



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:42 PM UTC

PDB ID : 3QM3 / pdb_00003qm3
Title : 1.85 Angstrom Resolution Crystal Structure of Fructose-bisphosphate Aldolase (Fba) from Campylobacter jejuni
Authors : Minasov, G.; Wawrzak, Z.; Skarina, T.; Onopriyenko, O.; Papazisi, L.; Savchenko, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2011-02-03
Resolution : 1.85 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:

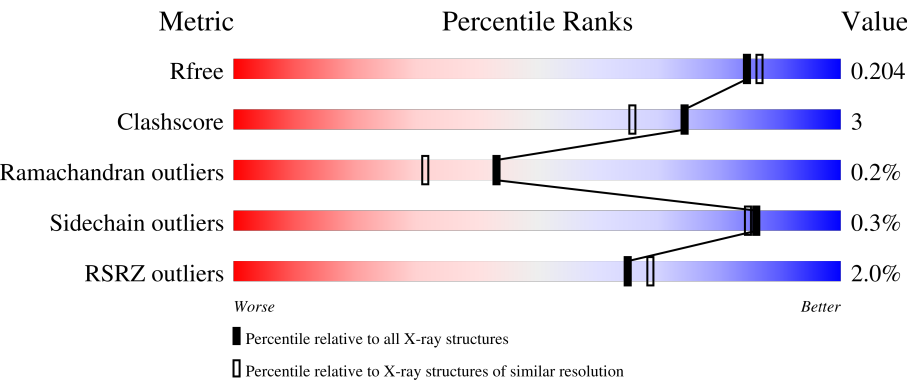
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	357	2% 92% 6%
1	B	357	3% 89% 8%
1	C	357	% 91% 5%
1	D	357	2% 88% 9%

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Mol	Chain	Length	Quality of chain
1	E	357	2% 92% 6%
1	F	357	3% 88% 8%
1	G	357	2% 92% 6%
1	H	357	2% 87% 8% 5%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 25480 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 Fructose-bisphosphate aldolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	6	0
			2748	1747	464	529	8			
1	B	344	Total	C	N	O	S	0	6	0
			2695	1713	455	518	9			
1	C	344	Total	C	N	O	S	0	4	0
			2685	1705	454	518	8			
1	D	344	Total	C	N	O	S	0	5	0
			2694	1710	456	519	9			
1	E	350	Total	C	N	O	S	0	6	0
			2750	1746	465	531	8			
1	F	343	Total	C	N	O	S	0	7	0
			2702	1718	459	517	8			
1	G	350	Total	C	N	O	S	0	2	0
			2716	1724	458	526	8			
1	H	339	Total	C	N	O	S	0	9	0
			2693	1714	454	516	9			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q0PAS0
A	-1	ASN	-	expression tag	UNP Q0PAS0
A	0	ALA	-	expression tag	UNP Q0PAS0
B	-2	SER	-	expression tag	UNP Q0PAS0
B	-1	ASN	-	expression tag	UNP Q0PAS0
B	0	ALA	-	expression tag	UNP Q0PAS0
C	-2	SER	-	expression tag	UNP Q0PAS0
C	-1	ASN	-	expression tag	UNP Q0PAS0
C	0	ALA	-	expression tag	UNP Q0PAS0
D	-2	SER	-	expression tag	UNP Q0PAS0
D	-1	ASN	-	expression tag	UNP Q0PAS0
D	0	ALA	-	expression tag	UNP Q0PAS0
E	-2	SER	-	expression tag	UNP Q0PAS0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	ASN	-	expression tag	UNP Q0PAS0
E	0	ALA	-	expression tag	UNP Q0PAS0
F	-2	SER	-	expression tag	UNP Q0PAS0
F	-1	ASN	-	expression tag	UNP Q0PAS0
F	0	ALA	-	expression tag	UNP Q0PAS0
G	-2	SER	-	expression tag	UNP Q0PAS0
G	-1	ASN	-	expression tag	UNP Q0PAS0
G	0	ALA	-	expression tag	UNP Q0PAS0
H	-2	SER	-	expression tag	UNP Q0PAS0
H	-1	ASN	-	expression tag	UNP Q0PAS0
H	0	ALA	-	expression tag	UNP Q0PAS0

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

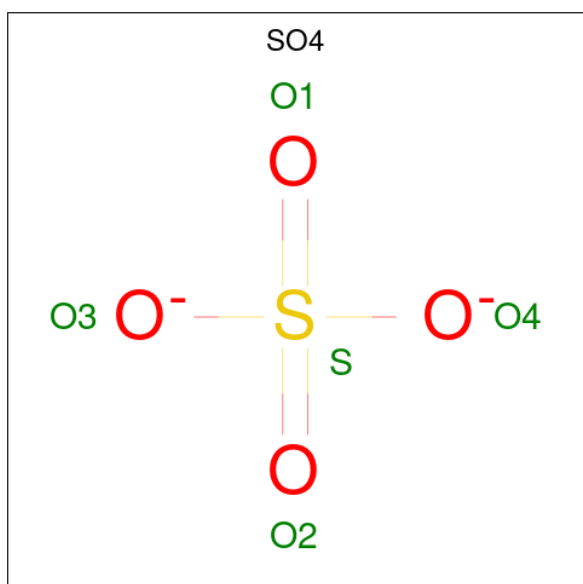
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0
2	G	1	Total Zn 1 1	0	0
2	H	1	Total Zn 1 1	0	0

