



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:39 AM GMT

PDB ID : 3FG6
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

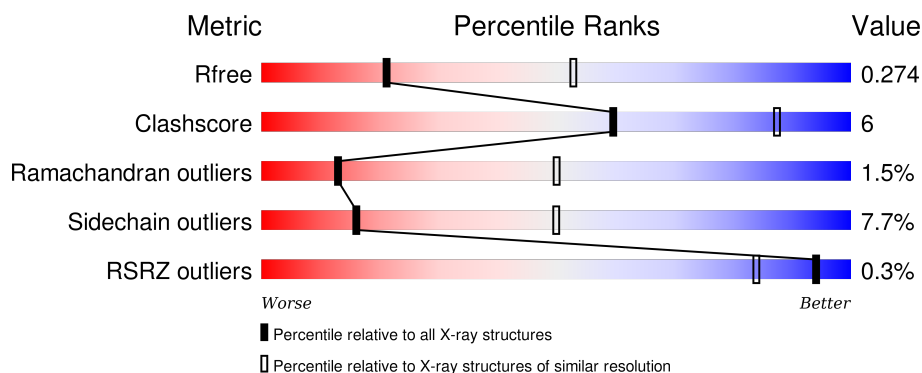
1 Overall quality at a glance

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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	
1	B	371	
1	C	371	
1	D	371	
1	E	371	

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Mol	Chain	Length	Quality of chain
1	F	371	<div><div><div>%</div><div><div></div><div>67%</div><div>13%</div><div>•</div><div>19%</div></div></div></div>
1	G	371	<div><div><div></div><div>66%</div><div>12%</div><div>•</div><div>20%</div></div></div>
1	H	371	<div><div><div>%</div><div><div></div><div>68%</div><div>12%</div><div>•</div><div>18%</div></div></div></div>

2 Entry composition

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 (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	3	Total	Ca	0	0
			3	3		
2	D	3	Total	Ca	0	0
			3	3		
2	E	3	Total	Ca	0	0
			3	3		
2	H	3	Total	Ca	0	0
			3	3		
2	B	3	Total	Ca	0	0
			3	3		
2	C	3	Total	Ca	0	0
			3	3		

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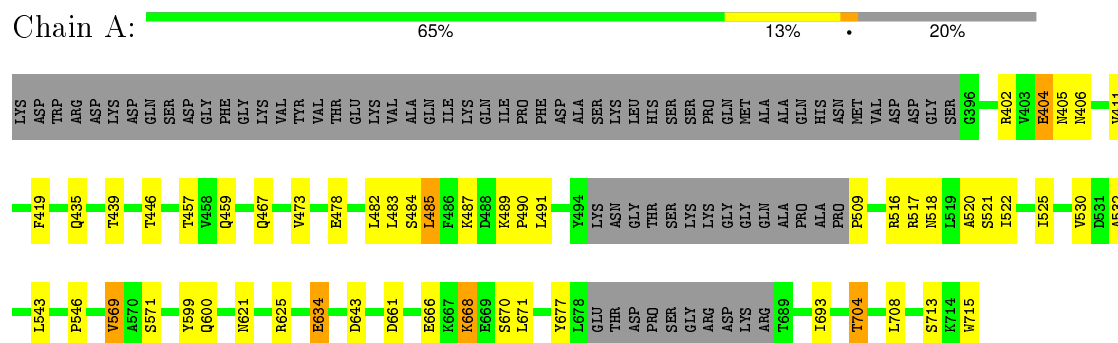
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total 3	Ca 3	0	0
2	F	2	Total 2	Ca 2	0	0

