



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:39 PM UTC

PDB ID : 2XG6 / pdb_00002xg6
Title : Molecular insights into clinically isolated OmpC mutants and their role in multi-drug resistance
Authors : Lou, H.; Naismith, J.H.
Deposited on : 2010-05-31
Resolution : 3.47 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

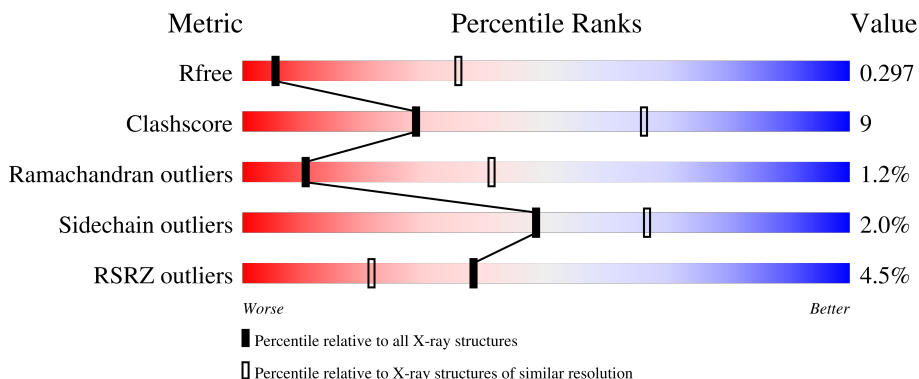
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.47 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	1083 (3.52-3.44)
Clashscore	190562	1139 (3.52-3.44)
Ramachandran outliers	187476	1111 (3.52-3.44)
Sidechain outliers	187428	1112 (3.52-3.44)
RSRZ outliers	180081	1082 (3.52-3.44)

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	343	4% 83% 16% .
1	B	343	2% 82% 17% .
1	C	343	4% 81% 19% .
1	D	343	5% 82% 17% .
1	E	343	6% 83% 17% .

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Mol	Chain	Length	Quality of chain
1	F	343	6% 80% 20%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16299 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 OMPC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	0	0
			2714	1705	451	554	4			
1	B	343	Total	C	N	O	S	0	0	0
			2714	1705	451	554	4			
1	C	343	Total	C	N	O	S	0	0	0
			2714	1705	451	554	4			
1	D	343	Total	C	N	O	S	0	0	0
			2714	1705	451	554	4			
1	E	343	Total	C	N	O	S	0	0	0
			2714	1705	451	554	4			
1	F	343	Total	C	N	O	S	0	0	0
			2714	1705	451	554	4			

There are 18 discrepancies between the modelled and reference sequences:

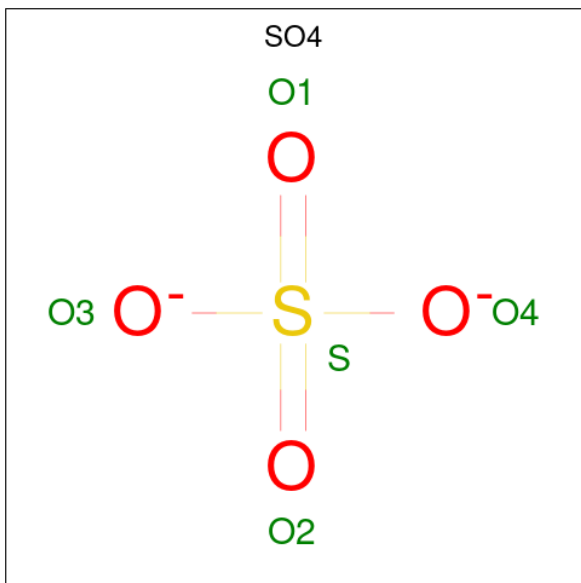
Chain	Residue	Modelled	Actual	Comment	Reference
A	18	GLU	ASP	SEE REMARK 999	UNP Q9K597
A	124	HIS	ARG	SEE REMARK 999	UNP Q9K597
A	271	PHE	SER	SEE REMARK 999	UNP Q9K597
B	18	GLU	ASP	SEE REMARK 999	UNP Q9K597
B	124	HIS	ARG	SEE REMARK 999	UNP Q9K597
B	271	PHE	SER	SEE REMARK 999	UNP Q9K597
C	18	GLU	ASP	SEE REMARK 999	UNP Q9K597
C	124	HIS	ARG	SEE REMARK 999	UNP Q9K597
C	271	PHE	SER	SEE REMARK 999	UNP Q9K597
D	18	GLU	ASP	SEE REMARK 999	UNP Q9K597
D	124	HIS	ARG	SEE REMARK 999	UNP Q9K597
D	271	PHE	SER	SEE REMARK 999	UNP Q9K597
E	18	GLU	ASP	SEE REMARK 999	UNP Q9K597
E	124	HIS	ARG	SEE REMARK 999	UNP Q9K597
E	271	PHE	SER	SEE REMARK 999	UNP Q9K597
F	18	GLU	ASP	SEE REMARK 999	UNP Q9K597
F	124	HIS	ARG	SEE REMARK 999	UNP Q9K597

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Chain	Residue	Modelled	Actual	Comment	Reference
F	271	PHE	SER	SEE REMARK 999	UNP Q9K597

