



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:13 PM UTC

PDB ID : 3RFZ / pdb_00003rfz
Title : Crystal structure of the FimD usher bound to its cognate FimC:FimH substrate
Authors : Phan, G.; Remaut, H.; Lebedev, A.; Geibel, S.; Waksman, G.
Deposited on : 2011-04-07
Resolution : 2.80 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

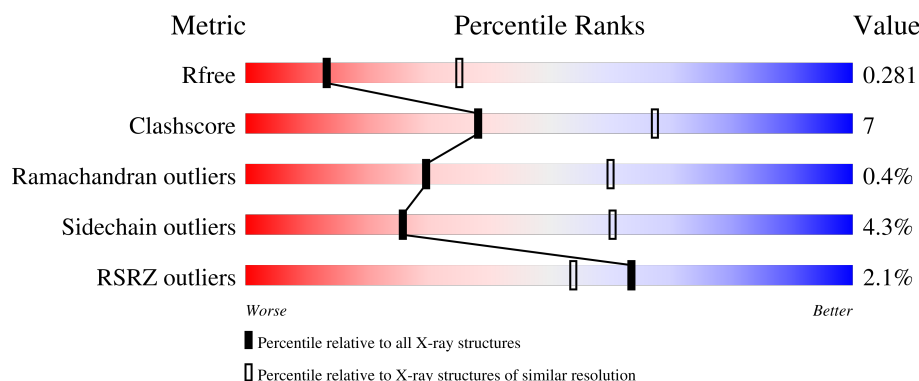
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	279	
1	D	279	
2	B	843	
2	E	843	
3	C	211	

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Mol	Chain	Length	Quality of chain
3	F	211	2% 75% 18% • 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19119 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 Type 1 fimbrial adhesin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	0	0	0
			2034	1290	335	405	4			
1	D	279	Total	C	N	O	S	0	0	0
			2036	1288	336	408	4			

- Molecule 2 is a protein called Outer membrane usher protein, type 1 fimbrial synthesis.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	778	Total	C	N	O	S	0	0	0
			5948	3712	1054	1163	19			
2	E	778	Total	C	N	O	S	0	0	0
			5969	3725	1057	1168	19			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	834	SER	-	expression tag	UNP C6UL88
B	835	ALA	-	expression tag	UNP C6UL88
B	836	TRP	-	expression tag	UNP C6UL88
B	837	SER	-	expression tag	UNP C6UL88
B	838	HIS	-	expression tag	UNP C6UL88
B	839	PRO	-	expression tag	UNP C6UL88
B	840	GLN	-	expression tag	UNP C6UL88
B	841	PHE	-	expression tag	UNP C6UL88
B	842	GLU	-	expression tag	UNP C6UL88
B	843	LYS	-	expression tag	UNP C6UL88
E	834	SER	-	expression tag	UNP C6UL88
E	835	ALA	-	expression tag	UNP C6UL88
E	836	TRP	-	expression tag	UNP C6UL88
E	837	SER	-	expression tag	UNP C6UL88
E	838	HIS	-	expression tag	UNP C6UL88
E	839	PRO	-	expression tag	UNP C6UL88

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Chain	Residue	Modelled	Actual	Comment	Reference
E	840	GLN	-	expression tag	UNP C6UL88
E	841	PHE	-	expression tag	UNP C6UL88
E	842	GLU	-	expression tag	UNP C6UL88
E	843	LYS	-	expression tag	UNP C6UL88

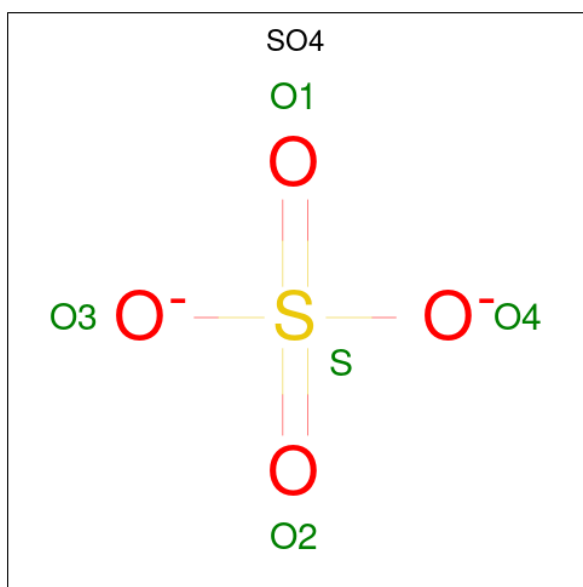
- Molecule 3 is a protein called Chaperone protein fimC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	201	Total	C	N	O	S	0	0	0
			1539	978	262	293	6			
3	F	201	Total	C	N	O	S	0	0	0
			1542	982	262	293	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	206	HIS	-	expression tag	UNP P59590
C	207	HIS	-	expression tag	UNP P59590
C	208	HIS	-	expression tag	UNP P59590
C	209	HIS	-	expression tag	UNP P59590
C	210	HIS	-	expression tag	UNP P59590
C	211	HIS	-	expression tag	UNP P59590
F	206	HIS	-	expression tag	UNP P59590
F	207	HIS	-	expression tag	UNP P59590
F	208	HIS	-	expression tag	UNP P59590
F	209	HIS	-	expression tag	UNP P59590
F	210	HIS	-	expression tag	UNP P59590
F	211	HIS	-	expression tag	UNP P59590

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

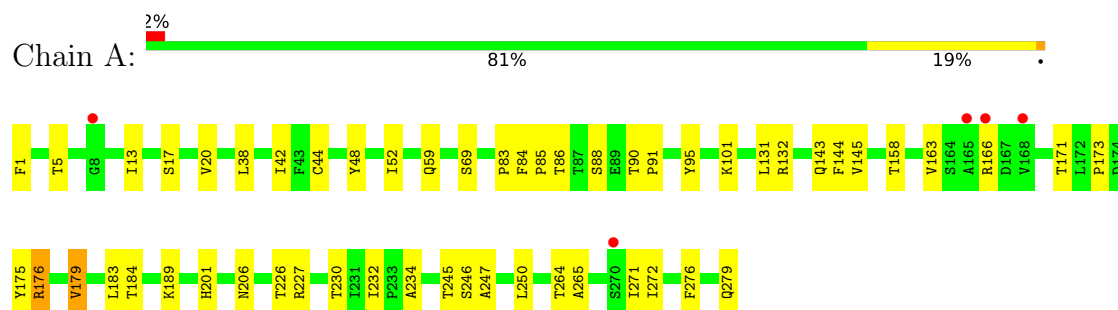
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	O	0	0
			2	2		
5	B	22	Total	O	0	0
			22	22		
5	C	4	Total	O	0	0
			4	4		
5	D	1	Total	O	0	0
			1	1		
5	E	8	Total	O	0	0
			8	8		
5	F	4	Total	O	0	0
			4	4		