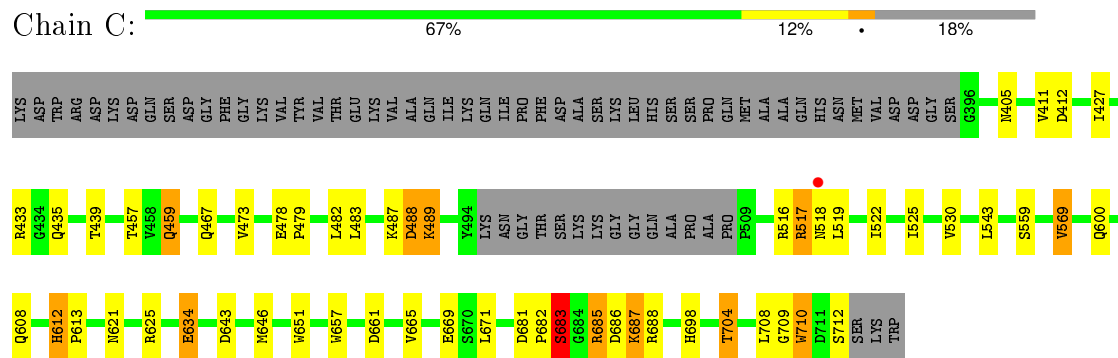
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