- Molecule 3 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			3	1	2		
3	D	1	Total	C	O	0	0
			3	1	2		
3	D	1	Total	C	O	0	0
			3	1	2		
3	F	1	Total	C	O	0	0
			3	1	2		
3	H	1	Total	C	O	0	0
			3	1	2		

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	1
4	E	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	1

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Cl	0	1
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	547	Total	O	0	16
			561	561		
7	B	356	Total	O	0	6
			362	362		
7	C	514	Total	O	0	10
			524	524		

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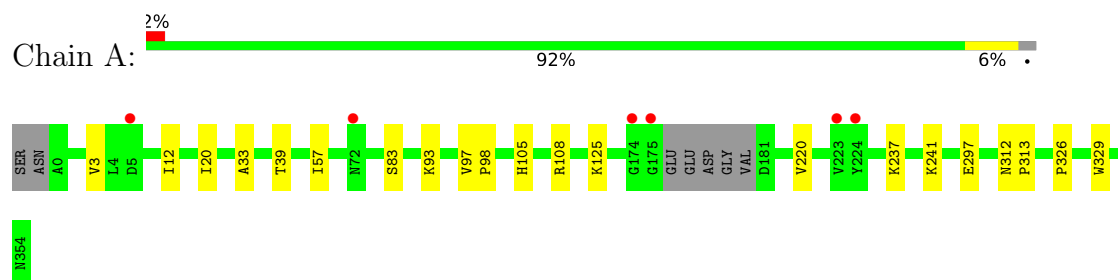
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	390	Total 400	O 400	0	12
7	E	499	Total 506	O 506	0	8
7	F	342	Total 347	O 347	0	7
7	G	546	Total 560	O 560	0	14
7	H	368	Total 378	O 378	0	11

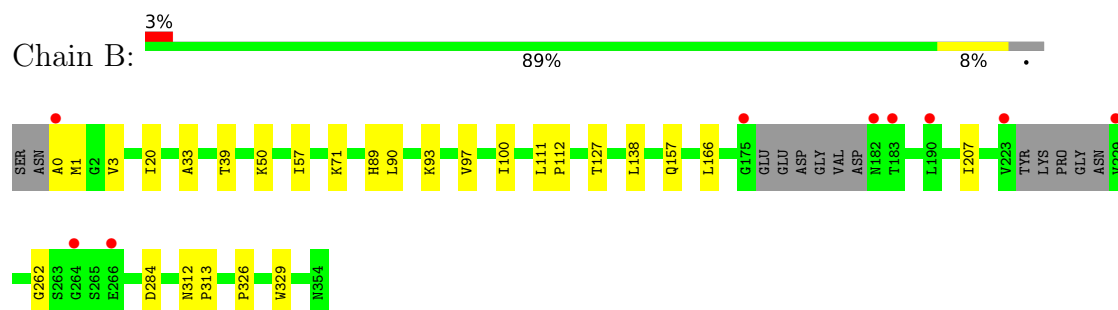
3 Residue-property plots

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.

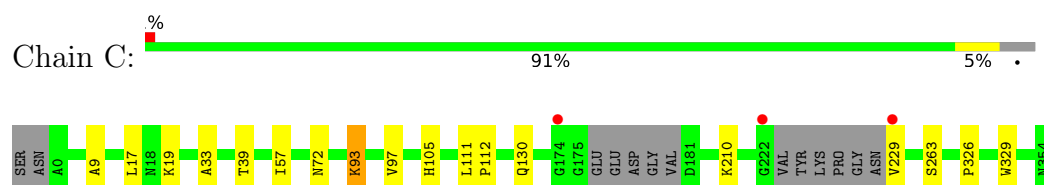
- Molecule 1: Fructose-bisphosphate aldolase



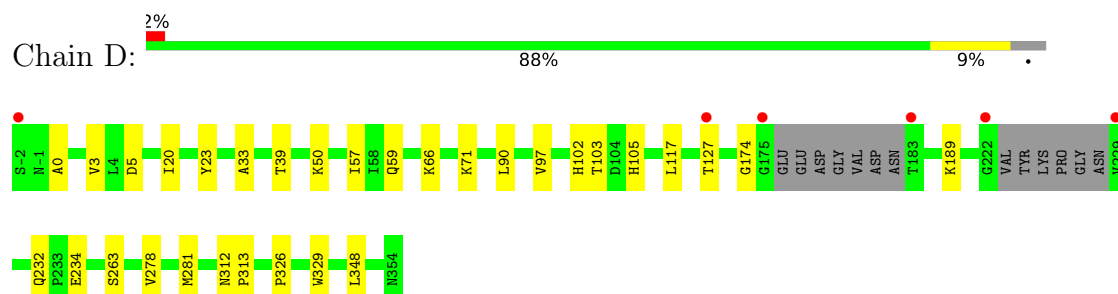
- Molecule 1: Fructose-bisphosphate aldolase