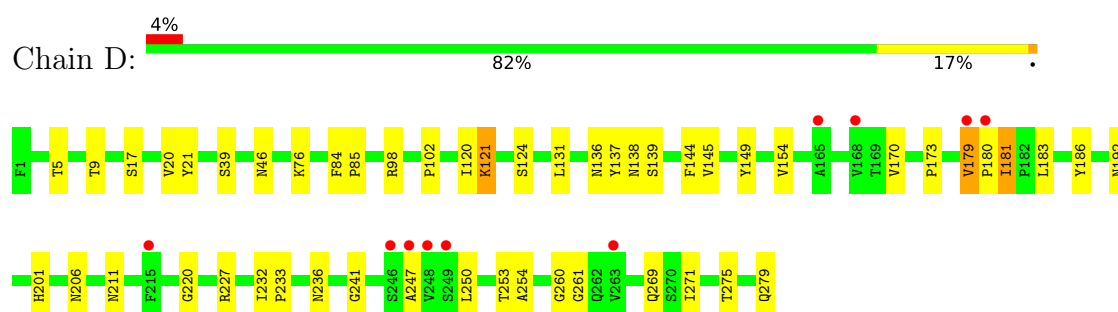
3 Residue-property plots [i](#)

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.

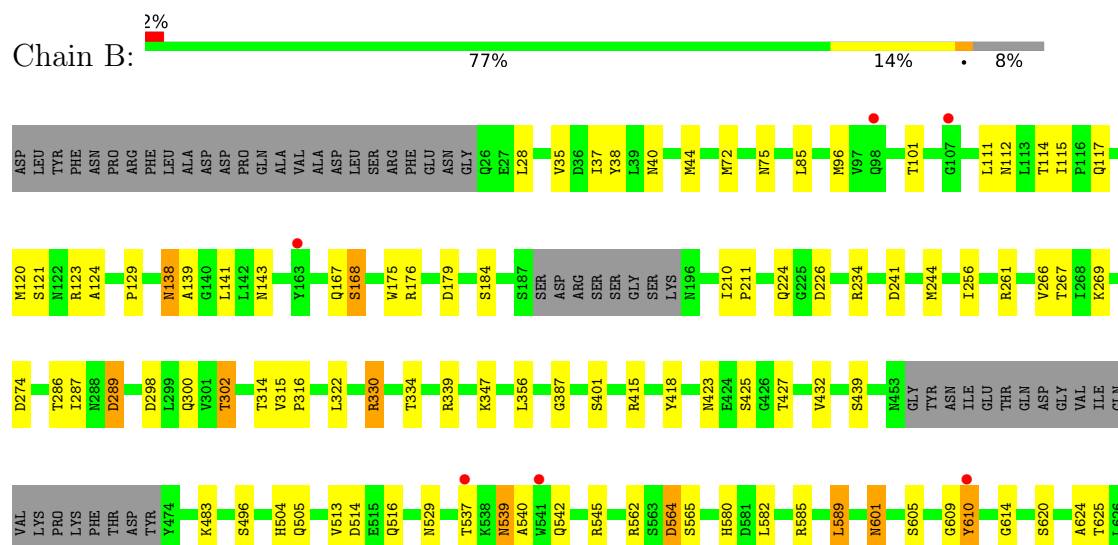
- Molecule 1: Type 1 fimbrial adhesin

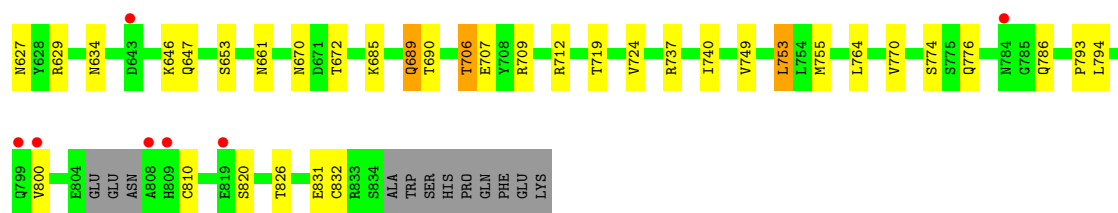


- Molecule 1: Type 1 fimbrial adhesin

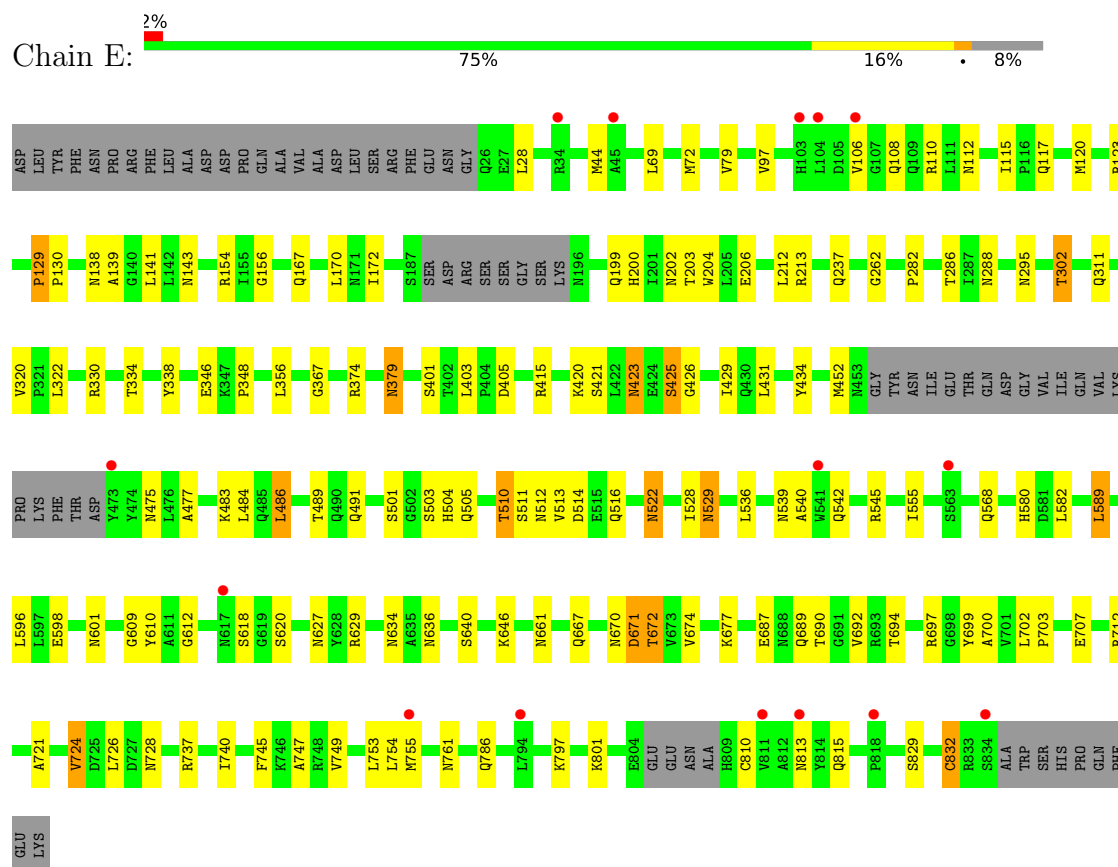


- Molecule 2: Outer membrane usher protein, type 1 fimbrial synthesis

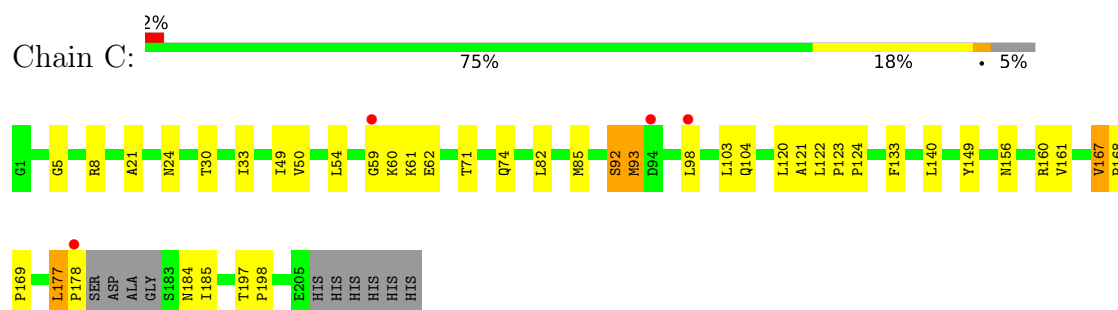




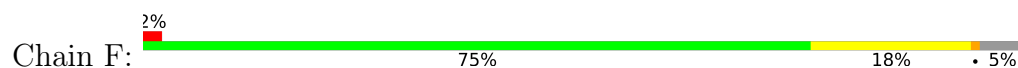
• Molecule 2: Outer membrane usher protein, type 1 fimbrial synthesis

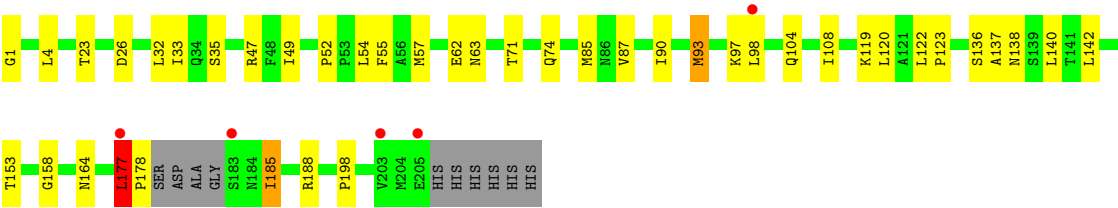


• Molecule 3: Chaperone protein fimC



• Molecule 3: Chaperone protein fimC





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	126.19Å 95.90Å 144.57Å 90.00° 112.13° 90.00°	Depositor
Resolution (Å)	59.13 – 2.80 59.13 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.3 (59.13-2.80) 97.3 (59.13-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.6.0077	Depositor
R, R_{free}	0.223 , 0.282 0.222 , 0.281	Depositor DCC
R_{free} test set	3845 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	53.7	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 34.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	19119	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.02 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.2235e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: SO4