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

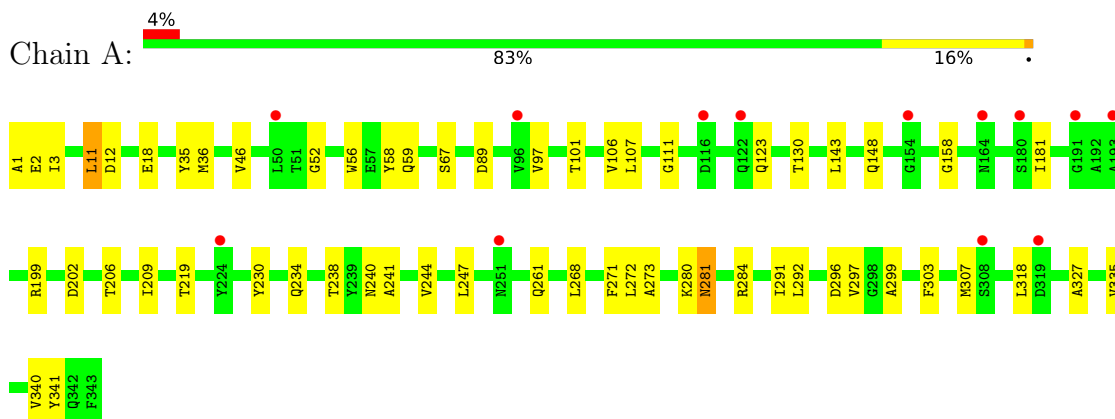


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

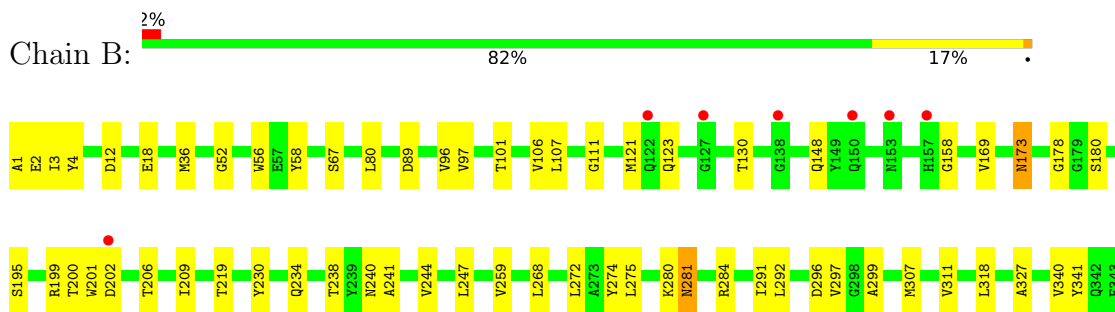
3 Residue-property plots [i](#)

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.

