2.34	0.53
1:A:363:ASP:OD2	1:A:380:SER:HB2	2.09	0.53
1:D:471:ASP:C	1:D:473:PRO:HD2	2.34	0.52
1:A:289:THR:OG1	1:A:291:GLU:HG2	2.10	0.52
1:C:329:VAL:HG22	1:C:405:LEU:HD21	1.91	0.52
1:B:513:THR:HB	1:B:532:THR:HG22	1.91	0.52
1:D:328:THR:HA	1:D:453:TYR:OH	2.09	0.52
1:B:264:VAL:HG22	1:B:570:ILE:HG23	1.90	0.52
1:B:386:ARG:O	1:B:390:ARG:HG3	2.09	0.52
1:D:286:ASP:O	1:D:290:GLY:N	2.35	0.52
1:B:288:ARG:CA	1:B:463:ARG:HH21	2.23	0.51
1:B:525:VAL:HG12	1:B:526:ASN:N	2.24	0.51
1:C:356:LEU:HD22	1:C:389:LEU:HD21	1.91	0.51
1:B:268:ILE:HD11	1:B:282:ALA:CB	2.39	0.51
1:C:446:PRO:HG3	1:C:548:LEU:HD22	1.92	0.51
1:C:508:ARG:HG3	1:C:583:ASP:O	2.10	0.51
1:B:277:ALA:HB2	1:B:552:PRO:HA	1.92	0.51
1:B:405:LEU:HD23	1:B:448:GLN:HB3	1.92	0.51
1:B:263:MET:SD	1:B:573:TYR:HB2	2.50	0.51
1:A:322:THR:HG22	1:A:445:THR:HG22	1.93	0.51
1:A:489:VAL:HG13	1:A:535:ILE:HD11	1.93	0.51
1:A:520:GLU:OE2	1:A:527:LYS:NZ	2.41	0.51
1:B:270:LYS:O	1:B:274:GLU:HB2	2.10	0.51
1:A:275:ASN:CG	1:A:562:VAL:HG11	2.36	0.51
1:D:569:ASN:O	1:D:573:TYR:HD1	1.94	0.51
1:A:336:THR:HG22	1:A:391:MET:SD	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:ASP:CG	1:D:289:THR:OG1	2.54	0.50
1:C:536:ALA:HB3	1:C:571:MET:HE2	1.94	0.50
1:D:370:GLN:HE22	1:D:380:SER:HB2	1.76	0.50
1:B:287:VAL:C	1:B:463:ARG:NH2	2.63	0.50
1:D:529:VAL:HG11	1:D:548:LEU:HD11	1.93	0.50
1:C:493:GLU:OE2	1:C:508:ARG:NH2	2.43	0.50
1:B:500:LYS:HG3	1:B:503:MET:CG	2.42	0.49
1:C:564:ALA:HB3	1:C:565:PRO:HD3	1.94	0.49
1:A:506:GLY:O	1:A:584:ALA:N	2.42	0.49
1:C:342:VAL:HG13	1:C:390:ARG:HG2	1.95	0.49
1:D:449:ILE:HG23	1:D:453:TYR:CE1	2.48	0.49
1:C:355:LYS:HE2	1:C:360:GLU:HB2	1.94	0.49
1:B:402:ASN:HB3	1:B:479:VAL:HG11	1.94	0.49
1:B:562:VAL:HG12	1:B:562:VAL:O	2.13	0.48
1:D:351:THR:HG22	1:D:351:THR:O	2.13	0.48
1:B:500:LYS:HG3	1:B:503:MET:SD	2.53	0.48
1:A:290:GLY:O	1:A:465:LEU:HA	2.13	0.48
1:B:517:ARG:NE	1:B:524:TYR:HB2	2.27	0.48
1:A:405:LEU:O	1:A:406:SER:C	2.57	0.48
1:B:507:TYR:CG	1:B:575:LEU:HD13	2.48	0.48
1:C:385:SER:O	1:C:388:ALA:HB3	2.14	0.48
1:C:529:VAL:HG13	1:C:548:LEU:HD11	1.94	0.48
1:B:342:VAL:CG1	1:B:390:ARG:HB2	2.44	0.48
1:C:335:LEU:HB2	1:C:488:ILE:HG13	1.96	0.48