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	0.53	0/2079	0.77	0/2859
1	D	0.53	0/2081	0.78	0/2861
2	B	0.50	0/6076	0.79	3/8273 (0.0%)
2	E	0.49	0/6097	0.77	3/8299 (0.0%)
3	C	0.49	0/1567	0.84	2/2138 (0.1%)
3	F	0.49	0/1570	0.81	2/2140 (0.1%)
All	All	0.50	0/19470	0.79	10/26570 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	167	VAL	CA-C-N	9.67	126.72	119.66
3	C	167	VAL	C-N-CA	9.67	126.72	119.66
2	B	647	GLN	N-CA-C	5.75	117.93	109.24
2	B	129	PRO	CA-C-N	5.75	126.14	119.47
2	B	129	PRO	C-N-CA	5.75	126.14	119.47
2	E	129	PRO	CA-C-N	5.47	125.30	119.28
2	E	129	PRO	C-N-CA	5.47	125.30	119.28
3	F	52	PRO	CA-C-N	5.12	124.91	119.28
3	F	52	PRO	C-N-CA	5.12	124.91	119.28
2	E	423	ASN	N-CA-C	5.11	116.69	110.41

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	2034	0	1969	31	0
1	D	2036	0	1961	30	0
2	B	5948	0	5647	78	0
2	E	5969	0	5692	80	0
3	C	1539	0	1542	29	0
3	F	1542	0	1560	28	0
4	B	10	0	0	0	0
5	A	2	0	0	0	0
5	B	22	0	0	0	0
5	C	4	0	0	0	0
5	D	1	0	0	0	0
5	E	8	0	0	0	0
5	F	4	0	0	0	0
All	All	19119	0	18371	259	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 7.

