



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:25 PM UTC

PDB ID : 3FG6 / pdb_00003fg6
Title : Structure of the C-terminus of Adseverin
Authors : Robinson, R.C.
Deposited on : 2008-12-05
Resolution : 3.00 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

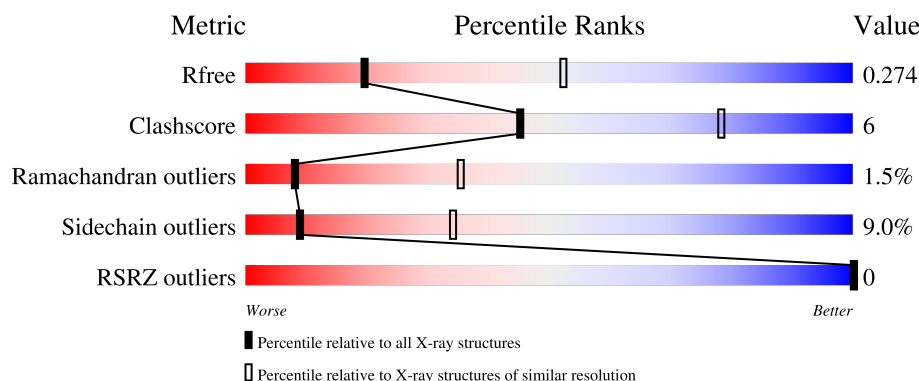
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	371	 64% 14% • 20%
1	B	371	 61% 17% • 20%
1	C	371	 66% 12% • • 18%
1	D	371	 65% 13% • 21%
1	E	371	 60% 14% • 23%

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Mol	Chain	Length	Quality of chain
1	F	371	 65%15%•19%
1	G	371	 65%13%•20%
1	H	371	 65%14%••18%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 19112 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 Adseverin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2381	1521	398	457	5			
1	C	303	Total	C	N	O	S	0	0	0
			2432	1546	410	471	5			
1	G	296	Total	C	N	O	S	0	0	0
			2381	1521	398	457	5			
1	E	285	Total	C	N	O	S	0	0	0
			2291	1468	383	435	5			
1	F	300	Total	C	N	O	S	0	0	0
			2410	1535	405	465	5			
1	H	306	Total	C	N	O	S	0	0	0
			2461	1566	415	475	5			
1	D	293	Total	C	N	O	S	0	0	0
			2352	1501	393	453	5			
1	B	296	Total	C	N	O	S	0	0	0
			2381	1521	398	457	5			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Ca	0	0
			3	3		
2	C	3	Total	Ca	0	0
			3	3		
2	G	3	Total	Ca	0	0
			3	3		
2	E	3	Total	Ca	0	0
			3	3		
2	F	2	Total	Ca	0	0
			2	2		
2	H	3	Total	Ca	0	0
			3	3		

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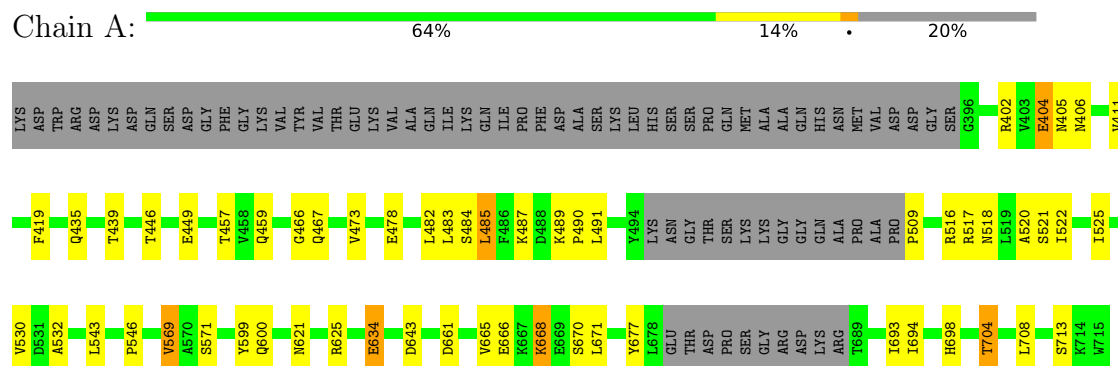
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	3	Total 3	Ca 3	0	0
2	B	3	Total 3	Ca 3	0	0

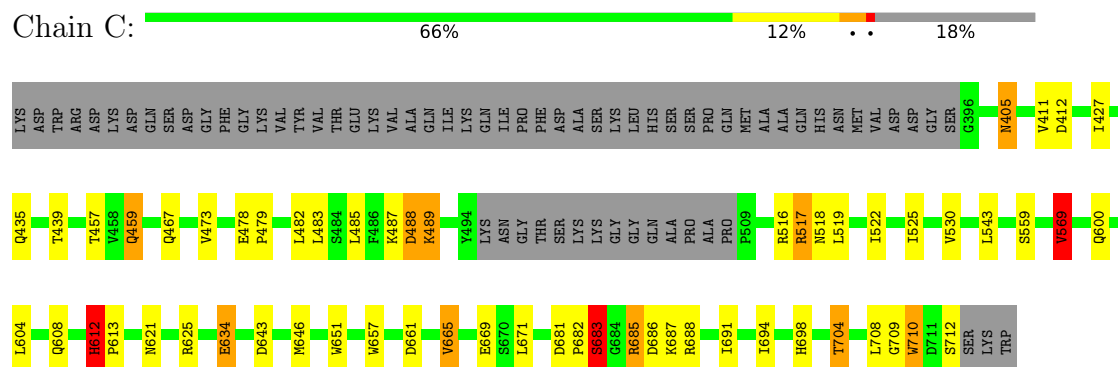
3 Residue-property plots

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.