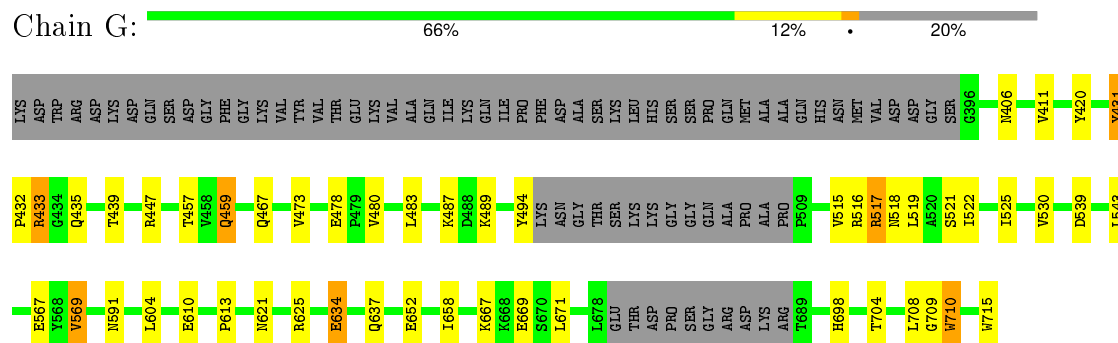
• Molecule 1: Adseverin



• Molecule 1: Adseverin

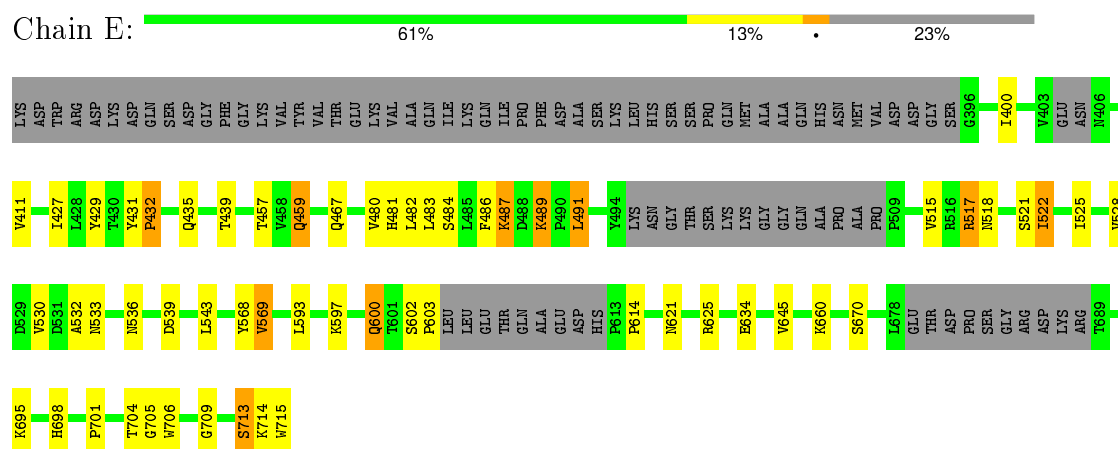


• Molecule 1: Adseverin



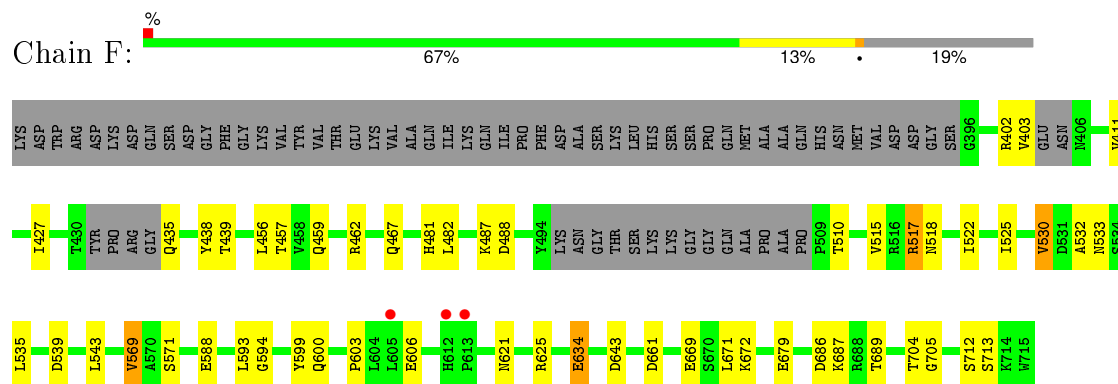
• Molecule 1: Adseverin

Chain E:



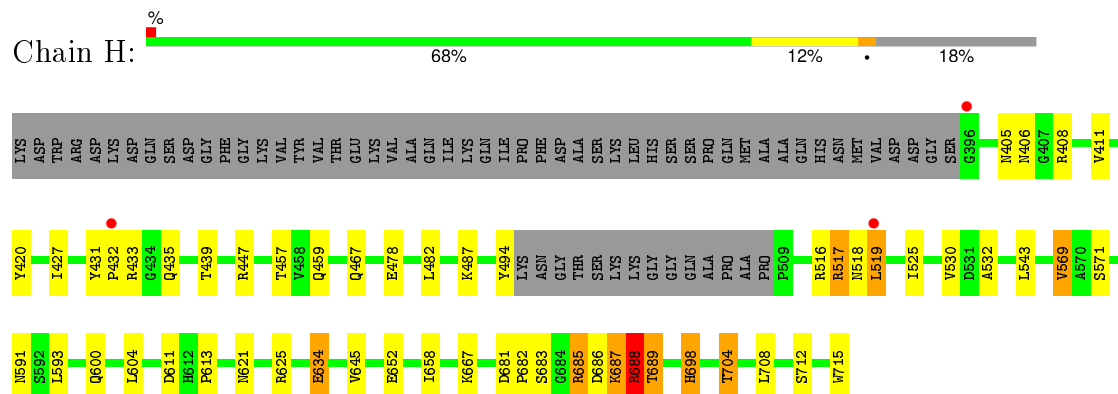
- Molecule 1: Adseverin

Chain F:



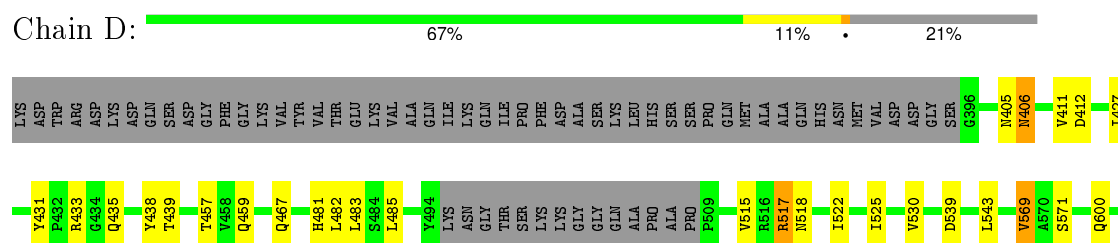
- Molecule 1: Adseverin

Chain H:



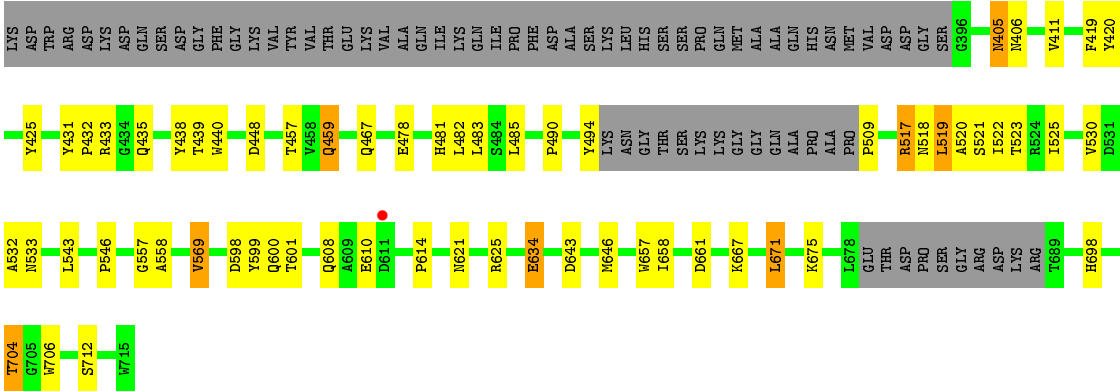
- Molecule 1: Adseverin

Chain D:





● 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 – 2.99	Depositor EDS
% Data completeness (in resolution range)	90.2 (29.92-3.00) 89.9 (29.92-2.99)	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 5.2.0019	Depositor
R, R_{free}	0.244 , 0.295 0.233 , 0.274	Depositor DCC
R_{free} test set	2078 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	54.5	Xtriage
Anisotropy	0.873	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.8	EDS
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 41214 reflections	Xtriage
F_o, F_c correlation	0.92	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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.37	0/2435	0.52	0/3299
1	B	0.36	0/2435	0.52	0/3299
1	C	0.39	0/2486	0.54	0/3368
1	D	0.36	0/2404	0.51	0/3257
1	E	0.37	0/2342	0.52	0/3168
1	F	0.35	0/2462	0.52	0/3332
1	G	0.37	0/2435	0.52	0/3299
1	H	0.39	0/2517	0.54	0/3410
All	All	0.37	0/19516	0.52	0/26432