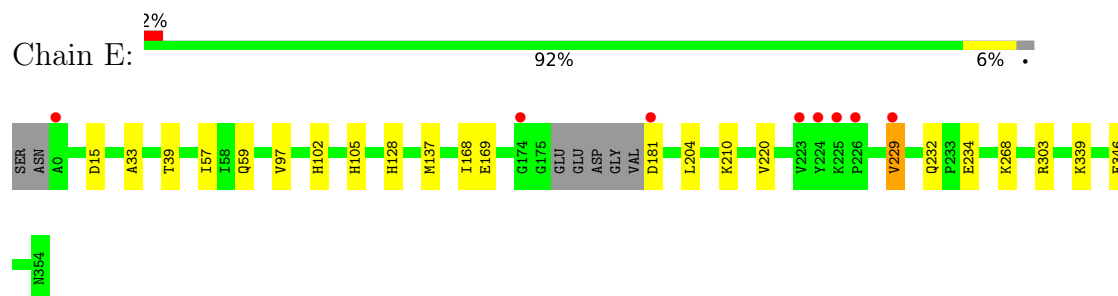
- Molecule 1: Fructose-bisphosphate aldolase



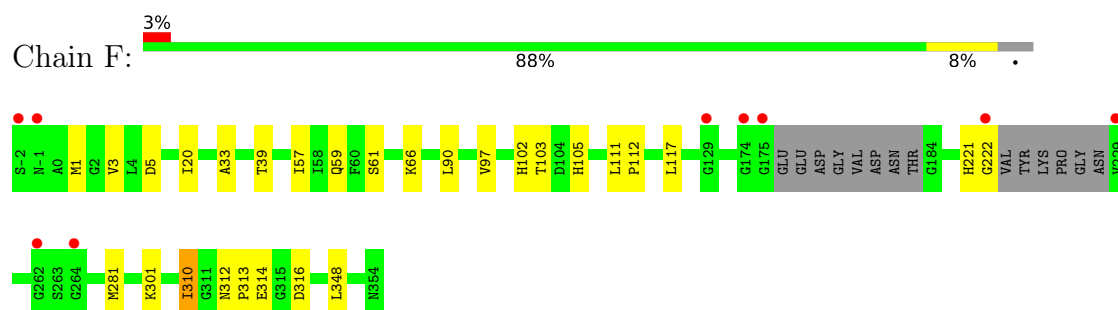
- Molecule 1: Fructose-bisphosphate aldolase



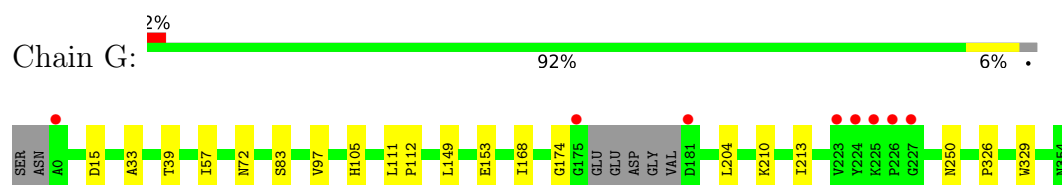
- Molecule 1: Fructose-bisphosphate aldolase



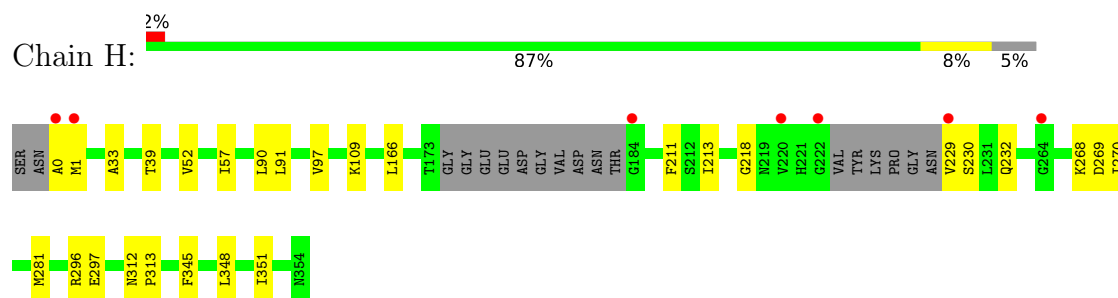
- Molecule 1: Fructose-bisphosphate aldolase



- Molecule 1: Fructose-bisphosphate aldolase



- Molecule 1: Fructose-bisphosphate aldolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	77.00Å 101.97Å 105.66Å 113.27° 95.34° 95.75°	Depositor
Resolution (Å)	29.66 – 1.85 29.66 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.6 (29.66-1.85) 97.6 (29.66-1.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.87 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.149 , 0.191 0.163 , 0.204	Depositor DCC
R_{free} test set	12186 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	16.6	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.001 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	25480	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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 53.20 % 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 4.3615e-05. 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: CL, ZN, SO4, FMT, GOL