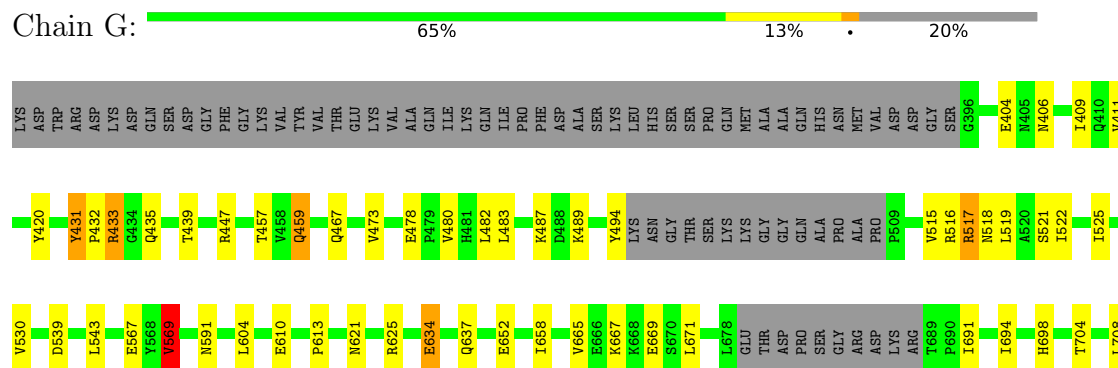
• Molecule 1: Adseverin



• Molecule 1: Adseverin



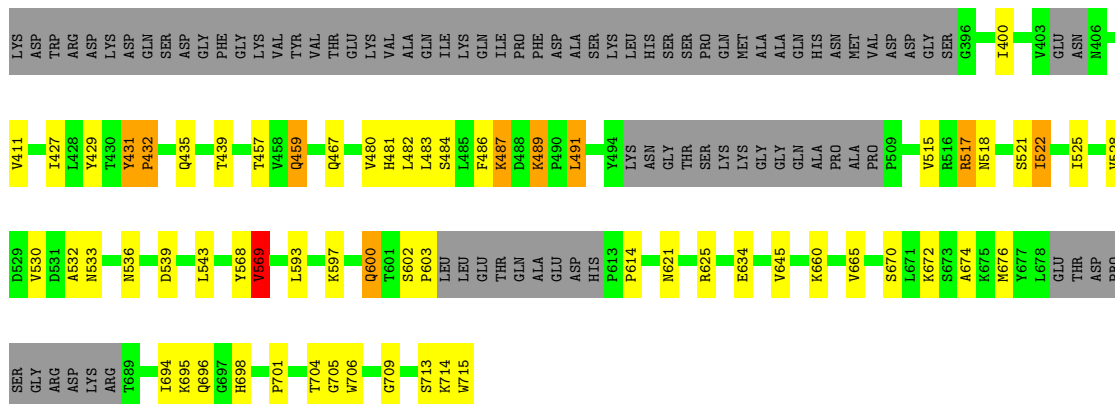
• Molecule 1: Adseverin





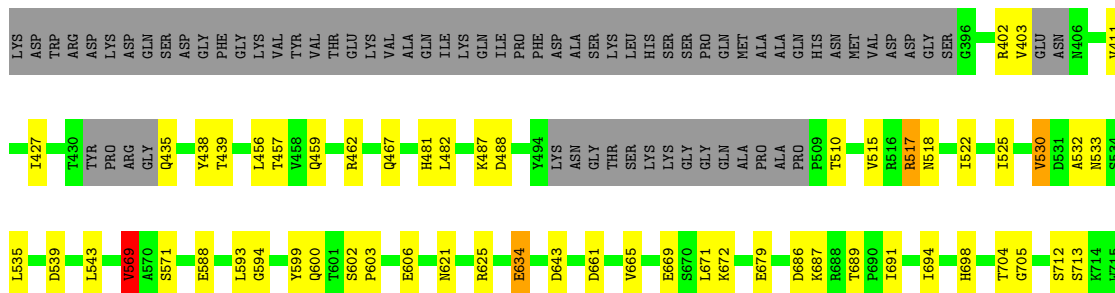
- Molecule 1: Adseverin

Chain E: 60% 14% 23%



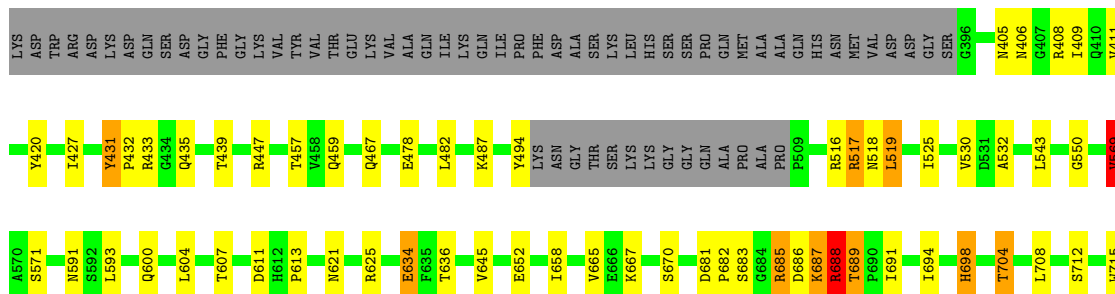
- Molecule 1: Adseverin

Chain F: 65% 15% 19%



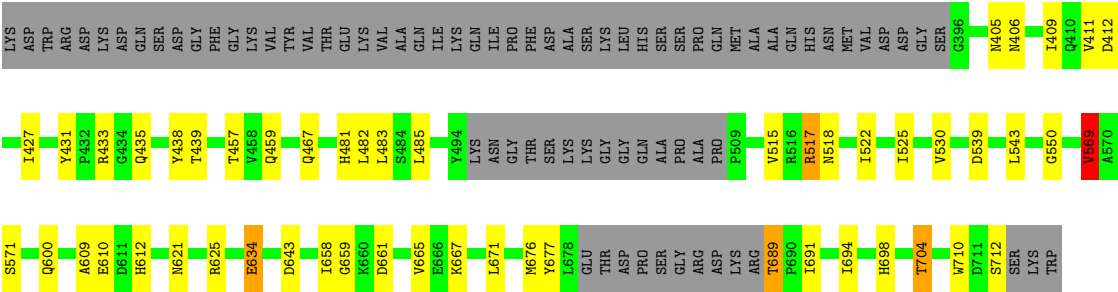
- Molecule 1: Adseverin

Chain H: 65% 14% 18%

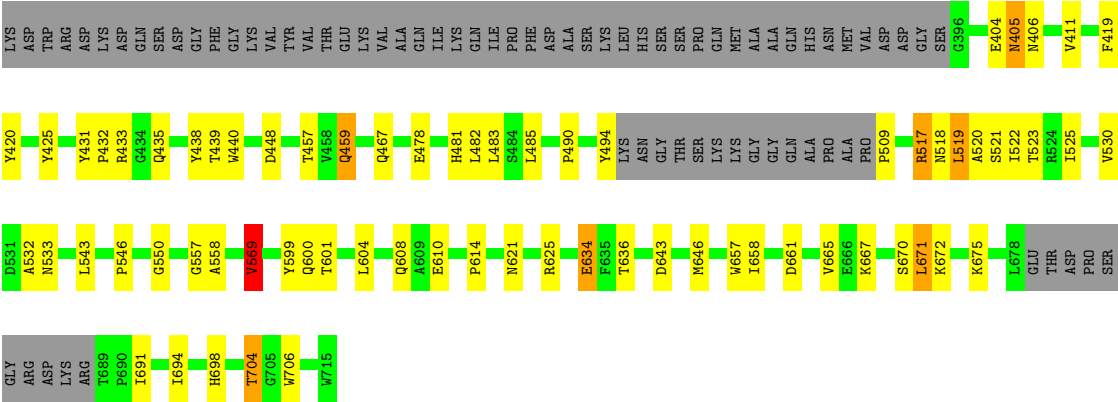


- Molecule 1: Adseverin

Chain D: 65% 13% 21%



● Molecule 1: Adseverin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	67.64Å 90.38Å 98.84Å 88.79° 88.26° 76.26°	Depositor
Resolution (Å)	29.92 – 3.00 29.92 – 3.00	Depositor EDS
% Data completeness (in resolution range)	90.2 (29.92-3.00) 90.3 (29.92-3.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.61 (at 3.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.244 , 0.295 0.233 , 0.274	Depositor DCC
R_{free} test set	2084 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	54.5	Xtriage
Anisotropy	0.873	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 69.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	19112	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section:
CA

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	0.45	0/2435	0.80	1/3299 (0.0%)
1	B	0.43	0/2435	0.79	2/3299 (0.1%)
1	C	0.46	0/2486	0.83	4/3368 (0.1%)
1	D	0.46	0/2404	0.83	6/3257 (0.2%)
1	E	0.44	0/2342	0.79	3/3168 (0.1%)
1	F	0.43	0/2462	0.78	3/3332 (0.1%)
1	G	0.44	0/2435	0.78	1/3299 (0.0%)