1:A:513:THR:HG23	1:A:532:THR:HG22	1.95	0.48
1:B:277:ALA:HA	1:B:551:ASP:O	2.14	0.48
1:B:342:VAL:HG21	1:B:391:MET:HG2	1.94	0.48
1:A:324:GLU:HB2	1:A:516:ALA:HB1	1.95	0.48
1:C:459:PHE:HA	1:C:485:THR:CG2	2.43	0.48
1:D:445:THR:OG1	1:D:448:GLN:HG3	2.14	0.48
1:D:564:ALA:HB3	1:D:565:PRO:HD3	1.96	0.48
1:A:451:ARG:O	1:A:454:ALA:HB3	2.14	0.47
1:B:282:ALA:HA	1:B:546:VAL:O	2.14	0.47
1:B:342:VAL:HG11	1:B:390:ARG:HB2	1.96	0.47
1:B:402:ASN:HB3	1:B:479:VAL:HG13	1.95	0.47
1:A:513:THR:OG1	1:A:532:THR:CG2	2.63	0.47
1:A:330:LYS:HG2	1:A:384:VAL:HG11	1.97	0.47
1:B:453:TYR:O	1:B:535:ILE:HD11	2.14	0.47
1:D:288:ARG:HH22	1:D:540:ASP:CG	2.23	0.47
1:D:342:VAL:HG11	1:D:390:ARG:HB3	1.95	0.46
1:C:545:LEU:HD23	1:C:567:PHE:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:573:TYR:O	1:A:577:ALA:HB2	2.16	0.46
1:A:370:GLN:HE22	1:A:380:SER:HB3	1.80	0.46
1:A:335:LEU:CB	1:A:488:ILE:HD13	2.46	0.46
1:C:529:VAL:CG1	1:C:548:LEU:CD1	2.90	0.46
1:D:330:LYS:HE3	1:D:379:SER:HG	1.79	0.46
1:A:513:THR:CB	1:A:532:THR:HG22	2.46	0.46
1:B:322:THR:HG22	1:B:445:THR:HG22	1.98	0.46
1:D:508:ARG:HB3	1:D:538:ILE:HD12	1.98	0.46
1:D:537:PRO:HG3	1:D:580:ILE:HG21	1.98	0.46
1:D:566:VAL:O	1:D:570:ILE:HG12	2.16	0.46
1:D:327:SER:HA	1:D:330:LYS:HE2	1.97	0.45
1:A:268:ILE:O	1:A:272:VAL:HG23	2.16	0.45
1:B:573:TYR:O	1:B:577:ALA:HB2	2.16	0.45
1:D:289:THR:HA	1:D:474:VAL:HG21	1.97	0.45
1:B:495:VAL:O	1:B:498:LYS:O	2.34	0.45
1:B:503:MET:O	1:B:568:SER:HB2	2.16	0.45
1:B:270:LYS:O	1:B:274:GLU:CB	2.65	0.45
1:B:478:ARG:HH12	1:B:482:GLU:HB2	1.81	0.45
1:B:517:ARG:CD	1:B:524:TYR:CB	2.93	0.45
1:B:569:ASN:O	1:B:573:TYR:CD1	2.70	0.45
1:C:510:GLY:HA3	1:C:538:ILE:HD11	1.98	0.45
1:C:407:LYS:CG	1:C:448:GLN:HE21	2.25	0.45
1:A:446:PRO:HG3	1:A:548:LEU:HD13	1.99	0.45
1:C:355:LYS:HA	1:C:359:LYS:O	2.17	0.45
1:C:356:LEU:CD2	1:C:389:LEU:HD21	2.47	0.45
1:C:403:ALA:O	1:C:452:ALA:HA	2.17	0.45
1:A:569:ASN:O	1:A:573:TYR:HD2	2.00	0.44
1:B:536:ALA:HB1	1:B:537:PRO:HA	1.99	0.44
1:D:537:PRO:O	1:D:541:PRO:HA	2.16	0.44
1:A:551:ASP:N	1:A:552:PRO:CD	2.80	0.44
1:B:488:ILE:HA	1:B:491:ILE:HD12	1.98	0.44
1:B:535:ILE:HG23	1:B:541:PRO:HB3	1.99	0.44
1:A:506:GLY:O	1:A:584:ALA:CB	2.64	0.44