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	0.74	0/2803	0.86	1/3783 (0.0%)
1	B	0.67	0/2744	0.86	1/3703 (0.0%)
1	C	0.75	0/2734	0.87	2/3689 (0.1%)
1	D	0.72	0/2743	0.85	3/3699 (0.1%)
1	E	0.72	0/2802	0.87	4/3783 (0.1%)
1	F	0.69	0/2751	0.86	2/3709 (0.1%)
1	G	0.77	0/2768	0.90	4/3739 (0.1%)
1	H	0.65	0/2742	0.86	3/3697 (0.1%)
All	All	0.72	0/22087	0.87	20/29802 (0.1%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	97	VAL	N-CA-C	7.46	116.85	108.05
1	G	97	VAL	N-CA-C	6.85	115.36	107.89
1	D	97	VAL	CB-CA-C	-6.39	103.53	110.37
1	G	174	GLY	N-CA-C	6.36	118.80	111.36
1	F	97	VAL	N-CA-C	6.29	115.47	108.05
1	B	97	VAL	N-CA-C	6.12	115.27	108.05
1	C	97	VAL	N-CA-C	5.97	114.40	107.89
1	C	17	LEU	N-CA-C	5.77	117.56	111.28
1	E	97	VAL	N-CA-C	5.75	114.16	107.89
1	F	61	SER	N-CA-C	-5.64	103.26	110.53
1	A	97	VAL	N-CA-C	5.59	113.99	107.89
1	H	91	LEU	N-CA-C	5.54	120.83	113.73
1	E	128	HIS	N-CA-C	5.40	120.02	113.38
1	D	5	ASP	N-CA-C	-5.36	106.78	113.38
1	G	97	VAL	CB-CA-C	-5.36	104.63	110.37
1	D	278	VAL	N-CA-C	-5.34	102.62	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	303	ARG	N-CA-C	5.08	117.21	111.11
1	G	213	ILE	N-CA-C	5.08	115.59	108.17
1	H	213	ILE	N-CA-C	5.06	115.41	108.12
1	E	97	VAL	CB-CA-C	-5.05	104.96	110.37

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	2748	0	2735	17	0
1	B	2695	0	2682	22	0
1	C	2685	0	2667	18	0
1	D	2694	0	2677	21	0
1	E	2750	0	2727	12	0
1	F	2702	0	2698	20	0
1	G	2716	0	2688	11	0
1	H	2693	0	2685	18	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	3	0	1	0	0
3	D	6	0	2	0	0
3	F	3	0	1	0	0
3	H	3	0	1	0	0
4	A	10	0	0	0	0
4	B	15	0	0	1	0
4	C	15	0	0	1	0
4	D	10	0	0	1	0
4	E	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	5	0	0	0	0
4	G	20	0	0	0	0
4	H	10	0	0	0	0
5	B	12	0	16	4	0
5	C	6	0	8	0	0
5	E	6	0	8	0	0
5	F	6	0	8	1	0
6	D	1	0	0	1	0
7	A	561	0	0	5	0
7	B	362	0	0	3	0
7	C	524	0	0	8	0
7	D	400	0	0	4	0
7	E	506	0	0	4	0
7	F	347	0	0	6	0
7	G	560	0	0	4	0
7	H	378	0	0	3	0
All	All	25480	0	21604	133	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 3.