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

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	27	0
1	B	2381	0	2329	35	1
1	C	2432	0	2377	31	0
1	D	2352	0	2301	23	0
1	E	2291	0	2251	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2410	0	2359	29	1
1	G	2381	0	2329	37	0
1	H	2461	0	2405	36	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	214	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 (214) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:669:GLU:OE2	1:F:672:LYS:HD2	1.99	0.63
1:F:427:ILE:HD13	1:F:482:LEU:HD11	1.80	0.63
1:E:459:GLN:HE21	1:H:571:SER:HA	1.63	0.63
1:C:600:GLN:OE1	1:C:704:THR:HG22	1.98	0.63
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:B:533:ASN:HA	1:B:599:TYR:CB	2.31	0.60
1:H:686:ASP:HB3	1:H:689:THR:OG1	2.01	0.60
1:A:439:THR:OG1	1:A:457:THR:HG21	2.01	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:E:660:LYS:NZ	1:F:530:VAL:HG21	2.18	0.59
1:C:439:THR:OG1	1:C:457:THR:HG21	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:THR:OG1	1:B:457:THR:HG21	2.04	0.57
1:H:600:GLN:OE1	1:H:704:THR:HG22	2.05	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:C:709:GLY:O	1:C:710:TRP:HB2	2.06	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:C:600:GLN:OE1	1:C:704:THR:CG2	2.54	0.55
1:E:429:TYR:CE2	1:E:431:TYR:HB3	2.43	0.54
1:A:473:VAL:HG11	1:A:478:GLU:HG3	1.89	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
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: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:B:405:ASN:CG	1:B:406:ASN:H	2.13	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:F:600:GLN:OE1	1:F:600:GLN:N	2.44	0.50
1:A:402:ARG:HH21	1:A:404:GLU:HG3	1.76	0.50
1:D:427:ILE:HD13	1:D:482:LEU:HD11	1.92	0.50
1:H:681:ASP:C	1:H:683:SER:H	2.15	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:B:420:TYR:CD1	1:B:494:TYR:HB2	2.47	0.50
1:G:447:ARG:HH11	1:B:509:PRO:HB3	1.71	0.49
1:C:710:TRP:CD1	1:C:712:SER:HA	2.48	0.49
1:D:405:ASN:C	1:D:406:ASN:HD22	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:516:ARG:HB3	1:H:708:LEU:HD13	1.93	0.49
1:A:532:ALA:O	1:A:599:TYR:HB3	2.12	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:643:ASP:HA	1:C:661:ASP:HB2	1.95	0.48
1:G:517:ARG:HH21	1:G:517:ARG:CG	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:E:487:LYS:C	1:E:489:LYS:H	2.17	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:O	1:E:491:LEU:HD23	2.14	0.47
1:F:517:ARG:HH22	1:F:522:ILE:HA	1.80	0.47
1:G:447:ARG:HH12	1:B:509:PRO:CB	2.27	0.47
1:G:637:GLN:HG3	1:G:710:TRP:CZ3	2.50	0.47
1:G:473:VAL:HG11	1:G:478:GLU:HG3	1.97	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:B:517:ARG:HH21	1:B:517:ARG:CG	2.27	0.46
1:B:558:ALA:O	1:B:608:GLN:NE2	2.48	0.46
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:E:715:TRP:O	1:F:530:VAL:HG22	2.15	0.46
1:C:473:VAL:HG11	1:C:478:GLU:HG3	1.96	0.46
1:B:519:LEU:HD21	1:B:610:GLU:HG3	1.98	0.46
1:E:660:LYS:NZ	1:F:510:THR:HB	2.26	0.46
1:A:634:GLU:H	1:A:634:GLU:HG2	1.49	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:E:532:ALA:HA	1:E:593:LEU:HD13	1.98	0.46
1:A:483:LEU:HD23	1:A:522:ILE:CG2	2.46	0.46
1:A:404:GLU:HA	1:A:405:ASN:HA	1.68	0.46
1:G:567:GLU:HB3	1:F:462:ARG:NE	2.31	0.46
1:C:634:GLU:HG2	1:C:634:GLU:H	1.54	0.46
1:E:517:ARG:HH21	1:E:517:ARG:CG	2.29	0.46
1:G:634:GLU:H	1:G:634:GLU:HG2	1.50	0.46
1:C:517:ARG:CG	1:C:517:ARG:HH21	2.29	0.46
1:H:687:LYS:O	1:H:689:THR:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:517:ARG:CG	1:F:517:ARG:HH21	2.30	0.45
1:H:431:TYR:C	1:H:433:ARG:H	2.14	0.45
1:B:517:ARG:NH2	1:B:520:ALA:O	2.50	0.45
1:G:658:ILE:HD13	1:G:667:LYS:HD3	1.98	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:OE1	1:C:608:GLN:HA	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:C:681:ASP:C	1:C:683:SER:H	2.21	0.44
1:E:645:VAL:HG11	1:E:670:SER:OG	2.18	0.44
1:E:481:HIS:O	1:E:484:SER:N	2.46	0.44
1:A:643:ASP:HA	1:A:661:ASP:HB2	1.99	0.44
1:A:546:PRO:HB3	1:H:447:ARG:HH12	1.82	0.44
1:H:687:LYS:C	1:H:689:THR:H	2.21	0.44
1:F:634:GLU:HG2	1:F:634:GLU:H	1.49	0.44
1:C:487:LYS:C	1:C:489:LYS:H	2.21	0.43
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: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:HG2	1:H:634:GLU:H	1.48	0.43
1:B:646:MET:HB2	1:B:657:TRP:HB3	2.01	0.43
1:H:517:ARG:CG	1:H:517:ARG:HH21	2.32	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:H:686:ASP:O	1:H:687:LYS:C	2.56	0.42
1:B:532:ALA:O	1:B:599:TYR:HB3	2.18	0.42
1:C:600:GLN:HG2	1:C:704:THR:HG22	2.02	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: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:D:515:VAL:O	1:D:539:ASP:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:634:GLU:H	1:B:634:GLU:HG2	1.54	0.42
1:G:669:GLU:HA	1:G:669:GLU:OE2	2.20	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:535:LEU:O	1:F:600:GLN:OE1	2.38	0.41
1:F:532:ALA:HA	1:F:593:LEU:HD13	2.02	0.41
1:D:658:ILE:HD13	1:D:667:LYS:HD3	2.01	0.41
1:D:710:TRP:CD1	1:D:712:SER:HA	2.56	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:G:515:VAL:O	1:G:539:ASP:HB3	2.21	0.41
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:H:604:LEU:HB2	1:H:652:GLU:CD	2.41	0.41
1:G:516:ARG:HD2	1:G:708:LEU:HB2	2.03	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:H:420:TYR:CD1	1:H:494:TYR:HB2	2.56	0.41
1:G:431:TYR:CD2	1:G:431:TYR:N	2.89	0.40
1:B:517:ARG:HH22	1:B:522:ILE:HA	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:C:612:HIS:HA	1:C:613:PRO:HD2	1.86	0.40
1:F:686:ASP:O	1:F:687:LYS:HG2	2.21	0.40
1:F:487:LYS:H	1:F:487:LYS:HG2	1.71	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