1	H	0.47	0/2517	0.82	4/3410 (0.1%)
All	All	0.45	0/19516	0.80	24/26432 (0.1%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	431	TYR	CA-C-N	8.49	130.45	119.84
1	H	431	TYR	C-N-CA	8.49	130.45	119.84
1	D	689	THR	CA-C-N	6.82	126.81	119.78
1	D	689	THR	C-N-CA	6.82	126.81	119.78
1	C	612	HIS	CA-C-N	6.56	124.39	119.66
1	C	612	HIS	C-N-CA	6.56	124.39	119.66
1	D	612	HIS	CA-C-N	6.40	124.33	119.66
1	D	612	HIS	C-N-CA	6.40	124.33	119.66
1	C	569	VAL	CB-CA-C	-5.59	104.59	112.14
1	H	569	VAL	CB-CA-C	-5.59	104.60	112.14
1	D	569	VAL	CB-CA-C	-5.56	104.63	112.14
1	F	602	SER	CA-C-N	5.49	126.70	119.84
1	F	602	SER	C-N-CA	5.49	126.70	119.84
1	E	569	VAL	CB-CA-C	-5.49	104.73	112.14
1	B	569	VAL	CB-CA-C	-5.42	104.82	112.14
1	B	550	GLY	N-CA-C	5.22	117.24	110.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	550	GLY	N-CA-C	5.18	117.19	110.45
1	C	405	ASN	N-CA-C	5.17	117.59	107.57
1	G	569	VAL	CB-CA-C	-5.14	105.20	112.14
1	E	431	TYR	CA-C-N	5.14	126.26	119.84
1	E	431	TYR	C-N-CA	5.14	126.26	119.84
1	F	569	VAL	CB-CA-C	-5.13	105.22	112.14
1	D	550	GLY	N-CA-C	5.11	117.09	110.45
1	A	466	GLY	N-CA-C	-5.07	108.29	115.43

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	2381	0	2329	28	0
1	B	2381	0	2329	37	1
1	C	2432	0	2377	32	0
1	D	2352	0	2301	24	0
1	E	2291	0	2251	35	0
1	F	2410	0	2359	29	1
1	G	2381	0	2329	38	0
1	H	2461	0	2405	37	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	3	0	0	0	0
2	F	2	0	0	0	0
2	G	3	0	0	0	0
2	H	3	0	0	0	0
All	All	19112	0	18680	222	1

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 6.