1:B:268:ILE:O	1:B:271:ALA:N	2.51	0.44
1:C:286:ASP:HB3	1:C:289:THR:OG1	2.18	0.44
1:C:325:PRO:HG2	1:C:442:ILE:HG23	1.99	0.44
1:A:322:THR:HG22	1:A:445:THR:CG2	2.47	0.44
1:D:451:ARG:HE	1:D:465:LEU:CG	2.31	0.44
1:D:503:MET:O	1:D:568:SER:OG	2.23	0.44
1:B:324:GLU:HG3	1:B:519:ILE:HD11	1.98	0.44
1:B:500:LYS:HG3	1:B:503:MET:HG3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:507:TYR:CZ	1:B:575:LEU:HB3	2.53	0.44
1:C:490:GLY:O	1:C:493:GLU:HB3	2.18	0.44
1:D:263:MET:HE1	1:D:574:ALA:HB2	1.99	0.44
1:D:350:ASP:O	1:D:386:ARG:NE	2.38	0.44
1:D:493:GLU:CB	1:D:538:ILE:HD13	2.45	0.44
1:A:272:VAL:O	1:A:276:ASN:N	2.51	0.43
1:D:272:VAL:HA	1:D:277:ALA:HB3	2.00	0.43
1:B:513:THR:HG22	1:B:532:THR:CB	2.48	0.43
1:D:406:SER:O	1:D:406:SER:OG	2.34	0.43
1:D:265:TYR:CA	1:D:268:ILE:HG22	2.47	0.43
1:D:325:PRO:O	1:D:328:THR:OG1	2.33	0.43
1:D:285:VAL:HG21	1:D:465:LEU:HD21	2.00	0.43
1:A:531:PHE:HA	1:A:547:VAL:O	2.18	0.43
1:D:479:VAL:HG12	1:D:480:PHE:CD1	2.53	0.43
1:D:518:LYS:NZ	1:D:520:GLU:OE2	2.44	0.43
1:A:325:PRO:HB2	1:A:329:VAL:HG13	2.00	0.43
1:B:459:PHE:CD1	1:B:486:LYS:CG	2.99	0.43
1:D:535:ILE:HD13	1:D:544:ALA:HA	2.00	0.43
1:B:531:PHE:HB3	1:B:548:LEU:CD1	2.46	0.43
1:D:445:THR:HG23	1:D:448:GLN:OE1	2.19	0.42
1:B:263:MET:CE	1:B:573:TYR:HB2	2.49	0.42
1:D:490:GLY:O	1:D:493:GLU:HB3	2.19	0.42
1:B:330:LYS:N	1:B:331:PRO:CD	2.82	0.42
1:D:496:ALA:HB3	1:D:509:VAL:O	2.19	0.42
1:A:260:ILE:O	1:A:264:VAL:HG23	2.20	0.42
1:A:395:ALA:HB3	2:A:601:HOH:O	2.20	0.42
1:A:573:TYR:O	1:A:577:ALA:CB	2.68	0.42
1:A:564:ALA:HB3	1:A:565:PRO:CD	2.49	0.42
1:B:444:ALA:HA	1:B:448:GLN:OE1	2.19	0.42
1:D:493:GLU:HB2	1:D:538:ILE:CD1	2.45	0.42
1:B:264:VAL:HG12	1:B:296:ALA:CB	2.50	0.42
1:B:284:LEU:HD11	1:B:543:TYR:HB3	2.01	0.42
1:B:478:ARG:HD2	1:B:480:PHE:O	2.20	0.42
1:C:325:PRO:HD2	1:C:442:ILE:HG23	2.02	0.42
1:C:351:THR:HG21	1:C:370:GLN:NE2	2.35	0.42
1:C:510:GLY:N	1:C:538:ILE:HD11	2.35	0.42
1:D:328:THR:HB	1:D:453:TYR:OH	2.20	0.42
1:D:370:GLN:HE22	1:D:380:SER:CB	2.32	0.42
1:B:370:GLN:HE22	1:B:380:SER:HB2	1.84	0.42
1:D:264:VAL:O	1:D:268:ILE:HG22	2.20	0.42
1:D:284:LEU:HG	1:D:293:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:285:VAL:HA	1:D:291:GLU:O	2.20	0.42