All (133) 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:E:220:VAL:HG13	7:E:3143:HOH:O	1.40	1.20
1:C:93:LYS:O	1:C:93:LYS:HD3	1.54	1.06
1:H:281:MET:HE2	1:H:348:LEU:HD21	1.56	0.88
1:C:93:LYS:HD3	1:C:93:LYS:C	2.00	0.86
7:G:1291:HOH:O	1:H:90[A]:LEU:HD11	1.75	0.86
1:D:90:LEU:HD12	7:D:871:HOH:O	1.77	0.84
1:F:1:MET:HE2	1:F:5:ASP:HB3	1.60	0.82
1:H:90[A]:LEU:HD12	7:H:720:HOH:O	1.77	0.82
1:D:281:MET:HE2	1:D:348:LEU:HD21	1.69	0.75
1:G:15:ASP:OD1	1:G:210:LYS:HE2	1.91	0.71
1:D:232:GLN:NE2	1:D:234[B]:GLU:OE2	2.23	0.71
7:E:2221:HOH:O	1:F:90[A]:LEU:HD11	1.94	0.66
1:H:230:SER:O	1:H:232:GLN:HG2	1.96	0.65
1:F:310:ILE:HD13	7:F:1582:HOH:O	1.97	0.65
1:E:229:VAL:HG13	7:E:3143:HOH:O	1.98	0.64
1:H:1[A]:MET:HE2	7:H:2244:HOH:O	1.99	0.63
1:D:3:VAL:HG13	1:D:20:ILE:HD12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237[B]:LYS:HB3	1:A:237[B]:LYS:NZ	2.15	0.61
1:B:3:VAL:HG13	1:B:20:ILE:HD12	1.83	0.61
1:E:168:ILE:HD13	1:E:204:LEU:HD11	1.83	0.61
5:B:357:GOL:H31	7:B:2637:HOH:O	2.01	0.60
1:C:93:LYS:O	1:C:93:LYS:CD	2.43	0.60
1:A:39:THR:HG23	1:B:39:THR:HG23	1.84	0.60
1:G:72:ASN:ND2	7:G:2616:HOH:O	2.34	0.59
1:A:237[B]:LYS:HB3	1:A:237[B]:LYS:HZ3	1.66	0.58
1:A:220:VAL:HG11	7:A:2107:HOH:O	2.04	0.58
1:B:71:LYS:NZ	4:B:360:SO4:O3	2.24	0.57
1:C:130:GLN:NE2	7:C:1576:HOH:O	2.39	0.56
1:B:157:GLN:OE1	1:B:207[A]:ILE:HD12	2.06	0.56
1:C:72:ASN:ND2	7:C:3174:HOH:O	2.39	0.55
1:C:9:ALA:HB3	1:C:93:LYS:HE2	1.89	0.54
1:E:33:ALA:HA	1:E:57:ILE:HB	1.89	0.54
1:C:19:LYS:HE2	7:C:1825:HOH:O	2.06	0.54
1:D:33:ALA:HA	1:D:57:ILE:HB	1.89	0.54
1:F:103:THR:HG21	1:F:117:LEU:HD13	1.90	0.53
1:H:90[A]:LEU:CD1	7:H:720:HOH:O	2.46	0.53
1:B:127:THR:O	1:B:127:THR:CG2	2.56	0.53
1:D:263:SER:HB3	6:D:356[B]:CL:CL	2.46	0.53
1:C:39:THR:HG23	1:D:39:THR:HG23	1.91	0.53
1:B:33:ALA:HA	1:B:57:ILE:HB	1.91	0.53
1:B:138:LEU:HD13	1:B:166:LEU:HD11	1.91	0.53
1:F:281:MET:HE2	1:F:348:LEU:HD21	1.90	0.53
1:H:33:ALA:HA	1:H:57:ILE:HB	1.90	0.52
1:B:127:THR:O	1:B:127:THR:HG22	2.10	0.52
1:H:296:ARG:NH2	1:H:297:GLU:HG2	2.24	0.52
1:E:39:THR:HG23	1:F:39:THR:HG23	1.92	0.52
1:F:310:ILE:HD13	1:F:310:ILE:N	2.24	0.52
1:E:137:MET:CE	1:E:169:GLU:HB2	2.41	0.51
1:A:33:ALA:HA	1:A:57:ILE:HB	1.92	0.51
1:A:237[B]:LYS:NZ	1:A:237[B]:LYS:CB	2.73	0.51
1:A:125:LYS:NZ	7:A:3391[A]:HOH:O	2.43	0.51
1:C:33:ALA:HA	1:C:57:ILE:HB	1.91	0.51
1:E:15:ASP:OD1	1:E:210:LYS:HE2	2.11	0.51
1:D:174:GLY:HA2	1:D:189:LYS:HA	1.93	0.51
1:G:33:ALA:HA	1:G:57:ILE:HB	1.91	0.50
1:H:166:LEU:O	1:H:211:PHE:HA	2.11	0.50
1:G:39:THR:HG23	1:H:39:THR:HG23	1.94	0.49
1:F:3:VAL:HG13	1:F:20:ILE:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:THR:HG22	1:D:127:THR:O	2.12	0.49
1:C:130:GLN:NE2	7:C:1515:HOH:O	2.37	0.49
1:B:284:ASP:H	5:B:357:GOL:H32	1.78	0.48
1:A:108:ARG:NH1	7:A:2905:HOH:O	2.41	0.48
1:B:50:LYS:HE2	7:G:2461:HOH:O	2.12	0.48
1:F:1:MET:HE2	1:F:5:ASP:CB	2.38	0.48
1:H:218:GLY:HA2	1:H:229:VAL:HG13	1.94	0.48
1:D:103:THR:HG21	1:D:117:LEU:HD13	1.96	0.48
1:F:90[A]:LEU:HD12	7:F:1578:HOH:O	2.12	0.48
1:G:15:ASP:OD2	7:G:2934:HOH:O	2.20	0.48
1:D:90:LEU:CD1	7:D:871:HOH:O	2.50	0.48
1:C:93:LYS:HG2	7:C:3398:HOH:O	2.13	0.48
1:F:310:ILE:HD13	1:F:310:ILE:H	1.79	0.47
1:C:19:LYS:CE	7:C:1825:HOH:O	2.63	0.47
1:F:310:ILE:CD1	7:F:1582:HOH:O	2.58	0.47
1:B:93:LYS:HD3	7:B:912:HOH:O	2.15	0.47
1:B:89:HIS:ND1	5:B:356:GOL:H11	2.30	0.46
1:C:326:PRO:HA	1:C:329:TRP:CE2	2.49	0.46
1:A:83:SER:HB2	1:B:90:LEU:HD23	1.98	0.46
1:F:111:LEU:N	1:F:112:PRO:CD	2.79	0.46
1:D:281:MET:CE	1:D:348:LEU:HD21	2.43	0.45
5:F:357:GOL:H2	7:F:3596:HOH:O	2.15	0.45
1:F:59:GLN:HA	1:F:102:HIS:O	2.16	0.45
1:F:312:ASN:HB2	1:F:313:PRO:CD	2.47	0.45
1:D:50:LYS:HE3	1:E:346:GLU:OE1	2.17	0.45
1:E:339:LYS:NZ	7:E:3587:HOH:O	2.46	0.45
1:D:66:LYS:NZ	7:D:748:HOH:O	2.48	0.44
1:F:66[A]:LYS:HG3	7:F:2364:HOH:O	2.16	0.44
1:D:71[A]:LYS:NZ	4:D:359:SO4:O3	2.44	0.44
1:H:52[B]:VAL:HG13	1:H:351:ILE:HD13	1.99	0.44
1:C:229:VAL:O	1:C:229:VAL:HG13	2.17	0.44
1:F:33:ALA:HA	1:F:57:ILE:HB	1.98	0.44
1:F:221:HIS:O	1:F:222:GLY:C	2.61	0.44
1:C:210:LYS:HE3	7:C:3328:HOH:O	2.17	0.43
1:A:241[B]:LYS:NZ	7:A:3502:HOH:O	2.50	0.43
1:B:262:GLY:N	7:B:2637:HOH:O	2.51	0.43
1:B:284:ASP:N	5:B:357:GOL:H32	2.33	0.43
1:B:0:ALA:C	1:B:1[A]:MET:O	2.58	0.43
1:B:312:ASN:HB2	1:B:313:PRO:CD	2.49	0.43
1:D:0:ALA:HB1	1:D:23:TYR:OH	2.19	0.43
1:G:83:SER:HB2	1:H:90[A]:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ASN:HB2	1:A:313:PRO:HD2	2.01	0.43
1:B:57:ILE:HG12	1:B:100:ILE:HB	2.01	0.43
1:D:312:ASN:HB2	1:D:313:PRO:CD	2.48	0.43
1:G:149:LEU:O	1:G:153:GLU:HG3	2.19	0.43
1:G:111:LEU:N	1:G:112:PRO:CD	2.82	0.43
1:C:263:SER:OG	4:C:359:SO4:O1	2.26	0.42
1:H:268:LYS:HG3	1:H:269:ASP:N	2.33	0.42
1:G:326:PRO:HA	1:G:329:TRP:CE2	2.54	0.42
1:C:93:LYS:NZ	7:C:3409:HOH:O	2.51	0.42
1:H:270:ILE:HD13	1:H:281:MET:HE1	2.02	0.42
1:A:3:VAL:HG13	1:A:20:ILE:HD12	2.02	0.42
1:D:59:GLN:HA	1:D:102:HIS:O	2.20	0.42
1:E:268[B]:LYS:HE3	1:E:268[B]:LYS:HB2	1.67	0.42
1:F:301[B]:LYS:HD3	7:F:1211:HOH:O	2.19	0.42
1:H:312:ASN:HB2	1:H:313:PRO:CD	2.49	0.42
1:A:93[A]:LYS:O	1:A:93[A]:LYS:HD3	2.19	0.42
1:A:326:PRO:HA	1:A:329:TRP:CE2	2.55	0.41
1:D:71[A]:LYS:NZ	7:D:2725:HOH:O	2.51	0.41
1:H:0:ALA:O	1:H:1[A]:MET:HB2	2.20	0.41
1:G:168:ILE:HD13	1:G:204:LEU:HD11	2.02	0.41
1:E:232:GLN:NE2	1:E:234:GLU:OE2	2.51	0.41
1:C:111:LEU:N	1:C:112:PRO:CD	2.84	0.41
1:H:52[B]:VAL:HG21	1:H:345:PHE:CD2	2.56	0.41
1:F:316:ASP:OD1	1:G:250:ASN:ND2	2.54	0.41
1:B:93:LYS:O	1:B:93:LYS:HD2	2.21	0.41
1:A:12:ILE:HD11	1:A:98:PRO:HB2	2.03	0.41
1:B:326:PRO:HA	1:B:329:TRP:CE2	2.56	0.41
1:B:111:LEU:N	1:B:112:PRO:CD	2.84	0.40
1:D:326:PRO:HA	1:D:329:TRP:CE2	2.55	0.40
1:E:59:GLN:HA	1:E:102:HIS:O	2.21	0.40
1:A:297:GLU:HG2	7:A:3583:HOH:O	2.20	0.40
1:A:312:ASN:HB2	1:A:313:PRO:CD	2.52	0.40
1:D:127:THR:O	1:D:127:THR:CG2	2.69	0.40
1:B:3:VAL:HG13	1:B:20:ILE:CD1	2.50	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	352/357 (99%)	345 (98%)	6 (2%)	1 (0%)	36	25
1	B	344/357 (96%)	337 (98%)	7 (2%)	0	100	100
1	C	342/357 (96%)	336 (98%)	5 (2%)	1 (0%)	36	25
1	D	343/357 (96%)	337 (98%)	5 (2%)	1 (0%)	36	25
1	E	352/357 (99%)	349 (99%)	2 (1%)	1 (0%)	36	25
1	F	344/357 (96%)	337 (98%)	6 (2%)	1 (0%)	36	25
1	G	348/357 (98%)	341 (98%)	6 (2%)	1 (0%)	36	25
1	H	342/357 (96%)	333 (97%)	9 (3%)	0	100	100
All	All	2767/2856 (97%)	2715 (98%)	46 (2%)	6 (0%)	43	31