All (222) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:GLN:OE1	1:A:704:THR:HG22	1.61	0.99
1:G:525:ILE:HD13	1:G:569:VAL:HG22	1.50	0.90
1:H:525:ILE:HD13	1:H:569:VAL:HG22	1.51	0.90
1:C:525:ILE:HD13	1:C:569:VAL:HG22	1.55	0.88
1:D:483:LEU:HD22	1:D:522:ILE:HG21	1.57	0.84
1:B:482:LEU:O	1:B:485:LEU:HB2	1.78	0.83
1:D:525:ILE:HD13	1:D:569:VAL:HG22	1.61	0.83
1:B:525:ILE:HD13	1:B:569:VAL:HG22	1.61	0.82
1:G:567:GLU:HG2	1:F:462:ARG:NH2	1.93	0.82
1:C:651:TRP:HH2	1:C:683:SER:HG	1.26	0.80
1:F:525:ILE:HD13	1:F:569:VAL:HG22	1.63	0.80
1:E:517:ARG:HH22	1:E:522:ILE:HA	1.46	0.78
1:H:431:TYR:O	1:H:433:ARG:N	2.13	0.78
1:G:447:ARG:NH1	1:B:509:PRO:HB3	1.98	0.77
1:A:525:ILE:HD13	1:A:569:VAL:HG22	1.69	0.76
1:A:446:THR:OG1	1:H:698:HIS:HE1	1.69	0.75
1:E:660:LYS:HZ2	1:F:510:THR:HB	1.52	0.75
1:B:438:TYR:OH	1:B:481:HIS:HD2	1.69	0.74
1:G:591:ASN:HD21	1:D:412:ASP:CA	2.03	0.71
1:B:600:GLN:OE1	1:B:704:THR:HG22	1.90	0.71
1:E:660:LYS:HZ1	1:F:530:VAL:HG21	1.58	0.69
1:B:483:LEU:HD22	1:B:522:ILE:HG21	1.74	0.69
1:C:459:GLN:HE21	1:F:571:SER:HA	1.59	0.68
1:G:483:LEU:HD22	1:G:522:ILE:HG21	1.76	0.67
1:G:591:ASN:HD21	1:D:412:ASP:HB2	1.59	0.67
1:D:600:GLN:OE1	1:D:704:THR:HG22	1.95	0.67
1:E:525:ILE:HD13	1:E:569:VAL:HG22	1.77	0.67
1:E:517:ARG:NH2	1:E:522:ILE:HA	2.11	0.65
1:E:533:ASN:HB2	1:E:701:PRO:HB3	1.79	0.65
1:C:487:LYS:O	1:C:489:LYS:N	2.30	0.65
1:G:591:ASN:HD21	1:D:412:ASP:CB	2.11	0.64
1:A:446:THR:OG1	1:H:698:HIS:CE1	2.50	0.64
1:B:533:ASN:HA	1:B:599:TYR:HB3	1.79	0.64
1:A:600:GLN:OE1	1:A:704:THR:CG2	2.42	0.64
1:H:427:ILE:HD13	1:H:482:LEU:HD11	1.80	0.63
1:G:439:THR:OG1	1:G:457:THR:HG21	1.98	0.63
1:C:412:ASP:HB2	1:H:591:ASN:HD21	1.63	0.63
1:E:459:GLN:HE21	1:H:571:SER:HA	1.63	0.63
1:F:427:ILE:HD13	1:F:482:LEU:HD11	1.80	0.63
1:F:669:GLU:OE2	1:F:672:LYS:HD2	1.99	0.63
1:C:600:GLN:OE1	1:C:704:THR:HG22	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:PRO:HB3	1:H:447:ARG:NH1	2.13	0.62
1:G:591:ASN:ND2	1:D:412:ASP:HB2	2.15	0.62
1:C:651:TRP:HH2	1:C:683:SER:OG	1.81	0.61
1:A:666:GLU:O	1:A:670:SER:OG	2.19	0.60
1:C:483:LEU:HD22	1:C:522:ILE:HG21	1.83	0.60
1:A:439:THR:OG1	1:A:457:THR:HG21	2.01	0.60
1:H:686:ASP:HB3	1:H:689:THR:OG1	2.01	0.60
1:B:533:ASN:HA	1:B:599:TYR:CB	2.31	0.60
1:F:439:THR:OG1	1:F:457:THR:HG21	2.01	0.60
1:B:557:GLY:HA2	1:B:608:GLN:HB2	1.83	0.60
1:A:509:PRO:HB3	1:H:447:ARG:HH12	1.67	0.60
1:G:447:ARG:NH1	1:B:546:PRO:HB3	2.17	0.59
1:C:439:THR:OG1	1:C:457:THR:HG21	2.01	0.59
1:E:660:LYS:NZ	1:F:530:VAL:HG21	2.18	0.59
1:C:427:ILE:HD13	1:C:482:LEU:HD11	1.84	0.59
1:A:482:LEU:HA	1:A:485:LEU:HD22	1.85	0.59
1:C:412:ASP:HB2	1:H:591:ASN:ND2	2.18	0.59
1:H:439:THR:OG1	1:H:457:THR:HG21	2.03	0.59
1:G:591:ASN:ND2	1:D:412:ASP:CA	2.66	0.58
1:E:431:TYR:HB2	1:E:432:PRO:HD2	1.84	0.58
1:A:509:PRO:CB	1:H:447:ARG:HH12	2.16	0.58
1:D:643:ASP:HA	1:D:661:ASP:HB2	1.84	0.57
1:H:600:GLN:OE1	1:H:704:THR:HG22	2.05	0.57
1:B:439:THR:OG1	1:B:457:THR:HG21	2.04	0.57
1:B:405:ASN:CG	1:B:406:ASN:H	2.13	0.57
1:D:431:TYR:CE1	1:D:433:ARG:HB2	2.41	0.56
1:G:447:ARG:NH1	1:B:509:PRO:CB	2.68	0.56
1:G:709:GLY:O	1:G:710:TRP:CB	2.53	0.56
1:C:412:ASP:OD2	1:H:591:ASN:ND2	2.39	0.56
1:E:439:THR:OG1	1:E:457:THR:HG21	2.05	0.56
1:G:591:ASN:ND2	1:D:412:ASP:CB	2.69	0.56