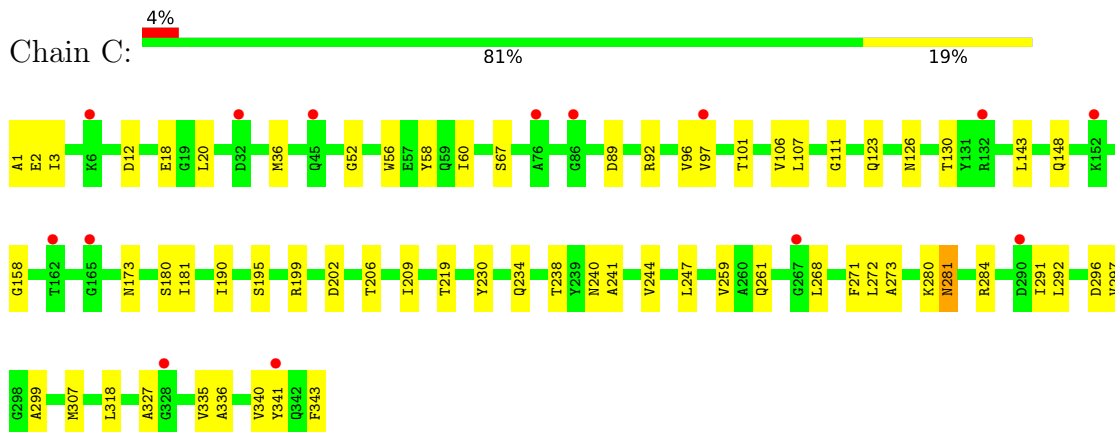
• Molecule 1: OMPC



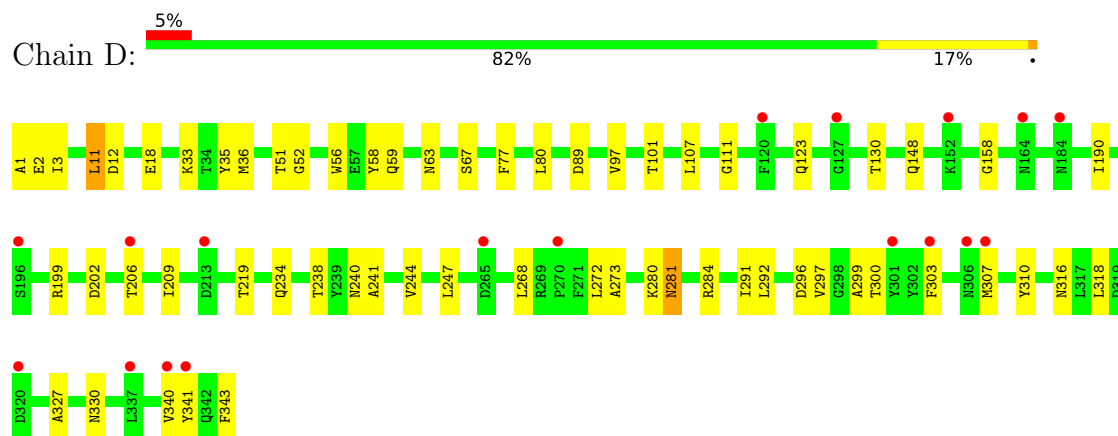
• Molecule 1: OMPC



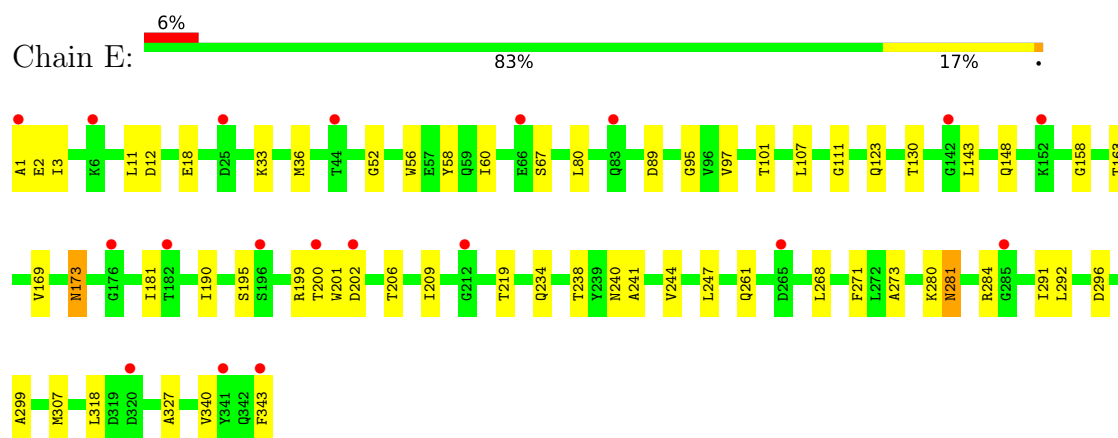
• Molecule 1: OMPC



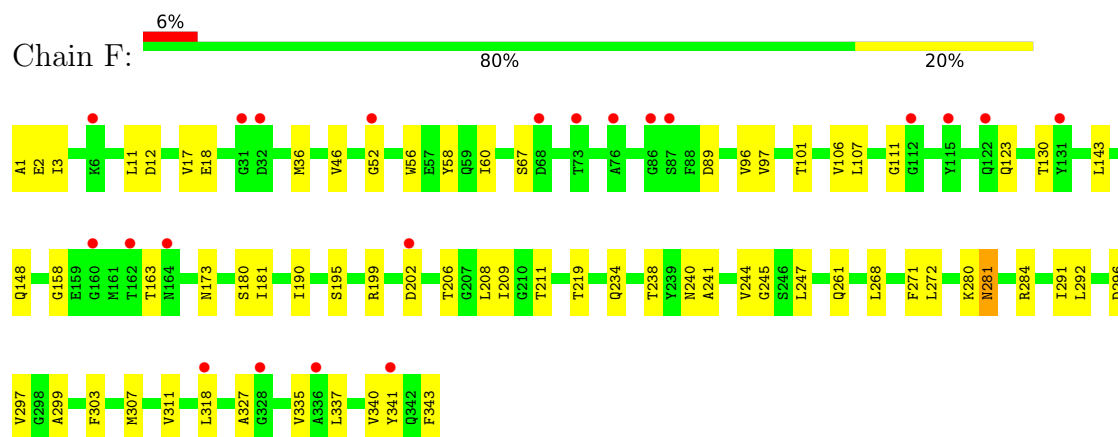
- Molecule 1: OMPC



- Molecule 1: OMPC



- Molecule 1: OMPC



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	142.82Å 159.72Å 164.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.19 – 3.47 53.19 – 3.47	Depositor EDS
% Data completeness (in resolution range)	82.4 (53.19-3.47) 82.4 (53.19-3.47)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.6.0073	Depositor
R, R_{free}	0.261 , 0.293 0.262 , 0.297	Depositor DCC
R_{free} test set	2053 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	121.1	Xtriage
Anisotropy	0.541	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 183.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	16299	wwPDB-VP
Average B, all atoms (Å ²)	53.0	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 36.10 % 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 5.2623e-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 [i](#)

5.1 Standard geometry [i](#)

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	0.47	0/2777	0.67	0/3758
1	B	0.48	0/2777	0.69	0/3758
1	C	0.46	0/2777	0.67	0/3758
1	D	0.48	0/2777	0.68	0/3758
1	E	0.48	0/2777	0.68	0/3758
1	F	0.46	0/2777	0.67	0/3758
All	All	0.47	0/16662	0.68	0/22548

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 [i](#)

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	2714	0	2479	50	0
1	B	2714	0	2479	49	0
1	C	2714	0	2479	56	0
1	D	2714	0	2479	52	0
1	E	2714	0	2479	56	0
1	F	2714	0	2479	58	0
2	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	5	0	0	0	0
2	D	5	0	0	0	0
All	All	16299	0	14874	275	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 9.