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	290/371 (78%)	271 (93%)	16 (6%)	3 (1%)	19	61
1	B	290/371 (78%)	267 (92%)	19 (7%)	4 (1%)	14	51
1	C	299/371 (81%)	274 (92%)	17 (6%)	8 (3%)	6	32
1	D	287/371 (77%)	269 (94%)	16 (6%)	2 (1%)	26	70
1	E	275/371 (74%)	258 (94%)	13 (5%)	4 (2%)	13	50
1	F	292/371 (79%)	267 (91%)	21 (7%)	4 (1%)	14	51
1	G	290/371 (78%)	273 (94%)	14 (5%)	3 (1%)	19	61
1	H	302/371 (81%)	278 (92%)	16 (5%)	8 (3%)	7	33
All	All	2325/2968 (78%)	2157 (93%)	132 (6%)	36 (2%)	13	50

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

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Mol	Chain	Res	Type
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
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%)	237 (92%)	21 (8%)	15	47
1	B	258/320 (81%)	240 (93%)	18 (7%)	19	55
1	C	264/320 (82%)	242 (92%)	22 (8%)	14	46
1	D	255/320 (80%)	235 (92%)	20 (8%)	16	49
1	E	248/320 (78%)	228 (92%)	20 (8%)	15	47
1	F	262/320 (82%)	245 (94%)	17 (6%)	21	58
1	G	258/320 (81%)	237 (92%)	21 (8%)	15	47
1	H	267/320 (83%)	247 (92%)	20 (8%)	17	51
All	All	2070/2560 (81%)	1911 (92%)	159 (8%)	16	50

All (159) 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
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	668	LYS
1	A	677	TYR
1	A	704	THR
1	A	713	SER
1	A	715	TRP
1	C	405	ASN
1	C	411	VAL
1	C	433	ARG
1	C	435	GLN
1	C	459	GLN
1	C	467	GLN
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	612	HIS
1	C	621	ASN
1	C	625	ARG
1	C	634	GLU
1	C	671	LEU
1	C	683	SER
1	C	685	ARG
1	C	687	LYS
1	C	698	HIS

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Mol	Chain	Res	Type
1	C	704	THR
1	G	406	ASN
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	671	LEU
1	G	698	HIS
1	G	704	THR
1	G	715	TRP
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	698	HIS
1	E	704	THR
1	E	713	SER
1	E	714	LYS

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Mol	Chain	Res	Type
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	671	LEU
1	F	679	GLU
1	F	704	THR
1	F	712	SER
1	H	406	ASN
1	H	408	ARG
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	621	ASN
1	H	625	ARG
1	H	634	GLU
1	H	685	ARG
1	H	688	ARG
1	H	698	HIS
1	H	704	THR
1	H	712	SER
1	H	715	TRP
1	D	406	ASN
1	D	411	VAL
1	D	435	GLN
1	D	459	GLN
1	D	467	GLN

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Mol	Chain	Res	Type
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	671	LEU
1	D	676	MET
1	D	677	TYR
1	D	689	THR
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	598	ASP
1	B	601	THR
1	B	621	ASN
1	B	625	ARG
1	B	634	GLU
1	B	671	LEU
1	B	698	HIS
1	B	704	THR
1	B	712	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	441	GLN
1	A	481	HIS
1	A	591	ASN
1	A	621	ASN
1	C	405	ASN