1:G:567:GLU:HG2	1:F:462:ARG:CZ	2.36	0.55
1:F:600:GLN:HG2	1:F:705:GLY:HA3	1.88	0.55
1:H:681:ASP:C	1:H:683:SER:H	2.15	0.55
1:C:600:GLN:OE1	1:C:704:THR:CG2	2.54	0.55
1:C:709:GLY:O	1:C:710:TRP:HB2	2.06	0.54
1:A:473:VAL:HG11	1:A:478:GLU:HG3	1.89	0.54
1:E:429:TYR:CE2	1:E:431:TYR:HB3	2.43	0.54
1:D:405:ASN:C	1:D:406:ASN:HD22	2.15	0.54
1:B:438:TYR:OH	1:B:481:HIS:CD2	2.56	0.54
1:B:643:ASP:HA	1:B:661:ASP:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:658:ILE:HD13	1:H:667:LYS:HD3	1.90	0.53
1:F:438:TYR:OH	1:F:481:HIS:HB3	2.08	0.53
1:E:487:LYS:C	1:E:489:LYS:H	2.17	0.53
1:G:591:ASN:ND2	1:D:412:ASP:HA	2.24	0.52
1:H:688:ARG:O	1:H:689:THR:O	2.26	0.52
1:C:516:ARG:HB3	1:C:708:LEU:HD13	1.92	0.52
1:E:528:VAL:HG12	1:E:709:GLY:HA2	1.92	0.51
1:E:532:ALA:HB3	1:E:597:LYS:HD2	1.93	0.51
1:B:431:TYR:HB2	1:B:432:PRO:HD2	1.93	0.51
1:A:516:ARG:HD2	1:A:708:LEU:HB2	1.92	0.51
1:A:671:LEU:HD22	1:A:693:ILE:HD11	1.93	0.51
1:A:402:ARG:HH21	1:A:404:GLU:HG3	1.76	0.50
1:F:600:GLN:OE1	1:F:600:GLN:N	2.44	0.50
1:D:427:ILE:HD13	1:D:482:LEU:HD11	1.92	0.50
1:E:400:ILE:HD11	1:E:486:PHE:HE2	1.76	0.50
1:D:439:THR:OG1	1:D:457:THR:HG21	2.11	0.50
1:A:419:PHE:HE1	1:A:491:LEU:HD11	1.77	0.50
1:B:419:PHE:HD2	1:B:425:TYR:CD1	2.30	0.50
1:G:591:ASN:HD21	1:D:412:ASP:N	2.09	0.50
1:B:440:TRP:NE1	1:B:478:GLU:OE2	2.40	0.50
1:H:431:TYR:C	1:H:433:ARG:H	2.14	0.50
1:B:420:TYR:CD1	1:B:494:TYR:HB2	2.47	0.50
1:C:710:TRP:CD1	1:C:712:SER:HA	2.48	0.49
1:G:447:ARG:HH11	1:B:509:PRO:HB3	1.71	0.49
1:H:516:ARG:HB3	1:H:708:LEU:HD13	1.93	0.49
1:C:681:ASP:C	1:C:683:SER:H	2.21	0.49
1:A:532:ALA:O	1:A:599:TYR:HB3	2.12	0.48
1:H:687:LYS:C	1:H:689:THR:H	2.21	0.48
1:E:427:ILE:HD13	1:E:482:LEU:HD11	1.96	0.48
1:C:559:SER:HB3	1:C:608:GLN:NE2	2.28	0.48
1:C:487:LYS:C	1:C:489:LYS:H	2.21	0.48
1:C:643:ASP:HA	1:C:661:ASP:HB2	1.95	0.48
1:G:517:ARG:CG	1:G:517:ARG:HH21	2.26	0.48
1:E:695:LYS:HE2	1:F:594:GLY:O	2.12	0.48
1:F:643:ASP:HA	1:F:661:ASP:HB2	1.94	0.48
1:H:532:ALA:HA	1:H:593:LEU:HD13	1.96	0.48
1:G:604:LEU:HB2	1:G:652:GLU:OE1	2.13	0.48
1:C:665:VAL:O	1:C:669:GLU:HG2	2.14	0.48
1:F:533:ASN:HA	1:F:599:TYR:HB3	1.96	0.48
1:C:686:ASP:O	1:C:687:LYS:HG2	2.14	0.47
1:E:491:LEU:HD23	1:E:491:LEU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:517:ARG:HH22	1:F:522:ILE:HA	1.80	0.47
1:H:686:ASP:O	1:H:687:LYS:C	2.56	0.47
1:G:447:ARG:HH12	1:B:509:PRO:CB	2.27	0.47
1:G:473:VAL:HG11	1:G:478:GLU:HG3	1.97	0.47
1:G:637:GLN:HG3	1:G:710:TRP:CZ3	2.50	0.47
1:G:709:GLY:O	1:G:710:TRP:HB2	2.15	0.47
1:D:571:SER:HA	1:B:459:GLN:HE21	1.80	0.47
1:A:419:PHE:CE1	1:A:491:LEU:HD11	2.50	0.46
1:E:536:ASN:ND2	1:E:705:GLY:O	2.48	0.46
1:B:517:ARG:CG	1:B:517:ARG:HH21	2.27	0.46
1:B:558:ALA:O	1:B:608:GLN:NE2	2.48	0.46
1:C:473:VAL:HG11	1:C:478:GLU:HG3	1.96	0.46
1:E:715:TRP:O	1:F:530:VAL:HG22	2.15	0.46
1:B:519:LEU:HD21	1:B:610:GLU:HG3	1.98	0.46
1:A:634:GLU:H	1:A:634:GLU:HG2	1.49	0.46
1:E:660:LYS:NZ	1:F:510:THR:HB	2.26	0.46
1:H:604:LEU:HB2	1:H:652:GLU:CD	2.41	0.46
1:E:489:LYS:HE3	1:E:568:TYR:OH	2.14	0.46
1:B:658:ILE:HD13	1:B:667:LYS:HD3	1.97	0.46
1:A:483:LEU:HD23	1:A:522:ILE:CG2	2.46	0.46
1:E:532:ALA:HA	1:E:593:LEU:HD13	1.98	0.46
1:A:404:GLU:HA	1:A:405:ASN:HA	1.68	0.46
1:C:634:GLU:H	1:C:634:GLU:HG2	1.54	0.46
1:G:567:GLU:HB3	1:F:462:ARG:NE	2.31	0.46