All (275) 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:130:THR:HG22	1:E:148:GLN:HG3	1.29	1.15
1:B:130:THR:HG22	1:B:148:GLN:HG3	1.32	1.11
1:F:130:THR:HG22	1:F:148:GLN:HG3	1.32	1.11
1:C:130:THR:HG22	1:C:148:GLN:HG3	1.31	1.11
1:A:130:THR:HG22	1:A:148:GLN:HG3	1.36	1.04
1:D:130:THR:HG22	1:D:148:GLN:HG3	1.36	1.01
1:E:36:MET:HE2	1:F:56:TRP:NE1	1.73	1.01
1:D:56:TRP:NE1	1:F:36:MET:HE2	1.82	0.94
1:F:36:MET:HE3	1:F:60:ILE:HB	1.54	0.90
1:F:36:MET:CE	1:F:60:ILE:HB	2.01	0.89
1:A:56:TRP:NE1	1:C:36:MET:HE2	1.89	0.87
1:C:36:MET:CE	1:C:60:ILE:HB	2.04	0.87
1:C:36:MET:HE3	1:C:60:ILE:HB	1.59	0.84
1:A:36:MET:HE3	1:B:56:TRP:CD2	2.17	0.79
1:D:36:MET:HE3	1:E:56:TRP:CD2	2.20	0.75
1:C:268:LEU:HD11	1:C:299:ALA:HB1	1.70	0.73
1:C:130:THR:CG2	1:C:148:GLN:HE21	2.01	0.73
1:E:36:MET:CE	1:E:60:ILE:HB	2.19	0.72
1:A:101:THR:HG23	1:A:219:THR:HG21	1.72	0.72
1:E:36:MET:HE3	1:E:60:ILE:HB	1.72	0.71
1:F:268:LEU:HD11	1:F:299:ALA:HB1	1.72	0.71
1:F:36:MET:HE1	1:F:60:ILE:HD12	1.73	0.70
1:E:36:MET:HE2	1:F:56:TRP:CE2	2.26	0.70
1:D:56:TRP:CE2	1:F:36:MET:HE2	2.26	0.69
1:F:130:THR:CG2	1:F:148:GLN:HE21	2.05	0.69
1:E:247:LEU:HD12	1:E:327:ALA:HB2	1.74	0.69
1:A:268:LEU:HD11	1:A:299:ALA:HB1	1.75	0.69
1:A:307:MET:HE1	1:A:341:TYR:HB2	1.74	0.68
1:B:130:THR:CG2	1:B:148:GLN:HE21	2.06	0.68
1:E:101:THR:HG23	1:E:219:THR:HG21	1.76	0.68
1:D:101:THR:HG23	1:D:219:THR:HG21	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:GLU:HG3	1:B:340:VAL:HG22	1.76	0.67
1:D:303:PHE:CZ	1:E:80:LEU:HD11	2.29	0.66
1:B:130:THR:HG22	1:B:148:GLN:CG	2.20	0.66
1:D:307:MET:HE1	1:D:341:TYR:HB2	1.76	0.66
1:A:130:THR:CG2	1:A:148:GLN:HE21	2.08	0.66
1:C:101:THR:HG23	1:C:219:THR:HG21	1.78	0.65
1:C:130:THR:HG22	1:C:148:GLN:CG	2.19	0.65
1:F:101:THR:HG23	1:F:219:THR:HG21	1.78	0.65
1:F:36:MET:HE1	1:F:60:ILE:HB	1.77	0.64
1:D:18:GLU:HG3	1:D:340:VAL:HG22	1.80	0.64
1:B:36:MET:HE3	1:C:56:TRP:CD2	2.33	0.64
1:C:247:LEU:HD12	1:C:327:ALA:HB2	1.80	0.64
1:E:268:LEU:HD11	1:E:299:ALA:HB1	1.79	0.64
1:E:36:MET:HE1	1:E:60:ILE:HD12	1.80	0.63
1:F:307:MET:HE1	1:F:341:TYR:HB2	1.79	0.63
1:C:36:MET:HE1	1:C:60:ILE:HB	1.78	0.63
1:B:101:THR:HG23	1:B:219:THR:HG21	1.80	0.63
1:D:247:LEU:HD12	1:D:327:ALA:HB2	1.81	0.62
1:C:130:THR:CG2	1:C:148:GLN:HG3	2.19	0.62
1:A:56:TRP:CE2	1:C:36:MET:HE2	2.34	0.62
1:C:107:LEU:HD12	1:C:111:GLY:HA3	1.81	0.62
1:E:130:THR:CG2	1:E:148:GLN:HE21	2.13	0.62
1:B:307:MET:HE3	1:C:52:GLY:HA3	1.82	0.61
1:E:18:GLU:HG3	1:E:340:VAL:HG22	1.80	0.61
1:E:130:THR:CG2	1:E:148:GLN:HG3	2.19	0.61
1:B:247:LEU:HD12	1:B:327:ALA:HB2	1.83	0.61
1:D:3:ILE:HD13	1:E:3:ILE:HD12	1.81	0.61
1:B:107:LEU:HD12	1:B:111:GLY:HA3	1.82	0.61
1:D:292:LEU:HD12	1:D:318:LEU:HD11	1.82	0.61
1:E:307:MET:HE3	1:F:52:GLY:HA3	1.82	0.60
1:A:36:MET:HE3	1:B:56:TRP:CE3	2.36	0.60
1:D:107:LEU:HD12	1:D:111:GLY:HA3	1.83	0.60
1:D:130:THR:CG2	1:D:148:GLN:HE21	2.14	0.60
1:D:268:LEU:HD11	1:D:299:ALA:HB1	1.85	0.59
1:B:307:MET:HE3	1:C:52:GLY:CA	2.33	0.58
1:E:107:LEU:HD12	1:E:111:GLY:HA3	1.85	0.58
1:A:247:LEU:HD12	1:A:327:ALA:HB2	1.85	0.58
1:E:130:THR:HG22	1:E:148:GLN:CG	2.20	0.58
1:F:209:ILE:CG2	1:F:284:ARG:HD3	2.34	0.57
1:B:130:THR:CG2	1:B:148:GLN:HG3	2.21	0.57
1:C:209:ILE:CG2	1:C:284:ARG:HD3	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:ILE:CG2	1:D:284:ARG:HD3	2.34	0.57
1:A:307:MET:HE3	1:B:52:GLY:C	2.29	0.57
1:F:130:THR:HG22	1:F:148:GLN:CG	2.21	0.57
1:C:18:GLU:HG3	1:C:340:VAL:HG22	1.87	0.57
1:A:107:LEU:HD12	1:A:111:GLY:HA3	1.87	0.57
1:C:36:MET:HE1	1:C:60:ILE:HD12	1.86	0.56
1:A:209:ILE:CG2	1:A:284:ARG:HD3	2.35	0.56
1:B:274:TYR:C	1:B:275:LEU:HD12	2.31	0.56
1:C:130:THR:HG21	1:C:148:GLN:HE21	1.68	0.56
1:B:209:ILE:CG2	1:B:284:ARG:HD3	2.36	0.56
1:E:209:ILE:CG2	1:E:284:ARG:HD3	2.36	0.56
1:A:35:TYR:CD2	1:A:59:GLN:NE2	2.73	0.56
1:C:106:VAL:HG11	1:C:230:TYR:CE2	2.41	0.56
1:D:36:MET:HE3	1:E:56:TRP:CE3	2.41	0.56
1:E:1:ALA:O	1:E:3:ILE:HG23	2.05	0.56
1:F:292:LEU:HD12	1:F:318:LEU:HD11	1.88	0.55
1:D:11:LEU:HD13	1:F:343:PHE:CD2	2.41	0.55
1:A:18:GLU:HG3	1:A:340:VAL:HG22	1.87	0.55
1:D:130:THR:HG22	1:D:148:GLN:CG	2.25	0.55
1:F:130:THR:CG2	1:F:148:GLN:HG3	2.21	0.55
1:A:292:LEU:HD12	1:A:318:LEU:HD11	1.88	0.55