All (259) 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:B:516:GLN:HG3	2:B:537:THR:HG22	1.53	0.91
2:B:514:ASP:OD1	2:B:540:ALA:HB2	1.74	0.87
1:A:173:PRO:HD3	1:A:179:VAL:HG22	1.56	0.86
2:E:797:LYS:HG2	2:E:813:ASN:HB3	1.62	0.80
2:E:627:ASN:HD22	2:E:636:ASN:HB3	1.47	0.80
2:E:539:ASN:HB2	2:E:542:GLN:HB3	1.63	0.79
2:E:237:GLN:HG3	2:E:334:THR:HG22	1.65	0.78
1:A:173:PRO:HD3	1:A:179:VAL:CG2	2.16	0.76
3:F:136:SER:H	3:F:137:ALA:HA	1.52	0.74
2:B:601:ASN:H	2:B:601:ASN:ND2	1.85	0.72
1:D:136:ASN:O	1:D:137:TYR:HB3	1.90	0.72
3:F:136:SER:N	3:F:137:ALA:HA	2.06	0.71
3:C:71:THR:O	3:C:74:GLN:HG2	1.90	0.71
2:B:75:ASN:HB2	2:B:121:SER:HB3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:MET:HE2	2:B:72:MET:HA	1.73	0.70
1:A:84:PHE:HA	1:A:85:PRO:C	2.16	0.69
2:B:820:SER:HB2	2:B:826:THR:HG21	1.75	0.69
2:B:300:GLN:HG3	2:B:314:THR:HG22	1.76	0.68
1:A:90:THR:HB	1:A:91:PRO:HD2	1.75	0.67
1:D:131:LEU:HB3	1:D:144:PHE:HB2	1.76	0.67
2:E:580:HIS:HD2	2:E:582:LEU:H	1.42	0.67
3:F:71:THR:O	3:F:74:GLN:HG2	1.95	0.67
2:B:601:ASN:H	2:B:601:ASN:HD22	1.42	0.67
2:B:505:GLN:HB2	2:B:514:ASP:HB2	1.77	0.67
2:B:423:ASN:HB2	2:B:427:THR:H	1.60	0.67
1:A:158:THR:HG22	1:A:189:LYS:HD3	1.77	0.67
2:B:38:TYR:HB2	2:B:112:ASN:HD22	1.60	0.66
2:E:712:ARG:NH1	3:F:62:GLU:OE1	2.29	0.65
2:E:117:GLN:HE21	2:E:286:THR:H	1.44	0.65
2:E:755:MET:O	2:E:786:GLN:HA	1.97	0.65
2:E:707:GLU:HG2	2:E:737:ARG:HA	1.80	0.64
2:E:514:ASP:OD1	2:E:540:ALA:HB2	1.98	0.64
2:B:117:GLN:OE1	2:B:123:ARG:HD2	1.97	0.64
2:E:322:LEU:HD11	2:E:415:ARG:HH21	1.63	0.63
2:E:138:ASN:ND2	2:E:172:ILE:HA	2.12	0.63
2:E:322:LEU:HD11	2:E:415:ARG:NH2	2.14	0.63
3:C:50:VAL:HG21	3:C:85:MET:HE1	1.81	0.63
3:F:93:MET:HA	3:F:104:GLN:HE22	1.62	0.63
3:C:156:ASN:O	3:C:185:ILE:HA	1.99	0.63
1:A:131:LEU:HB3	1:A:144:PHE:HB2	1.79	0.62
2:B:316:PRO:HB2	2:B:387:GLY:HA2	1.81	0.62
2:E:117:GLN:NE2	2:E:286:THR:H	1.96	0.62
2:E:110:ARG:HH11	2:E:112:ASN:HD21	1.48	0.62
2:B:831:GLU:HG3	2:B:832:CYS:H	1.64	0.61
2:B:226:ASP:O	2:B:415:ARG:NH2	2.34	0.61
2:B:330:ARG:HG2	2:B:356:LEU:HD13	1.82	0.61
1:D:201:HIS:CD2	1:D:206:ASN:HA	2.36	0.60
3:F:32:LEU:HB3	3:F:90:ILE:HB	1.84	0.59
1:D:220:GLY:HA2	1:D:260:GLY:H	1.67	0.59
2:B:562:ARG:HD3	2:B:564:ASP:HB2	1.83	0.59
2:B:601:ASN:HB3	2:B:629:ARG:O	2.02	0.59
2:B:707:GLU:HG2	2:B:737:ARG:HA	1.83	0.59
3:C:184:ASN:H	2:E:815:GLN:HE22	1.51	0.58
2:E:810:CYS:SG	2:E:832:CYS:HB2	2.44	0.58
1:D:192:ASN:HA	1:D:241:GLY:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:143:ASN:HB2	2:E:167:GLN:HB2	1.86	0.57
1:D:84:PHE:HA	1:D:85:PRO:C	2.29	0.57
2:E:44:MET:HE2	2:E:72:MET:HA	1.86	0.57
2:E:484:LEU:O	2:E:503:SER:HA	2.05	0.56
1:D:211:ASN:ND2	1:D:269:GLN:H	2.03	0.56
1:D:227:ARG:CB	1:D:232:ILE:HD11	2.36	0.56
2:E:330:ARG:HG2	2:E:356:LEU:HD13	1.88	0.56
2:B:423:ASN:HB3	2:B:425:SER:H	1.70	0.56
2:B:504:HIS:NE2	2:B:513:VAL:HG11	2.22	0.55
2:E:504:HIS:CD2	2:E:513:VAL:HG11	2.42	0.55
1:A:59:GLN:HB2	1:A:132:ARG:HB2	1.89	0.55
2:B:115:ILE:HB	2:B:120:MET:HE3	1.88	0.55
3:C:24:ASN:O	3:C:60:LYS:HA	2.06	0.54
2:E:141:LEU:HD11	2:E:740:ILE:HD11	1.87	0.54
2:E:420:LYS:HB3	2:E:429:ILE:HB	1.89	0.54
2:E:661:ASN:O	2:E:697:ARG:NH2	2.40	0.54
3:F:35:SER:HB3	3:F:85:MET:HE1	1.88	0.54
1:A:183:LEU:HD23	1:A:250:LEU:HD12	1.89	0.54
2:E:674:VAL:HB	2:E:702:LEU:HD12	1.90	0.54
2:E:536:LEU:HD11	2:E:545:ARG:HD3	1.90	0.54
2:B:339:ARG:HH11	2:B:347:LYS:HD3	1.73	0.53
1:D:21:TYR:CD2	1:D:149:TYR:HB2	2.43	0.53
1:A:59:GLN:HE22	1:A:143:GLN:HE21	1.57	0.53
1:D:17:SER:HB3	1:D:145:VAL:HB	1.91	0.53
2:B:562:ARG:HH12	3:C:121:ALA:C	2.17	0.53
1:D:138:ASN:OD1	1:D:139:SER:N	2.36	0.53
3:F:47:ARG:HB3	3:F:71:THR:HG22	1.90	0.53
3:F:122:LEU:HD12	3:F:123:PRO:HD2	1.91	0.53
2:B:37:ILE:HG12	2:B:111:LEU:HD23	1.91	0.53
2:B:755:MET:O	2:B:786:GLN:HA	2.09	0.53