1:C:517:ARG:HH21	1:C:517:ARG:CG	2.29	0.46
1:G:634:GLU:H	1:G:634:GLU:HG2	1.50	0.46
1:E:517:ARG:CG	1:E:517:ARG:HH21	2.29	0.46
1:H:687:LYS:O	1:H:689:THR:N	2.49	0.46
1:F:517:ARG:HH21	1:F:517:ARG:CG	2.30	0.45
1:G:658:ILE:HD13	1:G:667:LYS:HD3	1.98	0.45
1:B:517:ARG:NH2	1:B:520:ALA:O	2.50	0.45
1:D:517:ARG:CG	1:D:517:ARG:HH21	2.29	0.45
1:E:600:GLN:HG3	1:E:705:GLY:HA3	1.98	0.45
1:C:608:GLN:HA	1:C:608:GLN:OE1	2.17	0.44
1:G:420:TYR:CD1	1:G:494:TYR:HB2	2.51	0.44
1:H:600:GLN:OE1	1:H:704:THR:CG2	2.64	0.44
1:E:645:VAL:HG11	1:E:670:SER:OG	2.18	0.44
1:A:643:ASP:HA	1:A:661:ASP:HB2	1.99	0.44
1:E:481:HIS:O	1:E:484:SER:N	2.46	0.44
1:A:546:PRO:HB3	1:H:447:ARG:HH12	1.82	0.44
1:E:696:GLN:HE21	1:E:715:TRP:CG	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:634:GLU:H	1:F:634:GLU:HG2	1.49	0.44
1:H:681:ASP:OD2	1:H:682:PRO:HD2	2.19	0.43
1:B:482:LEU:O	1:B:485:LEU:CB	2.59	0.43
1:A:449:GLU:CD	1:H:698:HIS:CE1	2.97	0.43
1:C:487:LYS:C	1:C:489:LYS:N	2.76	0.43
1:G:517:ARG:HH22	1:G:522:ILE:HA	1.84	0.43
1:A:489:LYS:HA	1:A:490:PRO:HD3	1.89	0.43
1:H:634:GLU:H	1:H:634:GLU:HG2	1.48	0.43
1:H:517:ARG:HH21	1:H:517:ARG:CG	2.32	0.43
1:B:646:MET:HB2	1:B:657:TRP:HB3	2.01	0.43
1:A:668:LYS:HD2	1:A:668:LYS:N	2.33	0.43
1:B:671:LEU:O	1:B:675:LYS:HG3	2.18	0.43
1:C:600:GLN:HG2	1:C:704:THR:HG22	2.02	0.42
1:B:532:ALA:O	1:B:599:TYR:HB3	2.18	0.42
1:D:634:GLU:H	1:D:634:GLU:HG2	1.53	0.42
1:B:490:PRO:HB3	1:B:523:THR:HB	2.02	0.42
1:E:487:LYS:O	1:E:489:LYS:N	2.51	0.42
1:G:482:LEU:O	1:G:483:LEU:C	2.62	0.42
1:H:645:VAL:HG21	1:H:667:LYS:HA	2.01	0.42
1:B:614:PRO:HG3	1:B:706:TRP:CE3	2.54	0.42
1:E:602:SER:HA	1:E:603:PRO:HD3	1.93	0.42
1:D:438:TYR:OH	1:D:481:HIS:HD2	2.03	0.42
1:A:571:SER:HA	1:G:459:GLN:HE21	1.85	0.42
1:E:614:PRO:HG3	1:E:706:TRP:CE3	2.54	0.42
1:C:651:TRP:HH2	1:C:683:SER:CB	2.32	0.42
1:F:403:VAL:HG13	1:F:456:LEU:HD12	2.02	0.42
1:G:669:GLU:HA	1:G:669:GLU:OE2	2.20	0.42
1:D:515:VAL:O	1:D:539:ASP:HB3	2.20	0.42
1:B:634:GLU:H	1:B:634:GLU:HG2	1.54	0.42
1:E:483:LEU:HD13	1:E:522:ILE:HG22	2.02	0.41
1:H:487:LYS:H	1:H:487:LYS:HG2	1.63	0.41
1:G:519:LEU:HD11	1:G:613:PRO:HB3	2.02	0.41
1:F:515:VAL:O	1:F:539:ASP:HB3	2.20	0.41
1:F:532:ALA:HA	1:F:593:LEU:HD13	2.02	0.41
1:F:535:LEU:O	1:F:600:GLN:OE1	2.38	0.41
1:D:658:ILE:HD13	1:D:667:LYS:HD3	2.01	0.41
1:D:659:GLY:C	1:D:661:ASP:H	2.27	0.41
1:G:515:VAL:O	1:G:539:ASP:HB3	2.21	0.41
1:H:478:GLU:OE1	1:H:478:GLU:N	2.54	0.41
1:H:519:LEU:HD11	1:H:613:PRO:HG3	2.03	0.41
1:D:710:TRP:CD1	1:D:712:SER:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:713:SER:HB2	1:F:713:SER:H	1.86	0.41
1:A:546:PRO:HB3	1:H:447:ARG:NH1	2.35	0.41
1:G:516:ARG:HD2	1:G:708:LEU:HB2	2.03	0.41
1:B:670:SER:C	1:B:672:LYS:H	2.29	0.41
1:C:478:GLU:HA	1:C:479:PRO:HD3	1.92	0.41
1:E:515:VAL:O	1:E:539:ASP:HB3	2.21	0.41
1:E:674:ALA:C	1:E:676:MET:H	2.29	0.41
1:H:420:TYR:CD1	1:H:494:TYR:HB2	2.56	0.41
1:B:404:GLU:O	1:B:405:ASN:C	2.62	0.41
1:G:431:TYR:CD2	1:G:431:TYR:N	2.89	0.40
1:C:612:HIS:HA	1:C:613:PRO:HD2	1.86	0.40
1:C:646:MET:HB2	1:C:657:TRP:HB3	2.03	0.40
1:G:432:PRO:HB2	1:G:433:ARG:HD2	2.04	0.40
1:B:517:ARG:HH22	1:B:522:ILE:HA	1.86	0.40
1:F:487:LYS:H	1:F:487:LYS:HG2	1.71	0.40
1:F:686:ASP:O	1:F:687:LYS:HG2	2.21	0.40
1:G:487:LYS:H	1:G:487:LYS:HG2	1.67	0.40