1:F:130:THR:HG21	1:F:148:GLN:HE21	1.71	0.54
1:A:130:THR:HG22	1:A:148:GLN:CG	2.24	0.54
1:D:80:LEU:HD11	1:F:303:PHE:CZ	2.43	0.54
1:F:18:GLU:HG3	1:F:340:VAL:HG22	1.89	0.54
1:E:307:MET:HE3	1:F:52:GLY:CA	2.37	0.54
1:F:130:THR:HG22	1:F:148:GLN:HE21	1.73	0.54
1:A:130:THR:HG22	1:A:148:GLN:HE21	1.72	0.53
1:C:130:THR:HG22	1:C:148:GLN:HE21	1.74	0.53
1:D:35:TYR:CD2	1:D:59:GLN:NE2	2.77	0.53
1:A:272:LEU:HD13	1:A:297:VAL:CG2	2.40	0.52
1:B:307:MET:HE3	1:C:52:GLY:C	2.34	0.52
1:F:247:LEU:HD12	1:F:327:ALA:HB2	1.89	0.52
1:A:244:VAL:HG22	1:A:291:ILE:HD13	1.92	0.52
1:D:202:ASP:O	1:D:206:THR:HG23	2.10	0.52
1:C:143:LEU:HD11	1:C:181:ILE:HG23	1.91	0.51
1:B:292:LEU:HA	1:B:318:LEU:HD11	1.90	0.51
1:B:244:VAL:HG22	1:B:291:ILE:HD13	1.92	0.51
1:A:272:LEU:HD13	1:A:297:VAL:HG22	1.93	0.51
1:C:106:VAL:CG2	1:C:259:VAL:HG11	2.41	0.51
1:F:107:LEU:HD12	1:F:111:GLY:HA3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:THR:HG21	1:B:148:GLN:HE21	1.74	0.51
1:A:1:ALA:O	1:A:3:ILE:HG23	2.11	0.51
1:B:2:GLU:HA	1:B:12:ASP:HA	1.92	0.51
1:F:202:ASP:O	1:F:206:THR:HG23	2.11	0.51
1:A:202:ASP:O	1:A:206:THR:HG23	2.11	0.51
1:D:307:MET:HE3	1:E:52:GLY:C	2.36	0.51
1:E:2:GLU:HA	1:E:12:ASP:HA	1.92	0.51
1:C:202:ASP:O	1:C:206:THR:HG23	2.10	0.50
1:D:272:LEU:HD13	1:D:297:VAL:CG2	2.41	0.50
1:E:36:MET:HE1	1:E:60:ILE:HB	1.91	0.50
1:D:272:LEU:HD13	1:D:297:VAL:HG22	1.93	0.50
1:E:202:ASP:O	1:E:206:THR:HG23	2.11	0.50
1:F:2:GLU:HA	1:F:12:ASP:HA	1.93	0.50
1:B:130:THR:HG22	1:B:148:GLN:HE21	1.76	0.50
1:F:36:MET:HE1	1:F:60:ILE:CD1	2.41	0.50
1:A:2:GLU:HA	1:A:12:ASP:HA	1.94	0.50
1:B:202:ASP:O	1:B:206:THR:HG23	2.12	0.50
1:D:199:ARG:NH1	1:D:240:ASN:O	2.45	0.50
1:D:2:GLU:HA	1:D:12:ASP:HA	1.95	0.49
1:D:244:VAL:HG22	1:D:291:ILE:HD13	1.95	0.49
1:E:199:ARG:NH1	1:E:240:ASN:O	2.46	0.49
1:A:199:ARG:NH1	1:A:240:ASN:O	2.45	0.49
1:D:130:THR:HG22	1:D:148:GLN:HE21	1.76	0.49
1:B:199:ARG:NH1	1:B:240:ASN:O	2.46	0.49
1:C:199:ARG:NH1	1:C:240:ASN:O	2.46	0.49
1:A:143:LEU:HD11	1:A:181:ILE:HG23	1.94	0.49
1:C:2:GLU:HA	1:C:12:ASP:HA	1.94	0.49
1:E:143:LEU:HD11	1:E:181:ILE:HG23	1.94	0.48
1:A:130:THR:HG21	1:A:148:GLN:HE21	1.79	0.48
1:B:272:LEU:HD13	1:B:297:VAL:HG22	1.96	0.48
1:C:272:LEU:HD13	1:C:297:VAL:CG2	2.43	0.48
1:F:199:ARG:NH1	1:F:240:ASN:O	2.46	0.48
1:D:280:LYS:O	1:D:281:ASN:C	2.56	0.48
1:B:209:ILE:HG23	1:B:284:ARG:HH11	1.79	0.48
1:D:209:ILE:HG23	1:D:284:ARG:HH11	1.79	0.48
1:C:280:LYS:O	1:C:281:ASN:C	2.56	0.48
1:D:33:LYS:HD3	1:E:163:THR:HG21	1.96	0.48
1:B:106:VAL:HG11	1:B:230:TYR:CE2	2.48	0.47
1:A:280:LYS:O	1:A:281:ASN:C	2.57	0.47
1:F:209:ILE:HG23	1:F:284:ARG:HH11	1.79	0.47
1:E:247:LEU:CD1	1:E:327:ALA:HB2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:LEU:HD11	1:B:299:ALA:HB1	1.96	0.47
1:E:209:ILE:HG23	1:E:284:ARG:HH11	1.80	0.47
1:C:209:ILE:HG23	1:C:284:ARG:HH11	1.80	0.47
1:D:107:LEU:HD13	1:D:296:ASP:OD2	2.14	0.47
1:E:280:LYS:O	1:E:281:ASN:C	2.57	0.47
1:F:280:LYS:O	1:F:281:ASN:C	2.57	0.47
1:F:56:TRP:CZ2	1:F:58:TYR:HB2	2.50	0.47
1:F:238:THR:HB	1:F:241:ALA:HB3	1.95	0.47
1:E:36:MET:HE2	1:F:56:TRP:HE1	1.70	0.47
1:B:1:ALA:O	1:B:3:ILE:HG23	2.14	0.47
1:E:56:TRP:CZ2	1:E:58:TYR:HB2	2.50	0.47
1:E:33:LYS:HD3	1:F:163:THR:HG21	1.96	0.47
1:B:121:MET:HE1	1:B:178:GLY:N	2.29	0.46
1:B:307:MET:HE1	1:B:341:TYR:HB2	1.98	0.46
1:C:56:TRP:CZ2	1:C:58:TYR:HB2	2.50	0.46
1:F:36:MET:HE1	1:F:60:ILE:CB	2.44	0.46
1:D:1:ALA:O	1:D:3:ILE:HG23	2.15	0.46
1:B:280:LYS:O	1:B:281:ASN:C	2.58	0.46
1:C:92:ARG:HD2	1:C:126:ASN:ND2	2.31	0.46
1:A:268:LEU:HD11	1:A:299:ALA:CB	2.45	0.46
1:F:96:VAL:HG22	1:F:180:SER:HB3	1.98	0.46
1:A:1:ALA:HB1	1:B:4:TYR:CE1	2.51	0.46
1:A:209:ILE:HG23	1:A:284:ARG:HH11	1.79	0.46
1:B:56:TRP:CZ2	1:B:58:TYR:HB2	2.51	0.46
1:A:56:TRP:HE1	1:C:36:MET:HE2	1.79	0.45
1:A:101:THR:HG22	1:A:234:GLN:OE1	2.16	0.45
1:A:238:THR:HB	1:A:241:ALA:HB3	1.97	0.45
1:A:3:ILE:HD13	1:B:3:ILE:HD12	1.98	0.45
1:A:56:TRP:CZ2	1:A:58:TYR:HB2	2.51	0.45
1:F:36:MET:HE1	1:F:60:ILE:CG1	2.46	0.45
1:F:272:LEU:HD13	1:F:297:VAL:HG22	1.99	0.45
1:E:101:THR:HG22	1:E:234:GLN:OE1	2.16	0.45
1:F:1:ALA:O	1:F:3:ILE:HG23	2.15	0.45
1:C:36:MET:HE1	1:C:60:ILE:CB	2.46	0.45
1:C:307:MET:HE1	1:C:341:TYR:HB2	1.97	0.45
1:E:173:ASN:C	1:E:173:ASN:HD22	2.24	0.45