2:B:513:VAL:HG12	2:B:514:ASP:N	2.24	0.53
2:B:168:SER:HB3	2:B:179:ASP:HB3	1.91	0.52
2:B:539:ASN:HB3	2:B:542:GLN:HG2	1.91	0.52
1:D:183:LEU:HD23	1:D:250:LEU:HD12	1.90	0.52
2:B:418:TYR:HB3	2:B:432:VAL:HB	1.90	0.52
3:C:197:THR:HB	3:C:198:PRO:HD2	1.90	0.52
3:C:160:ARG:HD3	3:C:177:LEU:HD21	1.90	0.52
1:A:201:HIS:CE1	1:A:234:ALA:HB3	2.44	0.52
2:B:322:LEU:HD11	2:B:415:ARG:HH21	1.75	0.52
2:B:267:THR:OG1	2:B:302:THR:HG23	2.10	0.52
2:E:707:GLU:H	2:E:707:GLU:CD	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:580:HIS:HD2	2:B:582:LEU:H	1.58	0.51
3:F:33:ILE:O	3:F:54:LEU:HA	2.11	0.51
2:B:143:ASN:HB2	2:B:167:GLN:HB2	1.92	0.51
2:B:753:LEU:HD13	2:B:755:MET:HG3	1.92	0.51
1:A:17:SER:HB3	1:A:145:VAL:HB	1.93	0.51
2:E:115:ILE:HB	2:E:120:MET:HE3	1.93	0.51
2:E:423:ASN:HB3	2:E:425:SER:H	1.76	0.51
1:A:163:VAL:HG21	1:A:276:PHE:CE1	2.46	0.50
1:D:173:PRO:HD3	1:D:179:VAL:HG23	1.92	0.50
2:B:634:ASN:HB2	2:B:653:SER:OG	2.12	0.50
1:D:181:ILE:HD11	1:D:254:ALA:HB2	1.92	0.50
2:E:627:ASN:ND2	2:E:636:ASN:HB3	2.23	0.50
1:A:175:TYR:O	1:A:176:ARG:CB	2.59	0.50
1:D:275:THR:OG1	3:F:108:ILE:HB	2.12	0.50
2:E:200:HIS:HE1	2:E:203:THR:OG1	1.95	0.49
3:F:142:LEU:HD12	3:F:142:LEU:H	1.77	0.49
2:B:138:ASN:N	2:B:138:ASN:HD22	2.11	0.49
3:F:188:ARG:HH21	3:F:198:PRO:HA	1.77	0.49
2:B:562:ARG:HG3	3:C:123:PRO:HB3	1.95	0.49
2:B:124:ALA:HA	2:B:289:ASP:OD1	2.12	0.49
2:E:712:ARG:HD2	3:F:62:GLU:OE2	2.13	0.49
2:E:522:ASN:HD21	2:E:529:ASN:ND2	2.11	0.49
1:A:272:ILE:HD12	3:C:103:LEU:HD11	1.94	0.49
1:A:279:GLN:C	3:C:8:ARG:NH2	2.71	0.48
2:B:241:ASP:HB3	2:B:244:MET:HE3	1.95	0.48
3:C:133:PHE:HB3	3:C:140:LEU:HD11	1.94	0.48
1:A:227:ARG:HB2	1:A:232:ILE:HD11	1.95	0.48
2:B:322:LEU:HD11	2:B:415:ARG:NH2	2.28	0.48
2:B:40:ASN:OD1	2:B:114:THR:HA	2.14	0.48
2:E:670:ASN:O	2:E:672:THR:N	2.45	0.48
2:B:685:LYS:HB3	2:B:719:THR:HG21	1.96	0.48
3:C:33:ILE:O	3:C:54:LEU:HA	2.14	0.48
2:E:601:ASN:HB3	2:E:629:ARG:O	2.14	0.48
2:B:298:ASP:OD1	2:B:316:PRO:HA	2.14	0.47
2:B:712:ARG:HD2	3:C:62:GLU:OE2	2.14	0.47
1:D:5:THR:HG21	1:D:20:VAL:HG22	1.95	0.47
2:B:670:ASN:O	2:B:672:THR:N	2.48	0.47
2:E:580:HIS:HD2	2:E:582:LEU:N	2.12	0.47
2:B:269:LYS:HG2	2:B:274:ASP:HA	1.97	0.47
2:B:562:ARG:HG2	2:B:564:ASP:H	1.79	0.47
3:C:160:ARG:HH11	3:C:177:LEU:HD21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:LYS:O	1:D:124:SER:OG	2.32	0.47
3:F:4:LEU:HD21	3:F:87:VAL:HG21	1.97	0.47
3:C:30:THR:O	3:C:92:SER:HB2	2.15	0.46
1:D:180:PRO:HA	1:D:253:THR:HA	1.98	0.46
3:F:55:PHE:HE1	3:F:57:MET:HE3	1.80	0.46
3:F:153:THR:HA	3:F:164:ASN:HD22	1.80	0.46
2:B:423:ASN:HB3	2:B:425:SER:N	2.31	0.46
2:E:721:ALA:HB3	2:E:724:VAL:HG23	1.98	0.46
2:B:564:ASP:O	2:B:565:SER:C	2.58	0.46
1:D:120:ILE:HB	1:D:154:VAL:HB	1.98	0.46
3:F:87:VAL:O	3:F:108:ILE:HA	2.16	0.46
1:D:180:PRO:HD2	2:E:108:GLN:HG2	1.98	0.46
2:E:426:GLY:HA3	2:E:491:GLN:HB2	1.98	0.46
2:E:139:ALA:HB3	2:E:740:ILE:HD13	1.98	0.45
2:B:764:LEU:HD13	2:B:800:VAL:HG11	1.98	0.45
2:E:69:LEU:HD23	2:E:72:MET:HE3	1.98	0.45
2:B:770:VAL:HG22	2:B:800:VAL:HG22	1.99	0.45
2:E:504:HIS:NE2	2:E:513:VAL:HG11	2.32	0.45
2:B:141:LEU:HD12	2:B:740:ILE:HD11	1.96	0.45
1:D:170:VAL:HG21	1:D:181:ILE:HG23	1.97	0.45
3:C:24:ASN:ND2	3:C:59:GLY:O	2.49	0.45
2:E:726:LEU:HD23	2:E:747:ALA:HA	1.98	0.45
1:A:13:ILE:H	1:A:13:ILE:HG13	1.63	0.45
3:C:93:MET:H	3:C:93:MET:HG2	1.50	0.45
1:D:279:GLN:HE22	3:F:153:THR:HB	1.81	0.45
1:D:21:TYR:HD2	1:D:149:TYR:HB2	1.82	0.44
2:E:338:TYR:HB3	2:E:348:PRO:HD2	1.98	0.44
2:E:670:ASN:HB2	2:E:703:PRO:O	2.16	0.44
2:E:728:ASN:O	2:E:745:PHE:HD1	2.00	0.44
1:A:264:THR:HG22	1:A:265:ALA:N	2.32	0.44
2:B:139:ALA:HB3	2:B:740:ILE:HD13	1.98	0.44
1:A:38:LEU:HB3	1:A:42:ILE:HD12	2.00	0.44
2:B:564:ASP:OD2	3:C:124:PRO:HD2	2.17	0.44
3:C:120:LEU:C	3:C:122:LEU:H	2.26	0.44
2:E:79:VAL:HG11	2:E:97:VAL:HG22	1.99	0.44