All (1) 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:F:588:GLU:OE1	1:B:448:ASP:N[1_556]	2.07	0.13

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	290/371 (78%)	271 (93%)	16 (6%)	3 (1%)	12	45
1	B	290/371 (78%)	267 (92%)	19 (7%)	4 (1%)	9	36
1	C	299/371 (81%)	274 (92%)	17 (6%)	8 (3%)	4	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	287/371 (77%)	269 (94%)	16 (6%)	2 (1%)	18	53
1	E	275/371 (74%)	258 (94%)	13 (5%)	4 (2%)	8	35
1	F	292/371 (79%)	267 (91%)	21 (7%)	4 (1%)	9	36
1	G	290/371 (78%)	273 (94%)	14 (5%)	3 (1%)	12	45
1	H	302/371 (81%)	278 (92%)	16 (5%)	8 (3%)	4	23
All	All	2325/2968 (78%)	2157 (93%)	132 (6%)	36 (2%)	8	35

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	488	ASP
1	G	710	TRP
1	H	405	ASN
1	H	432	PRO
1	H	611	ASP
1	H	689	THR
1	B	405	ASN
1	A	487	LYS
1	C	519	LEU
1	C	710	TRP
1	E	487	LYS
1	E	521	SER
1	F	606	GLU
1	H	687	LYS
1	G	521	SER
1	F	603	PRO
1	F	689	THR
1	H	688	ARG
1	A	520	ALA
1	C	682	PRO
1	C	688	ARG
1	D	609	ALA
1	C	683	SER
1	E	432	PRO
1	H	685	ARG
1	B	521	SER
1	C	685	ARG
1	D	530	VAL
1	B	519	LEU
1	A	530	VAL

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Mol	Chain	Res	Type
1	C	530	VAL
1	G	530	VAL
1	E	530	VAL
1	F	530	VAL
1	H	530	VAL
1	B	530	VAL

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	258/320 (81%)	235 (91%)	23 (9%)	9	34
1	B	258/320 (81%)	237 (92%)	21 (8%)	11	38
1	C	264/320 (82%)	239 (90%)	25 (10%)	8	31
1	D	255/320 (80%)	232 (91%)	23 (9%)	9	34
1	E	248/320 (78%)	226 (91%)	22 (9%)	9	34
1	F	262/320 (82%)	241 (92%)	21 (8%)	11	38
1	G	258/320 (81%)	233 (90%)	25 (10%)	8	30
1	H	267/320 (83%)	240 (90%)	27 (10%)	7	29
All	All	2070/2560 (81%)	1883 (91%)	187 (9%)	9	34

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	404	GLU
1	A	406	ASN
1	A	411	VAL
1	A	435	GLN
1	A	459	GLN
1	A	467	GLN
1	A	484	SER
1	A	485	LEU
1	A	517	ARG

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Mol	Chain	Res	Type
1	A	518	ASN
1	A	521	SER
1	A	543	LEU
1	A	569	VAL
1	A	621	ASN
1	A	625	ARG
1	A	634	GLU
1	A	665	VAL
1	A	668	LYS
1	A	677	TYR
1	A	694	ILE
1	A	698	HIS
1	A	704	THR
1	A	713	SER
1	C	405	ASN
1	C	411	VAL
1	C	435	GLN
1	C	459	GLN
1	C	467	GLN
1	C	485	LEU
1	C	488	ASP
1	C	489	LYS
1	C	517	ARG
1	C	518	ASN
1	C	543	LEU
1	C	569	VAL
1	C	604	LEU
1	C	612	HIS
1	C	621	ASN
1	C	625	ARG
1	C	634	GLU
1	C	665	VAL
1	C	671	LEU
1	C	683	SER
1	C	685	ARG
1	C	691	ILE
1	C	694	ILE
1	C	698	HIS
1	C	704	THR
1	G	404	GLU
1	G	406	ASN
1	G	409	ILE

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Mol	Chain	Res	Type
1	G	411	VAL
1	G	431	TYR
1	G	433	ARG
1	G	435	GLN
1	G	459	GLN
1	G	467	GLN
1	G	480	VAL
1	G	489	LYS
1	G	517	ARG
1	G	518	ASN
1	G	543	LEU
1	G	569	VAL
1	G	610	GLU
1	G	621	ASN
1	G	625	ARG
1	G	634	GLU
1	G	665	VAL
1	G	671	LEU
1	G	691	ILE
1	G	694	ILE
1	G	698	HIS
1	G	704	THR
1	E	411	VAL
1	E	435	GLN
1	E	459	GLN
1	E	467	GLN
1	E	480	VAL
1	E	489	LYS
1	E	491	LEU
1	E	517	ARG
1	E	518	ASN
1	E	522	ILE
1	E	543	LEU
1	E	569	VAL
1	E	600	GLN
1	E	621	ASN
1	E	625	ARG
1	E	634	GLU
1	E	665	VAL
1	E	672	LYS
1	E	694	ILE
1	E	698	HIS

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Mol	Chain	Res	Type
1	E	704	THR
1	E	714	LYS
1	F	402	ARG
1	F	411	VAL
1	F	435	GLN
1	F	459	GLN
1	F	467	GLN
1	F	488	ASP
1	F	517	ARG
1	F	518	ASN
1	F	543	LEU
1	F	569	VAL
1	F	621	ASN
1	F	625	ARG
1	F	634	GLU
1	F	665	VAL
1	F	671	LEU
1	F	679	GLU
1	F	691	ILE
1	F	694	ILE
1	F	698	HIS
1	F	704	THR
1	F	712	SER
1	H	406	ASN
1	H	408	ARG
1	H	409	ILE
1	H	411	VAL
1	H	435	GLN
1	H	459	GLN
1	H	467	GLN
1	H	517	ARG
1	H	518	ASN
1	H	519	LEU
1	H	543	LEU
1	H	569	VAL
1	H	607	THR
1	H	621	ASN
1	H	625	ARG
1	H	634	GLU
1	H	636	THR
1	H	665	VAL
1	H	670	SER