1:C:107:LEU:HD13	1:C:296:ASP:OD2	2.17	0.45
1:D:130:THR:HG21	1:D:148:GLN:HE21	1.82	0.45
1:A:106:VAL:HG11	1:A:230:TYR:CE2	2.51	0.45
1:B:106:VAL:CG2	1:B:259:VAL:HG11	2.47	0.45
1:B:272:LEU:HD13	1:B:297:VAL:CG2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:THR:HB	1:C:241:ALA:HB3	1.97	0.45
1:D:300:THR:HG23	1:D:310:TYR:HB3	1.99	0.45
1:E:107:LEU:HD13	1:E:296:ASP:OD2	2.17	0.44
1:E:95:GLY:HA2	1:E:148:GLN:HE22	1.82	0.44
1:C:101:THR:HG22	1:C:234:GLN:OE1	2.17	0.44
1:F:272:LEU:HD13	1:F:297:VAL:CG2	2.48	0.44
1:B:107:LEU:HD13	1:B:296:ASP:OD2	2.17	0.44
1:A:11:LEU:HD13	1:C:343:PHE:CD2	2.53	0.44
1:D:238:THR:HB	1:D:241:ALA:HB3	1.98	0.44
1:A:307:MET:CE	1:A:341:TYR:HD1	2.30	0.44
1:C:272:LEU:HD13	1:C:297:VAL:HG22	1.99	0.44
1:D:107:LEU:HD21	1:D:273:ALA:HB2	2.00	0.44
1:A:107:LEU:HD13	1:A:296:ASP:OD2	2.18	0.43
1:B:101:THR:HG22	1:B:234:GLN:OE1	2.18	0.43
1:E:343:PHE:CG	1:F:11:LEU:HD13	2.52	0.43
1:A:52:GLY:HA3	1:C:307:MET:HE3	2.00	0.43
1:C:107:LEU:HD21	1:C:273:ALA:HB2	2.01	0.43
1:E:173:ASN:C	1:E:173:ASN:ND2	2.76	0.43
1:F:107:LEU:HD13	1:F:296:ASP:OD2	2.19	0.43
1:A:268:LEU:CD1	1:A:299:ALA:HB1	2.47	0.43
1:C:244:VAL:HG22	1:C:291:ILE:HD13	2.01	0.43
1:D:56:TRP:CZ2	1:D:58:TYR:HB2	2.53	0.43
1:A:303:PHE:CZ	1:B:80:LEU:HD11	2.54	0.43
1:A:107:LEU:HD21	1:A:273:ALA:HB2	2.01	0.43
1:B:36:MET:HE3	1:C:56:TRP:CE3	2.54	0.43
1:F:101:THR:HG22	1:F:234:GLN:OE1	2.18	0.43
1:E:36:MET:CE	1:F:56:TRP:CE2	3.00	0.42
1:F:244:VAL:HG22	1:F:291:ILE:HD13	2.01	0.42
1:C:20:LEU:HD11	1:C:336:ALA:HB1	2.01	0.42
1:D:307:MET:CE	1:D:341:TYR:HD1	2.32	0.42
1:E:238:THR:HB	1:E:241:ALA:HB3	2.00	0.42
1:D:268:LEU:CD1	1:D:299:ALA:HB1	2.49	0.42
1:D:343:PHE:CG	1:E:11:LEU:HD13	2.55	0.42
1:A:130:THR:CG2	1:A:148:GLN:HG3	2.27	0.42
1:E:107:LEU:HD21	1:E:273:ALA:HB2	2.01	0.42
1:F:143:LEU:HD11	1:F:181:ILE:HG23	2.02	0.42
1:C:1:ALA:O	1:C:3:ILE:HG23	2.19	0.42
1:E:292:LEU:HA	1:E:318:LEU:HD11	2.00	0.42
1:C:96:VAL:HG22	1:C:180:SER:HB3	2.01	0.42
1:E:130:THR:HG21	1:E:148:GLN:HE21	1.84	0.42
1:F:261:GLN:HG2	1:F:271:PHE:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:MET:HE3	1:C:36:MET:HB3	1.93	0.42
1:B:96:VAL:HG22	1:B:180:SER:HB3	2.02	0.41
1:F:311:VAL:HG22	1:F:337:LEU:HD13	2.01	0.41
1:A:52:GLY:CA	1:C:307:MET:HE3	2.50	0.41
1:D:292:LEU:HA	1:D:318:LEU:HD11	2.01	0.41
1:E:36:MET:HE2	1:F:56:TRP:CD1	2.49	0.41
1:B:200:THR:HG22	1:B:201:TRP:N	2.35	0.41
1:C:292:LEU:HD12	1:C:318:LEU:HD11	2.02	0.41
1:A:261:GLN:HG2	1:A:271:PHE:HB3	2.03	0.41
1:B:238:THR:HB	1:B:241:ALA:HB3	2.02	0.41
1:C:261:GLN:HG2	1:C:271:PHE:HB3	2.03	0.41
1:D:33:LYS:HA	1:D:63:ASN:HD22	1.86	0.41
1:D:77:PHE:C	1:F:17:VAL:HG11	2.46	0.41
1:D:101:THR:HG22	1:D:234:GLN:OE1	2.20	0.41
1:D:307:MET:HE3	1:E:52:GLY:HA3	2.03	0.41
1:E:200:THR:HG22	1:E:201:TRP:N	2.36	0.41
1:A:307:MET:HE3	1:B:52:GLY:HA3	2.03	0.41
1:D:316:ASN:ND2	1:D:330:ASN:O	2.53	0.41
1:A:307:MET:HE3	1:B:52:GLY:CA	2.51	0.41
1:B:169:VAL:HG21	1:B:206:THR:HG21	2.03	0.41
1:C:268:LEU:HD11	1:C:299:ALA:CB	2.46	0.41
1:C:268:LEU:CD1	1:C:299:ALA:HB1	2.47	0.41
1:D:36:MET:HE3	1:E:56:TRP:CE2	2.56	0.41
1:E:244:VAL:HG22	1:E:291:ILE:HD13	2.03	0.41
1:F:106:VAL:HG23	1:F:261:GLN:NE2	2.36	0.41
1:F:208:LEU:O	1:F:211:THR:HG23	2.22	0.41
1:C:36:MET:HE1	1:C:60:ILE:CG1	2.51	0.40
1:C:292:LEU:HA	1:C:318:LEU:HD11	2.01	0.40
1:E:261:GLN:HG2	1:E:271:PHE:HB3	2.03	0.40
1:A:36:MET:HE3	1:B:56:TRP:CE2	2.55	0.40
1:B:173:ASN:HD22	1:B:173:ASN:C	2.29	0.40
1:D:52:GLY:C	1:F:307:MET:HE3	2.46	0.40
1:D:303:PHE:CZ	1:E:80:LEU:CD1	3.00	0.40
1:E:169:VAL:HG21	1:E:206:THR:HG21	2.03	0.40
1:F:307:MET:CE	1:F:341:TYR:HD1	2.35	0.40
1:D:56:TRP:CE2	1:F:36:MET:CE	3.01	0.40
1:D:307:MET:HE2	1:D:341:TYR:HD1	1.86	0.40
1:E:292:LEU:HD12	1:E:318:LEU:HD11	2.02	0.40
1:F:245:GLY:HA3	1:F:327:ALA:HB1	2.02	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	341/343 (99%)	310 (91%)	27 (8%)	4 (1%)	10	41
1	B	341/343 (99%)	307 (90%)	30 (9%)	4 (1%)	10	41
1	C	341/343 (99%)	309 (91%)	28 (8%)	4 (1%)	10	41
1	D	341/343 (99%)	310 (91%)	27 (8%)	4 (1%)	10	41
1	E	341/343 (99%)	310 (91%)	27 (8%)	4 (1%)	10	41
1	F	341/343 (99%)	310 (91%)	27 (8%)	4 (1%)	10	41
All	All	2046/2058 (99%)	1856 (91%)	166 (8%)	24 (1%)	10	41