1:A:330:LYS:N	1:A:331:PRO:CD	2.82	0.41
1:B:463:ARG:HD2	1:B:474:VAL:HB	2.01	0.41
1:B:566:VAL:O	1:B:570:ILE:HG13	2.20	0.41
1:D:328:THR:C	1:D:453:TYR:OH	2.62	0.41
1:B:335:LEU:HD21	1:B:480:PHE:CG	2.55	0.41
1:B:500:LYS:CG	1:B:503:MET:SD	3.09	0.41
1:C:370:GLN:HG3	1:C:374:GLU:CB	2.51	0.41
1:B:500:LYS:CD	1:B:503:MET:SD	3.08	0.41
1:B:517:ARG:HD2	1:B:524:TYR:HD2	1.82	0.41
1:B:281:THR:HA	1:B:296:ALA:O	2.21	0.41
1:C:510:GLY:CA	1:C:538:ILE:HD11	2.50	0.41
1:D:373:ASP:OD1	1:D:491:ILE:HG12	2.21	0.41
1:A:445:THR:OG1	1:A:448:GLN:HG3	2.21	0.41
1:B:564:ALA:O	1:B:565:PRO:C	2.63	0.41
1:A:325:PRO:HG3	1:A:444:ALA:HB2	2.03	0.41
1:C:335:LEU:HD12	1:C:484:ILE:HG22	2.02	0.41
1:C:484:ILE:O	1:C:488:ILE:HG12	2.20	0.41
1:C:539:SER:HG	1:C:583:ASP:CG	2.28	0.41
1:D:344:LYS:HB2	1:D:347:GLU:HB2	2.02	0.41
1:D:458:SER:OG	1:D:461:VAL:O	2.27	0.41
1:A:272:VAL:HG21	1:A:298:ALA:HB3	2.01	0.41
1:A:513:THR:CG2	1:A:532:THR:HG22	2.51	0.41
1:D:513:THR:HG21	1:D:564:ALA:HB2	2.03	0.41
1:C:400:TYR:CD1	1:C:405:LEU:HD23	2.55	0.40
1:D:333:VAL:HA	1:D:396:LEU:HD21	2.02	0.40
1:A:275:ASN:ND2	1:A:562:VAL:HG11	2.36	0.40
1:B:262:THR:HG22	1:B:266:ARG:NH1	2.37	0.40
1:D:511:VAL:HG13	1:D:532:THR:HG23	2.02	0.40
1:B:440:TYR:CE2	1:B:517:ARG:NH2	2.90	0.40
1:A:297:THR:O	1:A:299:PRO:HD3	2.21	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:524:TYR:OH	1:C:430:ASP:OD1[1_556]	1.92	0.28
1:B:430:ASP:OD1	1:D:524:TYR:OH[1_565]	2.10	0.10
1:A:584:ALA:C	1:D:266:ARG:NH2[2_655]	2.14	0.06
1:B:430:ASP:OD2	1:D:524:TYR:OH[1_565]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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	277/325 (85%)	267 (96%)	10 (4%)	0	100	100
1	B	275/325 (85%)	258 (94%)	17 (6%)	0	100	100
1	C	276/325 (85%)	265 (96%)	11 (4%)	0	100	100
1	D	277/325 (85%)	256 (92%)	21 (8%)	0	100	100
All	All	1105/1300 (85%)	1046 (95%)	59 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	232/262 (88%)	232 (100%)	0	100	100
1	B	230/262 (88%)	230 (100%)	0	100	100
1	C	231/262 (88%)	231 (100%)	0	100	100
1	D	232/262 (88%)	232 (100%)	0	100	100
All	All	925/1048 (88%)	925 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	339	GLN