1:A:279:GLN:O	3:C:8:ARG:NH2	2.51	0.44
1:D:76:LYS:HD2	2:E:670:ASN:HB3	1.98	0.44
1:A:48:TYR:HB2	1:A:52:ILE:HD12	2.00	0.44
2:E:486:LEU:O	2:E:501:SER:HA	2.17	0.44
2:B:256:ILE:HG12	2:B:315:VAL:HG21	2.00	0.43
1:D:173:PRO:HD3	1:D:179:VAL:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:HIS:ND1	1:A:206:ASN:OD1	2.51	0.43
2:E:204:TRP:HE1	2:E:206:GLU:CD	2.26	0.43
1:A:1:PHE:CZ	1:A:44:CYS:HB3	2.53	0.43
2:B:689:GLN:HE21	2:B:689:GLN:HB3	1.60	0.43
2:E:129:PRO:HA	2:E:130:PRO:HD3	1.85	0.43
2:E:405:ASP:HB3	2:E:452:MET:HG3	2.00	0.43
2:E:580:HIS:CD2	2:E:582:LEU:H	2.30	0.43
2:E:123:ARG:HH21	2:E:288:ASN:HD21	1.65	0.43
2:E:510:THR:HB	2:E:511:SER:H	1.65	0.43
2:B:175:TRP:C	2:B:176:ARG:HD3	2.43	0.43
2:B:629:ARG:HA	2:B:634:ASN:OD1	2.19	0.43
1:A:271:ILE:HG12	3:C:104:GLN:HB2	2.01	0.43
2:B:774:SER:HB2	2:B:793:PRO:HG3	2.01	0.43
2:E:212:LEU:O	2:E:213:ARG:C	2.61	0.43
2:E:513:VAL:HG12	2:E:514:ASP:N	2.34	0.43
2:B:724:VAL:HG22	2:B:749:VAL:HG22	2.01	0.42
1:A:95:TYR:CE2	1:A:101:LYS:HE3	2.54	0.42
1:A:226:THR:HA	1:A:230:THR:O	2.19	0.42
2:B:513:VAL:HG12	2:B:514:ASP:H	1.84	0.42
2:B:707:GLU:CD	2:B:707:GLU:H	2.26	0.42
2:E:687:GLU:OE1	2:E:712:ARG:NH2	2.52	0.42
2:E:694:THR:HA	2:E:700:ALA:HB2	2.00	0.42
2:E:707:GLU:CG	2:E:737:ARG:HA	2.48	0.42
2:B:605:SER:O	2:B:624:ALA:HA	2.19	0.42
2:E:610:TYR:HA	2:E:620:SER:HA	2.00	0.42
2:E:677:LYS:HG3	2:E:699:TYR:CE1	2.54	0.42
1:A:83:PRO:O	1:A:86:THR:HA	2.20	0.42
1:D:233:PRO:HG2	1:D:236:ASN:HD22	1.84	0.42
2:E:505:GLN:HB2	2:E:514:ASP:HB2	2.02	0.42
2:E:689:GLN:HB3	2:E:692:VAL:HG21	2.02	0.42
3:F:1:GLY:N	3:F:26:ASP:HB2	2.34	0.42
2:B:234:ARG:CZ	2:B:339:ARG:HH21	2.33	0.42
2:E:295:ASN:HA	2:E:421:SER:HB2	2.01	0.42
3:F:47:ARG:HH12	3:F:74:GLN:HG3	1.85	0.42
3:C:82:LEU:HB2	3:C:149:TYR:CE2	2.55	0.42
2:E:707:GLU:HG2	2:E:737:ARG:CA	2.48	0.42
3:F:57:MET:CE	3:F:63:ASN:HB2	2.49	0.42
2:B:266:VAL:HG11	2:B:287:ILE:CD1	2.50	0.42
3:C:149:TYR:CE1	3:C:169:PRO:HD3	2.54	0.42
1:D:271:ILE:HG12	3:F:104:GLN:HB2	2.02	0.42
3:F:136:SER:OG	3:F:138:ASN:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:177:LEU:HD12	3:C:178:PRO:HD2	2.00	0.42
2:E:475:ASN:HD21	2:E:477:ALA:HB3	1.84	0.42
2:E:797:LYS:HG2	2:E:813:ASN:CB	2.42	0.42
1:D:186:TYR:HB3	1:D:247:ALA:HA	2.02	0.42
2:E:434:TYR:HA	2:E:483:LYS:O	2.19	0.42
2:E:367:GLY:HA2	2:E:379:ASN:HD22	1.85	0.41
3:C:122:LEU:HA	3:C:123:PRO:HD2	1.94	0.41
2:E:634:ASN:OD1	2:E:667:GLN:HG2	2.19	0.41
2:B:610:TYR:HB2	2:B:620:SER:HA	2.02	0.41
3:F:97:LYS:H	3:F:97:LYS:HG2	1.73	0.41
1:D:39:SER:O	1:D:102:PRO:HB3	2.21	0.41
1:A:88:SER:HB2	2:B:224:GLN:OE1	2.20	0.41
2:B:706:THR:OG1	2:B:709:ARG:HD3	2.20	0.41
3:C:167:VAL:HA	3:C:168:PRO:HD3	1.81	0.41
2:B:483:LYS:HD2	2:B:505:GLN:HE21	1.85	0.41
2:E:528:ILE:HG12	2:E:555:ILE:HG23	2.02	0.41
3:F:140:LEU:HD21	3:F:185:ILE:HD13	2.03	0.41
2:B:564:ASP:OD2	2:B:564:ASP:N	2.54	0.41
2:B:85:LEU:HD21	2:B:96:MET:HE1	2.02	0.41
2:B:589:LEU:HD12	2:B:609:GLY:HA3	2.03	0.41
2:E:589:LEU:HD12	2:E:609:GLY:HA3	2.03	0.41
2:E:612:GLY:HA2	2:E:618:SER:HA	2.02	0.41
3:F:57:MET:HE1	3:F:63:ASN:HB2	2.03	0.41
1:A:184:THR:HB	1:A:247:ALA:HB1	2.02	0.41
2:B:210:ILE:N	2:B:211:PRO:CD	2.84	0.41
3:C:82:LEU:HB2	3:C:149:TYR:CZ	2.56	0.41
2:E:262:GLY:HA2	2:E:282:PRO:HB3	2.02	0.41
3:F:177:LEU:HD13	3:F:178:PRO:HD2	2.03	0.41
2:B:545:ARG:H	2:B:545:ARG:HG2	1.74	0.40
2:E:568:GLN:HG2	2:E:596:LEU:HD23	2.03	0.40
2:B:585:ARG:HB2	2:B:614:GLY:HA3	2.03	0.40
2:B:831:GLU:HG3	2:B:832:CYS:N	2.33	0.40
1:A:5:THR:HG21	1:A:20:VAL:HG22	2.04	0.40
1:A:90:THR:HB	1:A:91:PRO:CD	2.45	0.40
2:B:101:THR:OG1	2:B:114:THR:OG1	2.36	0.40
3:C:5:GLY:HA3	3:C:21:ALA:HB3	2.03	0.40
2:E:302:THR:HA	2:E:311:GLN:O	2.21	0.40
2:E:374:ARG:NH2	2:E:403:LEU:O	2.54	0.40
1:D:46:ASN:O	1:D:98:ARG:HA	2.22	0.40
2:E:754:LEU:HD11	2:E:786:GLN:HE21	1.86	0.40