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	105	HIS
1	C	105	HIS
1	G	105	HIS
1	A	105	HIS
1	D	105	HIS
1	F	105	HIS

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	293/293 (100%)	293 (100%)	0	100	100
1	B	287/293 (98%)	287 (100%)	0	100	100
1	C	286/293 (98%)	285 (100%)	1 (0%)	86	85
1	D	287/293 (98%)	287 (100%)	0	100	100
1	E	293/293 (100%)	291 (99%)	2 (1%)	76	70
1	F	288/293 (98%)	286 (99%)	2 (1%)	76	70
1	G	289/293 (99%)	289 (100%)	0	100	100
1	H	287/293 (98%)	286 (100%)	1 (0%)	86	85
All	All	2310/2344 (98%)	2304 (100%)	6 (0%)	86	85

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	93	LYS
1	E	181	ASP
1	E	229	VAL
1	F	310	ILE
1	F	314	GLU
1	H	109	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	72	ASN
1	A	130	GLN
1	A	309	GLN
1	A	354	ASN
1	B	72	ASN
1	C	128	HIS
1	D	72	ASN
1	E	75	ASN
1	E	130	GLN
1	F	309	GLN
1	G	309	GLN
1	H	232	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 40 ligands modelled in this entry, 9 are monoatomic - leaving 31 for Mogul analysis.

