



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:33 AM GMT

PDB ID : 2XG6  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

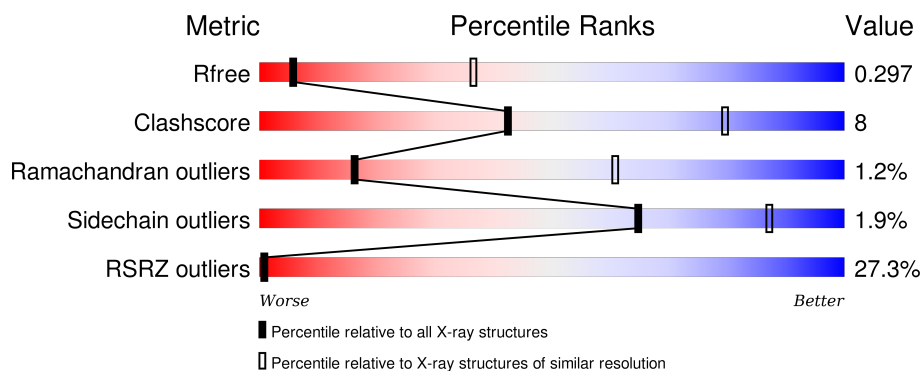
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.47 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))
$R_{free}$	91344	1173 (3.60-3.36)
Clashscore	102246	1010 (3.58-3.38)
Ramachandran outliers	100387	1245 (3.60-3.36)
Sidechain outliers	100360	1246 (3.60-3.36)
RSRZ outliers	91569	1180 (3.60-3.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	343	<div> <div>25%</div> <div>83%</div> <div>16%</div> </div>
1	B	343	<div> <div>21%</div> <div>83%</div> <div>17%</div> </div>
1	C	343	<div> <div>34%</div> <div>81%</div> <div>19%</div> </div>
1	D	343	<div> <div>25%</div> <div>83%</div> <div>17%</div> </div>
1	E	343	<div> <div>25%</div> <div>83%</div> <div>17%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	343	<div> <div>34%</div> <div>81%</div> <div>19%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	1344	-	-	-	X
2	SO4	C	1344	-	-	-	X
2	SO4	D	1344	-	-	-	X

## 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:

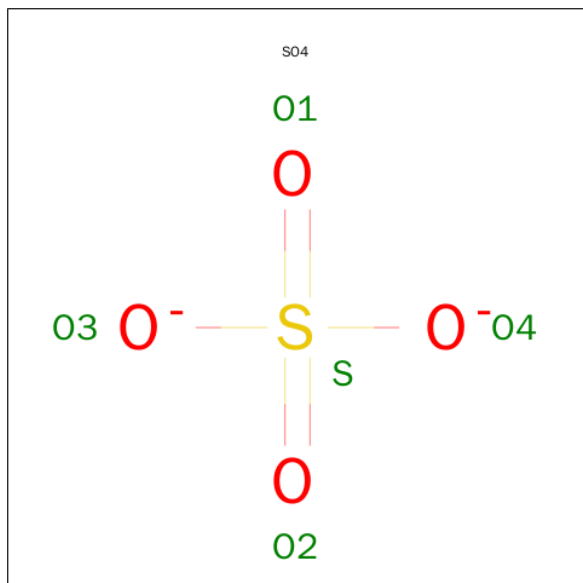
Chain	Residue	Modelled	Actual	Comment	Reference
A	18	GLU	ASP	SEE REMARK 999	UNP Q9K597
A	124	HIS	ARG	SEE REMARK 999	UNP Q9K597
A	271	PHE	SER	SEE REMARK 999	UNP Q9K597
B	18	GLU	ASP	SEE REMARK 999	UNP Q9K597
B	124	HIS	ARG	SEE REMARK 999	UNP Q9K597
B	271	PHE	SER	SEE REMARK 999	UNP Q9K597
C	18	GLU	ASP	SEE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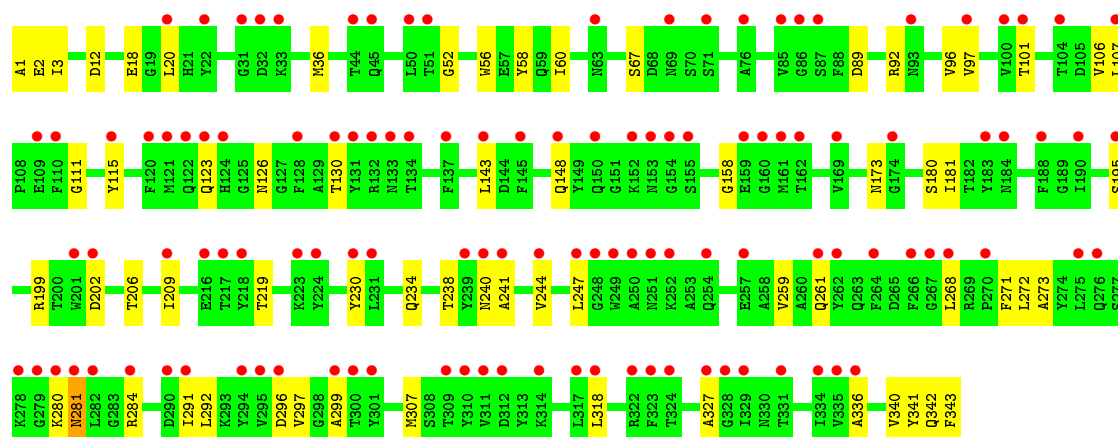
Chain	Residue	Modelled	Actual	Comment	Reference
F	271	PHE	SER	SEE REMARK 999	UNP Q9K597