1	B	369	GLN
1	D	521	ASN
1	D	578	ASN
1	D	582	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 oligosaccharides 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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	285/325 (87%)	0.21	15 (5%) 32 29	32, 55, 92, 143	0
1	B	283/325 (87%)	0.35	15 (5%) 32 29	32, 61, 106, 140	0
1	C	284/325 (87%)	0.56	22 (7%) 19 16	35, 60, 95, 136	0
1	D	285/325 (87%)	0.69	31 (10%) 10 8	36, 69, 121, 192	0
All	All	1137/1300 (87%)	0.45	83 (7%) 21 18	32, 61, 109, 192	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	560	GLY	5.6
1	A	300	GLY	4.9
1	A	467	PHE	4.3
1	C	499	ASN	3.9
1	D	535	ILE	3.9
1	A	524	TYR	3.8
1	D	300	GLY	3.8
1	D	256	LEU	3.8
1	A	263	MET	3.7
1	B	526	ASN	3.6
1	A	561	ALA	3.5
1	A	320	THR	3.5
1	A	358	GLY	3.5
1	B	525	VAL	3.3
1	B	562	VAL	3.3
1	B	524	TYR	3.2
1	D	571	MET	3.2
1	A	299	PRO	3.1
1	C	300	GLY	3.1
1	C	384	VAL	3.1
1	C	389	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	453	TYR	3.1
1	A	573	TYR	3.0
1	B	266	ARG	3.0
1	C	299	PRO	3.0
1	D	544	ALA	3.0
1	D	292	VAL	2.9
1	D	543	TYR	2.9
1	C	260	ILE	2.9
1	B	584	ALA	2.9
1	C	577	ALA	2.9
1	D	573	TYR	2.9
1	D	578	ASN	2.8
1	C	335	LEU	2.8
1	A	468	GLU	2.8
1	B	528	TYR	2.8
1	D	509	VAL	2.8
1	D	472	PRO	2.8
1	C	383	GLY	2.7
1	B	560	GLY	2.7
1	C	573	TYR	2.7
1	C	528	TYR	2.7
1	C	553	LYS	2.7
1	D	534	GLY	2.6
1	C	583	ASP	2.6
1	D	540	ASP	2.5
1	D	560	GLY	2.5
1	C	498	LYS	2.5
1	D	538	ILE	2.5
1	C	364	VAL	2.5
1	D	287	VAL	2.5
1	D	467	PHE	2.4
1	B	320	THR	2.4
1	C	469	LYS	2.4
1	D	451	ARG	2.4
1	A	528	TYR	2.4
1	C	288	ARG	2.4
1	D	266	ARG	2.3
1	D	497	ILE	2.3
1	D	545	LEU	2.3
1	B	260	ILE	2.3
1	B	519	ILE	2.3
1	D	549	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	553	LYS	2.3
1	A	298	ALA	2.2
1	D	561	ALA	2.2
1	D	539	SER	2.2
1	D	511	VAL	2.1
1	D	580	ILE	2.1
1	D	508	ARG	2.1
1	B	296	ALA	2.1
1	B	263	MET	2.1
1	A	429	ALA	2.1
1	C	259	ARG	2.1
1	B	268	ILE	2.1
1	C	535	ILE	2.1
1	D	260	ILE	2.1
1	D	265	TYR	2.1
1	C	467	PHE	2.0
1	C	475	ILE	2.0
1	B	300	GLY	2.0
1	C	348	ILE	2.0
1	A	466	SER	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 oligosaccharides 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.