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	$\# Z > 2$
3	FMT	D	357	-	2,2,2	0.67	0	1,1,1	0.46	0
4	SO4	D	360[A]	-	4,4,4	0.41	0	6,6,6	0.29	0
4	SO4	H	357	-	4,4,4	0.18	0	6,6,6	0.16	0
3	FMT	A	356	-	2,2,2	0.70	0	1,1,1	0.37	0
4	SO4	E	359	-	4,4,4	0.39	0	6,6,6	0.25	0
4	SO4	G	358	-	4,4,4	0.24	0	6,6,6	0.25	0
4	SO4	B	360	-	4,4,4	0.25	0	6,6,6	0.20	0
4	SO4	G	359	-	4,4,4	0.29	0	6,6,6	0.33	0
5	GOL	C	356	-	5,5,5	0.81	0	5,5,5	0.65	0
3	FMT	H	356	-	2,2,2	0.69	0	1,1,1	0.44	0
4	SO4	H	358[A]	-	4,4,4	0.14	0	6,6,6	0.16	0
4	SO4	G	357	-	4,4,4	0.51	0	6,6,6	0.41	0
5	GOL	F	357	-	5,5,5	0.46	0	5,5,5	0.31	0
4	SO4	A	358	-	4,4,4	0.31	0	6,6,6	0.49	0
4	SO4	B	359	-	4,4,4	0.33	0	6,6,6	0.71	0
4	SO4	A	357	-	4,4,4	0.26	0	6,6,6	0.18	0
4	SO4	E	360	-	4,4,4	0.22	0	6,6,6	0.24	0
5	GOL	E	356	-	5,5,5	0.45	0	5,5,5	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	D	359	-	4,4,4	0.26	0	6,6,6	0.28	0
5	GOL	B	357	-	5,5,5	0.85	0	5,5,5	0.66	0
4	SO4	C	357	-	4,4,4	0.26	0	6,6,6	0.28	0
4	SO4	E	358	-	4,4,4	0.67	0	6,6,6	0.55	0
3	FMT	D	358	-	2,2,2	0.66	0	1,1,1	0.36	0
4	SO4	F	358	-	4,4,4	0.22	0	6,6,6	0.05	0
4	SO4	G	356	-	4,4,4	0.34	0	6,6,6	0.46	0
4	SO4	C	359	-	4,4,4	0.19	0	6,6,6	0.33	0
4	SO4	B	358	-	4,4,4	0.35	0	6,6,6	0.34	0
4	SO4	E	357	-	4,4,4	0.32	0	6,6,6	0.42	0
5	GOL	B	356	-	5,5,5	0.33	0	5,5,5	0.27	0
3	FMT	F	356	-	2,2,2	0.71	0	1,1,1	0.47	0
4	SO4	C	358	-	4,4,4	0.17	0	6,6,6	0.68	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	C	356	-	-	2/4/4/4	-
5	GOL	E	356	-	-	2/4/4/4	-
5	GOL	F	357	-	-	0/4/4/4	-
5	GOL	B	357	-	-	1/4/4/4	-
5	GOL	B	356	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	356	GOL	O1-C1-C2-C3
5	E	356	GOL	O1-C1-C2-O2
5	C	356	GOL	O2-C2-C3-O3
5	B	356	GOL	C1-C2-C3-O3
5	B	357	GOL	C1-C2-C3-O3
5	C	356	GOL	C1-C2-C3-O3

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	360	SO4	1	0
5	F	357	GOL	1	0
4	D	359	SO4	1	0
5	B	357	GOL	3	0
4	C	359	SO4	1	0
5	B	356	GOL	1	0