There are no symmetry-related clashes.

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	277/279 (99%)	263 (95%)	12 (4%)	2 (1%)	18	47
1	D	277/279 (99%)	256 (92%)	20 (7%)	1 (0%)	30	60
2	B	770/843 (91%)	729 (95%)	41 (5%)	0	100	100
2	E	770/843 (91%)	722 (94%)	45 (6%)	3 (0%)	30	60
3	C	197/211 (93%)	185 (94%)	11 (6%)	1 (0%)	24	55
3	F	197/211 (93%)	187 (95%)	7 (4%)	3 (2%)	8	28
All	All	2488/2666 (93%)	2342 (94%)	136 (6%)	10 (0%)	30	60

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	ARG
2	E	156	GLY
2	E	671	ASP
3	C	177	LEU
3	F	119	LYS
3	F	177	LEU
1	A	166	ARG
2	E	154	ARG
1	D	261	GLY
3	F	158	GLY

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	220/226 (97%)	215 (98%)	5 (2%)	44	78
1	D	220/226 (97%)	216 (98%)	4 (2%)	51	82
2	B	620/694 (89%)	589 (95%)	31 (5%)	22	54
2	E	627/694 (90%)	594 (95%)	33 (5%)	20	52
3	C	163/181 (90%)	157 (96%)	6 (4%)	30	65
3	F	165/181 (91%)	158 (96%)	7 (4%)	26	61
All	All	2015/2202 (92%)	1929 (96%)	86 (4%)	26	60

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	SER
1	A	171	THR
1	A	179	VAL
1	A	245	THR
1	A	246	SER
2	B	28	LEU
2	B	35	VAL
2	B	138	ASN
2	B	168	SER
2	B	184	SER
2	B	261	ARG
2	B	286	THR
2	B	289	ASP
2	B	302	THR
2	B	330	ARG
2	B	334	THR
2	B	401	SER
2	B	439	SER
2	B	496	SER
2	B	529	ASN
2	B	539	ASN
2	B	564	ASP
2	B	589	LEU
2	B	601	ASN
2	B	610	TYR
2	B	625	THR
2	B	627	ASN
2	B	646	LYS
2	B	661	ASN
2	B	689	GLN