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Mol	Chain	Res	Type
1	H	685	ARG
1	H	688	ARG
1	H	691	ILE
1	H	694	ILE
1	H	698	HIS
1	H	704	THR
1	H	712	SER
1	H	715	TRP
1	D	409	ILE
1	D	411	VAL
1	D	435	GLN
1	D	459	GLN
1	D	467	GLN
1	D	485	LEU
1	D	517	ARG
1	D	518	ASN
1	D	543	LEU
1	D	569	VAL
1	D	610	GLU
1	D	621	ASN
1	D	625	ARG
1	D	634	GLU
1	D	665	VAL
1	D	671	LEU
1	D	676	MET
1	D	677	TYR
1	D	689	THR
1	D	691	ILE
1	D	694	ILE
1	D	698	HIS
1	D	704	THR
1	B	411	VAL
1	B	433	ARG
1	B	435	GLN
1	B	459	GLN
1	B	467	GLN
1	B	517	ARG
1	B	518	ASN
1	B	543	LEU
1	B	569	VAL
1	B	601	THR
1	B	604	LEU

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Mol	Chain	Res	Type
1	B	621	ASN
1	B	625	ARG
1	B	634	GLU
1	B	636	THR
1	B	665	VAL
1	B	671	LEU
1	B	691	ILE
1	B	694	ILE
1	B	698	HIS
1	B	704	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	414	ASN
1	A	441	GLN
1	A	481	HIS
1	A	581	GLN
1	A	591	ASN
1	A	621	ASN
1	C	405	ASN
1	C	413	GLN
1	C	414	ASN
1	C	441	GLN
1	C	459	GLN
1	C	518	ASN
1	C	591	ASN
1	C	621	ASN
1	G	414	ASN
1	G	441	GLN
1	G	459	GLN
1	G	481	HIS
1	G	518	ASN
1	G	591	ASN
1	G	600	GLN
1	G	621	ASN
1	E	414	ASN
1	E	441	GLN
1	E	459	GLN
1	E	514	GLN
1	E	518	ASN
1	E	591	ASN

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Mol	Chain	Res	Type
1	E	600	GLN
1	E	621	ASN
1	F	441	GLN
1	F	514	GLN
1	F	518	ASN
1	F	547	GLN
1	F	591	ASN
1	F	621	ASN
1	H	414	ASN
1	H	441	GLN
1	H	518	ASN
1	H	581	GLN
1	H	591	ASN
1	H	621	ASN
1	H	698	HIS
1	D	406	ASN
1	D	414	ASN
1	D	441	GLN
1	D	459	GLN
1	D	481	HIS
1	D	518	ASN
1	D	591	ASN
1	D	608	GLN
1	D	621	ASN
1	B	406	ASN
1	B	441	GLN
1	B	459	GLN
1	B	481	HIS
1	B	518	ASN
1	B	581	GLN
1	B	591	ASN
1	B	608	GLN
1	B	621	ASN
1	B	653	GLN
1	B	663	ASN

5.3.3 RNA ⓘ

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](#)

Of 23 ligands modelled in this entry, 23 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	296/371 (79%)	-1.61	0 100 100	24, 39, 40, 47	0
1	B	296/371 (79%)	-1.63	0 100 100	28, 39, 43, 48	0
1	C	303/371 (81%)	-1.61	0 100 100	17, 39, 40, 45	0
1	D	293/371 (78%)	-1.61	0 100 100	31, 39, 42, 45	0
1	E	285/371 (76%)	-1.57	0 100 100	21, 39, 41, 51	0
1	F	300/371 (80%)	-1.55	0 100 100	26, 39, 46, 49	0
1	G	296/371 (79%)	-1.55	0 100 100	31, 39, 42, 47	0
1	H	306/371 (82%)	-1.66	0 100 100	26, 39, 40, 46	0
All	All	2375/2968 (80%)	-1.60	0 100 100	17, 39, 42, 51	0

There are no RSRZ outliers to report.

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	A	2001	1/1	0.98	0.04	64,64,64,64	0
2	CA	B	2001	1/1	0.98	0.05	61,61,61,61	0
2	CA	G	2001	1/1	0.99	0.04	39,39,39,39	0
2	CA	E	2001	1/1	0.99	0.03	41,41,41,41	0
2	CA	E	2002	1/1	0.99	0.07	49,49,49,49	0
2	CA	D	2001	1/1	0.99	0.03	56,56,56,56	0
2	CA	C	2001	1/1	0.99	0.05	71,71,71,71	0
2	CA	G	2002	1/1	1.00	0.04	15,15,15,15	0
2	CA	G	2003	1/1	1.00	0.03	28,28,28,28	0
2	CA	A	2002	1/1	1.00	0.04	7,7,7,7	0
2	CA	C	2002	1/1	1.00	0.03	25,25,25,25	0
2	CA	E	2003	1/1	1.00	0.05	26,26,26,26	0
2	CA	F	2002	1/1	1.00	0.02	36,36,36,36	0
2	CA	F	2003	1/1	1.00	0.01	34,34,34,34	0
2	CA	H	2001	1/1	1.00	0.01	58,58,58,58	0
2	CA	H	2002	1/1	1.00	0.04	10,10,10,10	0
2	CA	H	2003	1/1	1.00	0.01	35,35,35,35	0
2	CA	C	2003	1/1	1.00	0.01	33,33,33,33	0
2	CA	D	2002	1/1	1.00	0.02	27,27,27,27	0
2	CA	D	2003	1/1	1.00	0.01	17,17,17,17	0
2	CA	A	2003	1/1	1.00	0.02	31,31,31,31	0
2	CA	B	2002	1/1	1.00	0.04	16,16,16,16	0
2	CA	B	2003	1/1	1.00	0.04	19,19,19,19	0

6.5 Other polymers

There are no such residues in this entry.