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

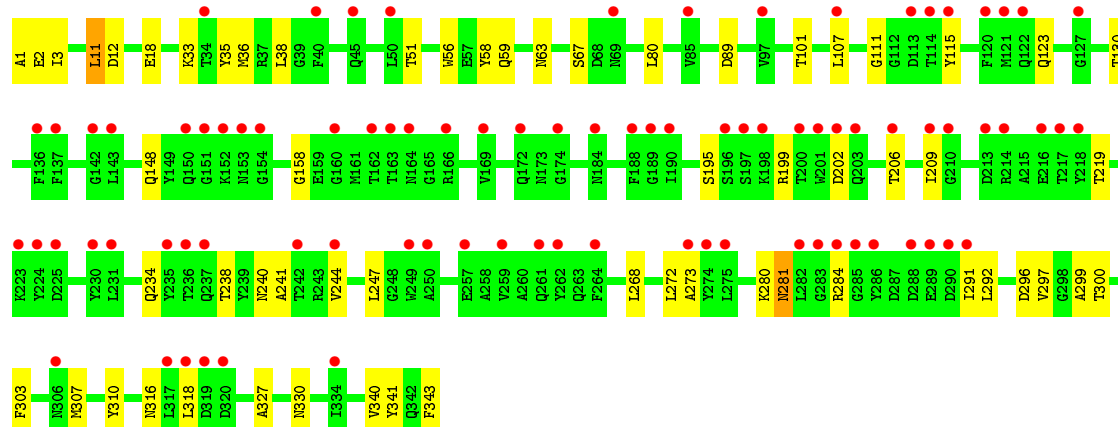
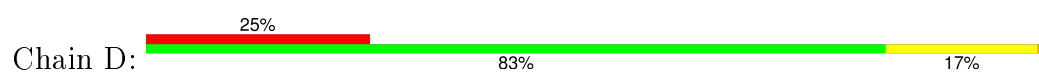


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

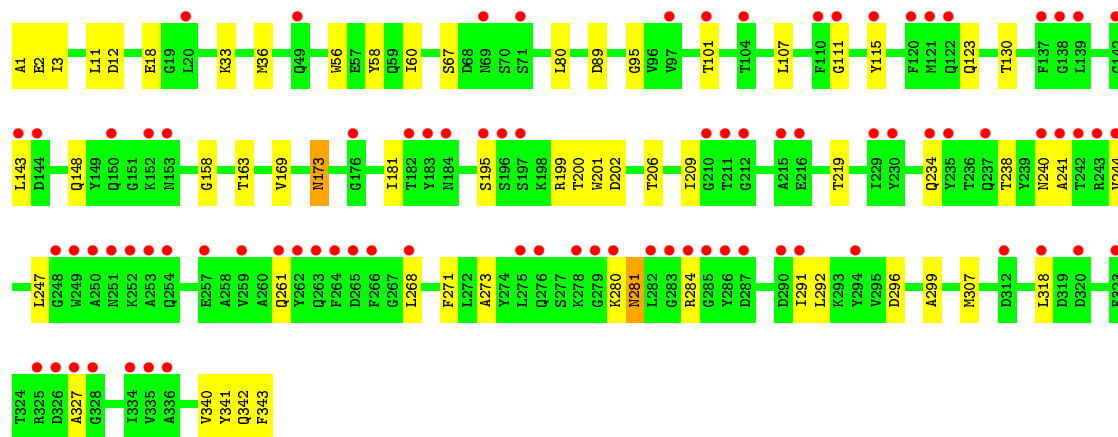
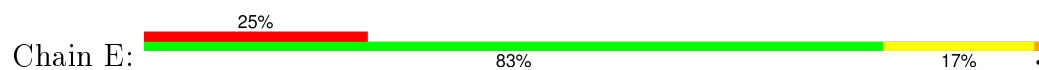