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	281	ASN
1	B	281	ASN
1	C	281	ASN
1	D	281	ASN
1	E	281	ASN
1	F	281	ASN
1	A	158	GLY
1	B	158	GLY
1	C	158	GLY
1	D	158	GLY
1	E	158	GLY
1	F	158	GLY
1	A	67	SER
1	B	67	SER
1	C	67	SER
1	D	67	SER
1	F	67	SER
1	A	123	GLN
1	B	123	GLN
1	C	123	GLN

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Mol	Chain	Res	Type
1	D	123	GLN
1	E	67	SER
1	E	123	GLN
1	F	123	GLN

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	277/277 (100%)	272 (98%)	5 (2%)	51	69
1	B	277/277 (100%)	272 (98%)	5 (2%)	51	69
1	C	277/277 (100%)	271 (98%)	6 (2%)	45	65
1	D	277/277 (100%)	272 (98%)	5 (2%)	51	69
1	E	277/277 (100%)	272 (98%)	5 (2%)	51	69
1	F	277/277 (100%)	270 (98%)	7 (2%)	42	63
All	All	1662/1662 (100%)	1629 (98%)	33 (2%)	48	66

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	46	VAL
1	A	89	ASP
1	A	97	VAL
1	A	335	VAL
1	B	89	ASP
1	B	97	VAL
1	B	173	ASN
1	B	195	SER
1	B	311	VAL
1	C	89	ASP
1	C	97	VAL
1	C	173	ASN
1	C	190	ILE