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Mol	Chain	Res	Type
1	C	441	GLN
1	C	459	GLN
1	C	591	ASN
1	C	621	ASN
1	G	441	GLN
1	G	459	GLN
1	G	481	HIS
1	G	591	ASN
1	G	600	GLN
1	G	621	ASN
1	G	698	HIS
1	E	441	GLN
1	E	459	GLN
1	E	591	ASN
1	E	621	ASN
1	F	441	GLN
1	F	459	GLN
1	F	591	ASN
1	F	621	ASN
1	H	441	GLN
1	H	459	GLN
1	H	591	ASN
1	H	621	ASN
1	H	698	HIS
1	D	406	ASN
1	D	441	GLN
1	D	459	GLN
1	D	481	HIS
1	D	591	ASN
1	D	608	GLN
1	D	621	ASN
1	B	441	GLN
1	B	459	GLN
1	B	481	HIS
1	B	591	ASN
1	B	608	GLN
1	B	621	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 carbohydrates 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 ⓘ

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	296/371 (79%)	-0.26	0 100 100	24, 39, 40, 47	0
1	B	296/371 (79%)	-0.34	1 (0%) 94 84	28, 39, 43, 48	0
1	C	303/371 (81%)	-0.29	1 (0%) 94 84	17, 39, 40, 45	0
1	D	293/371 (78%)	-0.35	0 100 100	31, 39, 42, 45	0
1	E	285/371 (76%)	-0.14	0 100 100	21, 39, 41, 51	0
1	F	300/371 (80%)	-0.17	3 (1%) 84 60	26, 39, 46, 49	0
1	G	296/371 (79%)	-0.18	0 100 100	31, 39, 42, 47	0
1	H	306/371 (82%)	-0.34	3 (0%) 84 60	26, 39, 40, 46	0
All	All	2375/2968 (80%)	-0.26	8 (0%) 94 84	17, 39, 42, 51	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	612	HIS	3.8
1	F	605	LEU	3.2
1	H	396	GLY	3.1
1	F	613	PRO	2.6
1	H	432	PRO	2.5
1	H	519	LEU	2.2
1	B	611	ASP	2.2
1	C	518	ASN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	CA	E	2002	1/1	0.96	0.19	-0.90	49,49,49,49	0
2	CA	A	2001	1/1	0.93	0.12	-1.11	64,64,64,64	0
2	CA	B	2001	1/1	0.93	0.14	-1.52	61,61,61,61	0
2	CA	D	2002	1/1	0.95	0.06	-2.50	27,27,27,27	0
2	CA	F	2002	1/1	0.94	0.07	-3.02	36,36,36,36	0
2	CA	B	2002	1/1	0.96	0.06	-3.09	16,16,16,16	0
2	CA	B	2003	1/1	0.98	0.06	-3.30	19,19,19,19	0
2	CA	E	2001	1/1	0.97	0.04	-3.40	41,41,41,41	0
2	CA	H	2003	1/1	0.97	0.04	-3.53	35,35,35,35	0
2	CA	A	2002	1/1	0.97	0.04	-3.71	7,7,7,7	0
2	CA	E	2003	1/1	0.98	0.05	-3.99	26,26,26,26	0
2	CA	C	2003	1/1	0.97	0.05	-4.02	33,33,33,33	0
2	CA	D	2001	1/1	0.98	0.07	-4.21	56,56,56,56	0
2	CA	G	2003	1/1	0.98	0.04	-4.57	28,28,28,28	0
2	CA	D	2003	1/1	0.99	0.07	-4.57	17,17,17,17	0
2	CA	H	2002	1/1	0.98	0.05	-4.76	10,10,10,10	0
2	CA	G	2002	1/1	0.99	0.05	-5.04	15,15,15,15	0
2	CA	C	2002	1/1	0.98	0.04	-5.15	25,25,25,25	0
2	CA	F	2003	1/1	0.97	0.03	-5.17	34,34,34,34	0
2	CA	A	2003	1/1	0.97	0.05	-5.35	31,31,31,31	0
2	CA	H	2001	1/1	0.97	0.07	-	58,58,58,58	0
2	CA	G	2001	1/1	0.95	0.09	-	39,39,39,39	0
2	CA	C	2001	1/1	0.88	0.11	-	71,71,71,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.