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Mol	Chain	Res	Type
2	B	690	THR
2	B	706	THR
2	B	753	LEU
2	B	776	GLN
2	B	794	LEU
2	B	810	CYS
3	C	49	ILE
3	C	61	LYS
3	C	92	SER
3	C	93	MET
3	C	98	LEU
3	C	161	VAL
1	D	9	THR
1	D	121	LYS
1	D	179	VAL
1	D	181	ILE
2	E	28	LEU
2	E	106	VAL
2	E	170	LEU
2	E	199	GLN
2	E	202	ASN
2	E	302	THR
2	E	320	VAL
2	E	346	GLU
2	E	379	ASN
2	E	401	SER
2	E	425	SER
2	E	431	LEU
2	E	486	LEU
2	E	489	THR
2	E	510	THR
2	E	512	ASN
2	E	516	GLN
2	E	522	ASN
2	E	529	ASN
2	E	589	LEU
2	E	598	GLU
2	E	640	SER
2	E	646	LYS
2	E	671	ASP
2	E	672	THR
2	E	690	THR

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Mol	Chain	Res	Type
2	E	724	VAL
2	E	749	VAL
2	E	753	LEU
2	E	761	ASN
2	E	801	LYS
2	E	829	SER
2	E	832	CYS
3	F	23	THR
3	F	49	ILE
3	F	93	MET
3	F	98	LEU
3	F	120	LEU
3	F	177	LEU
3	F	185	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	23	ASN
1	A	29	ASN
1	A	41	GLN
1	A	59	GLN
1	A	192	ASN
1	A	211	ASN
1	A	255	ASN
2	B	112	ASN
2	B	138	ASN
2	B	149	ASN
2	B	199	GLN
2	B	202	ASN
2	B	265	GLN
2	B	370	GLN
2	B	379	ASN
2	B	400	ASN
2	B	428	ASN
2	B	430	GLN
2	B	475	ASN
2	B	505	GLN
2	B	518	GLN
2	B	522	ASN
2	B	529	ASN

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Mol	Chain	Res	Type
2	B	552	ASN
2	B	554	ASN
2	B	559	HIS
2	B	580	HIS
2	B	588	ASN
2	B	601	ASN
2	B	647	GLN
2	B	661	ASN
2	B	689	GLN
2	B	759	HIS
2	B	786	GLN
2	B	813	ASN
3	C	73	ASN
3	C	77	GLN
3	C	164	ASN
1	D	29	ASN
1	D	33	ASN
1	D	59	GLN
1	D	201	HIS
1	D	211	ASN
1	D	224	GLN
1	D	228	ASN
1	D	236	ASN
1	D	279	GLN
2	E	75	ASN
2	E	98	GLN
2	E	112	ASN
2	E	117	GLN
2	E	138	ASN
2	E	149	ASN
2	E	153	ASN
2	E	167	GLN
2	E	196	ASN
2	E	200	HIS
2	E	202	ASN
2	E	237	GLN
2	E	249	GLN
2	E	295	ASN
2	E	379	ASN
2	E	408	GLN
2	E	419	ASN
2	E	475	ASN

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Mol	Chain	Res	Type
2	E	485	GLN
2	E	522	ASN
2	E	580	HIS
2	E	600	ASN
2	E	601	ASN
2	E	627	ASN
2	E	688	ASN
2	E	689	GLN
2	E	786	GLN
2	E	815	GLN
3	F	104	GLN
3	F	156	ASN
3	F	164	ASN

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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	B	844	-	4,4,4	0.24	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	B	845	-	4,4,4	0.21	0	6,6,6	0.23	0

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	279/279 (100%)	-0.00	5 (1%) 67 58	32, 52, 82, 125	0
1	D	279/279 (100%)	0.12	10 (3%) 46 37	32, 55, 94, 114	0
2	B	778/843 (92%)	0.02	13 (1%) 69 60	33, 54, 96, 127	2 (0%)
2	E	778/843 (92%)	0.16	15 (1%) 66 57	35, 59, 103, 136	2 (0%)
3	C	201/211 (95%)	0.04	4 (1%) 65 56	39, 57, 103, 121	0
3	F	201/211 (95%)	0.19	5 (2%) 58 48	42, 63, 107, 132	0
All	All	2516/2666 (94%)	0.09	52 (2%) 63 54	32, 57, 99, 136	4 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	165	ALA	4.6
1	A	168	VAL	4.0
2	B	808	ALA	3.5
2	E	106	VAL	3.3
2	B	643	ASP	3.2
2	B	537	THR	3.1
3	C	94	ASP	3.0
2	B	610	TYR	3.0
1	D	165	ALA	3.0
2	E	541	TRP	2.9
3	C	98	LEU	2.9
2	E	813	ASN	2.8
3	F	177	LEU	2.8
3	F	183	SER	2.8
2	E	811	VAL	2.7
2	E	34	ARG	2.7
2	B	163	TYR	2.6
3	C	178	PRO	2.6
2	E	617	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
2	E	473	TYR	2.6
1	D	168	VAL	2.6
2	E	818	PRO	2.5
2	B	784	ASN	2.5
2	B	541	TRP	2.5
1	D	215	PHE	2.5
2	B	809	HIS	2.4
3	F	203	VAL	2.3
3	C	59	GLY	2.3
1	D	247	ALA	2.3
2	E	794	LEU	2.3
1	A	270	SER	2.3
2	B	799	GLN	2.3
2	B	800	VAL	2.3
1	A	8	GLY	2.2
2	E	104	LEU	2.2
2	E	103	HIS	2.2
1	A	166	ARG	2.2
2	E	755	MET	2.2
1	D	246	SER	2.2
2	E	563	SER	2.2
2	B	98	GLN	2.1
3	F	98	LEU	2.1
2	B	819	GLU	2.1
2	E	834	SER	2.1
1	D	248	VAL	2.1
1	D	180	PRO	2.1
3	F	205	GLU	2.1
2	E	45	ALA	2.1
1	D	179	VAL	2.0
1	D	263	VAL	2.0
2	B	107	GLY	2.0
1	D	249	SER	2.0

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 ⓘ

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
4	SO4	B	844	5/5	0.97	0.15	65,66,67,71	0
4	SO4	B	845	5/5	0.97	0.07	60,61,63,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.