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Mol	Chain	Res	Type
1	C	195	SER
1	C	335	VAL
1	D	11	LEU
1	D	51	THR
1	D	89	ASP
1	D	97	VAL
1	D	190	ILE
1	E	89	ASP
1	E	97	VAL
1	E	173	ASN
1	E	190	ILE
1	E	195	SER
1	F	46	VAL
1	F	89	ASP
1	F	97	VAL
1	F	173	ASN
1	F	190	ILE
1	F	195	SER
1	F	335	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	69	ASN
1	A	157	HIS
1	A	205	ASN
1	A	237	GLN
1	B	9	ASN
1	B	61	GLN
1	B	69	ASN
1	B	119	ASN
1	B	123	GLN
1	B	157	HIS
1	B	205	ASN
1	B	237	GLN
1	C	69	ASN
1	C	150	GLN
1	C	157	HIS
1	C	205	ASN
1	C	281	ASN
1	D	9	ASN

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Mol	Chain	Res	Type
1	D	69	ASN
1	D	157	HIS
1	D	205	ASN
1	D	237	GLN
1	D	281	ASN
1	E	9	ASN
1	E	69	ASN
1	E	150	GLN
1	E	157	HIS
1	E	205	ASN
1	E	237	GLN
1	E	281	ASN
1	F	9	ASN
1	F	61	GLN
1	F	69	ASN
1	F	150	GLN
1	F	157	HIS
1	F	205	ASN
1	F	237	GLN
1	F	254	GLN
1	F	321	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](#)

3 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	$\# Z > 2$
2	SO4	A	1344	-	4,4,4	0.24	0	6,6,6	0.16	0
2	SO4	D	1344	-	4,4,4	0.26	0	6,6,6	0.22	0
2	SO4	C	1344	-	4,4,4	0.25	0	6,6,6	0.16	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	343/343 (100%)	0.31	13 (3%) 44 25	19, 49, 77, 95	0
1	B	343/343 (100%)	0.17	7 (2%) 65 40	10, 47, 73, 87	0
1	C	343/343 (100%)	0.35	14 (4%) 41 23	27, 61, 85, 131	0
1	D	343/343 (100%)	0.29	18 (5%) 33 19	20, 50, 74, 87	0
1	E	343/343 (100%)	0.44	19 (5%) 30 18	14, 46, 74, 96	0
1	F	343/343 (100%)	0.44	21 (6%) 27 17	30, 61, 84, 115	0
All	All	2058/2058 (100%)	0.33	92 (4%) 38 21	10, 53, 80, 131	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	86	GLY	6.3
1	A	251	ASN	4.8
1	F	160	GLY	4.5
1	A	164	ASN	4.5
1	D	164	ASN	4.4
1	F	87	SER	4.4
1	E	265	ASP	4.4
1	E	196	SER	4.3
1	B	153	ASN	4.3
1	C	86	GLY	4.2
1	F	112	GLY	3.7
1	D	184	ASN	3.6
1	C	290	ASP	3.6
1	F	202	ASP	3.6
1	E	176	GLY	3.5
1	B	150	GLN	3.5
1	D	303	PHE	3.4
1	F	336	ALA	3.4
1	A	50	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	76	ALA	3.2
1	A	319	ASP	3.1
1	A	193	ALA	3.0
1	C	6	LYS	2.9
1	A	191	GLY	2.9
1	D	337	LEU	2.9
1	D	120	PHE	2.9
1	E	25	ASP	2.9
1	F	162	THR	2.8
1	E	285	GLY	2.8
1	F	52	GLY	2.8
1	B	122	GLN	2.7
1	B	127	GLY	2.7
1	D	152	LYS	2.7
1	C	328	GLY	2.7
1	A	224	TYR	2.7
1	F	73	THR	2.6
1	E	200	THR	2.6
1	D	306	ASN	2.6
1	D	341	TYR	2.6
1	F	131	TYR	2.6
1	E	182	THR	2.6
1	C	341	TYR	2.6
1	D	127	GLY	2.5
1	E	66	GLU	2.5
1	E	152	LYS	2.5
1	D	213	ASP	2.5
1	E	212	GLY	2.5
1	E	320	ASP	2.5
1	F	115	TYR	2.5
1	A	154	GLY	2.5
1	F	68	ASP	2.5
1	A	308	SER	2.4
1	F	341	TYR	2.4
1	E	142	GLY	2.4
1	D	265	ASP	2.4
1	F	31	GLY	2.4
1	D	320	ASP	2.4
1	E	343	PHE	2.4
1	C	165	GLY	2.4
1	B	138	GLY	2.3
1	B	202	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	32	ASP	2.3
1	F	318	LEU	2.3
1	D	340	VAL	2.3
1	F	6	LYS	2.3
1	A	122	GLN	2.3
1	E	83	GLN	2.3
1	C	152	LYS	2.3
1	D	307	MET	2.2
1	F	164	ASN	2.2
1	E	1	ALA	2.2
1	C	162	THR	2.2
1	D	301	TYR	2.2
1	C	97	VAL	2.2
1	D	196	SER	2.2
1	C	132	ARG	2.2
1	A	116	ASP	2.2
1	E	341	TYR	2.1
1	C	45	GLN	2.1
1	D	270	PRO	2.1
1	F	32	ASP	2.1
1	A	180	SER	2.1
1	F	328	GLY	2.1
1	B	157	HIS	2.0
1	D	206	THR	2.0
1	C	267	GLY	2.0
1	F	122	GLN	2.0
1	A	96	VAL	2.0
1	E	44	THR	2.0
1	F	76	ALA	2.0
1	E	202	ASP	2.0
1	E	6	LYS	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
2	SO4	C	1344	5/5	0.60	0.09	190,214,217,225	0
2	SO4	D	1344	5/5	0.62	0.14	148,169,201,210	0
2	SO4	A	1344	5/5	0.69	0.09	170,179,185,186	0

6.5 Other polymers [i](#)

There are no such residues in this entry.