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	350/357 (98%)	-0.34	6 (1%) 69 73	7, 15, 31, 45	6 (1%)
1	B	344/357 (96%)	-0.10	9 (2%) 57 61	7, 21, 47, 74	6 (1%)
1	C	344/357 (96%)	-0.46	3 (0%) 81 84	6, 15, 27, 46	4 (1%)
1	D	344/357 (96%)	-0.19	6 (1%) 69 73	9, 19, 42, 62	5 (1%)
1	E	350/357 (98%)	-0.29	8 (2%) 61 64	7, 17, 36, 64	6 (1%)
1	F	343/357 (96%)	-0.04	9 (2%) 57 61	7, 23, 48, 64	7 (2%)
1	G	350/357 (98%)	-0.36	8 (2%) 61 64	9, 15, 32, 51	2 (0%)
1	H	339/357 (94%)	-0.14	7 (2%) 63 67	7, 21, 47, 64	9 (2%)
All	All	2764/2856 (96%)	-0.24	56 (2%) 65 68	6, 18, 42, 74	45 (1%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	0	ALA	6.6
1	B	223	VAL	5.2
1	E	224	TYR	5.0
1	D	-2	SER	5.0
1	E	0	ALA	4.5
1	G	223	VAL	4.3
1	B	183	THR	3.9
1	E	223	VAL	3.7
1	H	1[A]	MET	3.6
1	E	226	PRO	3.5
1	F	129	GLY	3.3
1	E	225	LYS	3.3
1	B	264	GLY	3.3
1	G	0	ALA	3.2
1	G	225	LYS	3.2
1	A	223	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	224	TYR	3.1
1	B	0	ALA	3.0
1	H	229	VAL	3.0
1	D	229	VAL	3.0
1	A	175	GLY	3.0
1	H	220	VAL	2.9
1	C	174	GLY	2.8
1	A	174	GLY	2.8
1	C	222	GLY	2.8
1	H	222	GLY	2.8
1	B	182	ASN	2.8
1	G	175	GLY	2.7
1	H	184	GLY	2.6
1	E	229	VAL	2.6
1	E	174	GLY	2.5
1	D	183	THR	2.5
1	D	175	GLY	2.5
1	G	181	ASP	2.5
1	A	224	TYR	2.4
1	C	229	VAL	2.4
1	F	175	GLY	2.4
1	A	5	ASP	2.4
1	D	127	THR	2.4
1	B	229	VAL	2.3
1	G	226	PRO	2.3
1	F	-2	SER	2.3
1	F	229	VAL	2.3
1	F	262	GLY	2.3
1	A	72	ASN	2.2
1	B	190	LEU	2.2
1	G	227	GLY	2.2
1	F	-1	ASN	2.1
1	F	264	GLY	2.1
1	B	266	GLU	2.1
1	F	174	GLY	2.1
1	D	222	GLY	2.0
1	F	222	GLY	2.0
1	H	264	GLY	2.0
1	E	181	ASP	2.0
1	B	175	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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	E	360	5/5	0.74	0.14	76,76,77,79	0
3	FMT	D	358	3/3	0.76	0.21	45,45,47,47	0
4	SO4	G	358	5/5	0.77	0.13	63,65,67,68	0
5	GOL	B	356	6/6	0.78	0.15	45,49,53,54	0
5	GOL	E	356	6/6	0.81	0.16	33,40,41,45	0
3	FMT	F	356	3/3	0.83	0.11	34,34,35,35	0
4	SO4	D	360[A]	5/5	0.83	0.13	8,24,31,32	5
4	SO4	H	358[A]	5/5	0.84	0.16	26,28,30,32	5
4	SO4	G	359	5/5	0.85	0.15	38,42,48,48	0
3	FMT	A	356	3/3	0.85	0.11	30,30,31,32	0
4	SO4	F	358	5/5	0.86	0.17	37,38,39,40	5
4	SO4	C	358	5/5	0.87	0.15	35,39,42,43	0
4	SO4	E	358	5/5	0.87	0.11	24,29,32,37	0
5	GOL	B	357	6/6	0.87	0.13	22,30,39,45	0
5	GOL	C	356	6/6	0.87	0.14	27,34,40,45	0
4	SO4	D	359	5/5	0.87	0.09	46,49,52,53	0
5	GOL	F	357	6/6	0.87	0.11	25,34,38,43	0
4	SO4	B	360	5/5	0.88	0.11	45,48,50,51	5
4	SO4	B	359	5/5	0.89	0.11	39,42,45,45	0
3	FMT	D	357	3/3	0.89	0.09	32,32,33,34	0
3	FMT	H	356	3/3	0.89	0.08	34,34,35,35	0
4	SO4	A	358	5/5	0.89	0.14	20,25,38,39	0
4	SO4	A	357	5/5	0.90	0.09	56,56,58,59	0
4	SO4	G	357	5/5	0.90	0.14	21,27,40,40	0
4	SO4	H	357	5/5	0.90	0.11	33,37,38,42	0
4	SO4	E	359	5/5	0.93	0.11	21,22,32,32	0
4	SO4	C	357	5/5	0.95	0.08	24,27,31,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	G	356	5/5	0.95	0.09	29,29,33,37	0
4	SO4	C	359	5/5	0.95	0.10	19,26,29,29	0
4	SO4	E	357	5/5	0.95	0.08	30,30,32,36	0
4	SO4	B	358	5/5	0.96	0.08	28,28,31,34	0
6	CL	D	356[B]	1/1	0.97	0.08	16,16,16,16	1
2	ZN	D	355	1/1	0.99	0.02	23,23,23,23	0
2	ZN	F	355	1/1	0.99	0.03	28,28,28,28	0
2	ZN	H	355	1/1	0.99	0.03	27,27,27,27	0
2	ZN	B	355	1/1	0.99	0.02	24,24,24,24	0
2	ZN	C	355	1/1	0.99	0.02	18,18,18,18	0
2	ZN	E	355	1/1	1.00	0.01	16,16,16,16	0
2	ZN	A	355	1/1	1.00	0.02	16,16,16,16	0
2	ZN	G	355	1/1	1.00	0.02	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.