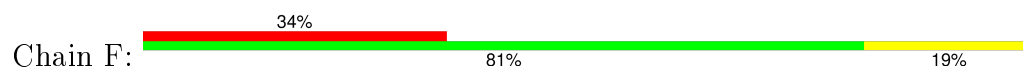
• Molecule 1: OMPC

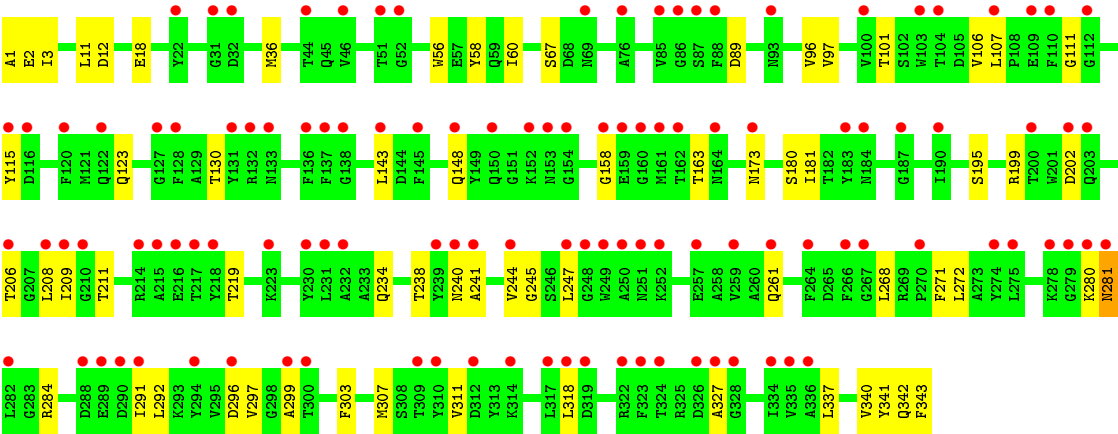


• Molecule 1: OMPC



• Molecule 1: OMPC







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	121.1	Xtriage
Anisotropy	0.541	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 133.0	EDS
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	4 of 40689 reflections (0.010%)	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	16299	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [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	0.39	0/2777	0.52	0/3758
1	B	0.40	0/2777	0.54	0/3758
1	C	0.38	0/2777	0.52	0/3758
1	D	0.40	0/2777	0.53	0/3758
1	E	0.41	0/2777	0.53	0/3758
1	F	0.37	0/2777	0.52	0/3758
All	All	0.39	0/16662	0.53	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	48	0
1	B	2714	0	2479	43	0
1	C	2714	0	2479	51	0
1	D	2714	0	2479	49	0
1	E	2714	0	2479	51	0
1	F	2714	0	2479	52	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	260	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 8.

All (260) 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:C:36:MET:HE3	1:C:60:ILE:HB	1.27	1.16
1:E:130:THR:HG22	1:E:148:GLN:HG3	1.29	1.15
1:F:130:THR:HG22	1:F:148:GLN:HG3	1.32	1.11
1:B:130:THR:HG22	1:B:148:GLN:HG3	1.32	1.11
1:E:36:MET:HE3	1:E:60:ILE:HB	1.31	1.11
1:C:130:THR:HG22	1:C:148:GLN:HG3	1.31	1.11
1:F:36:MET:HE3	1:F:60:ILE:HB	1.21	1.10
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:F:36:MET:CE	1:F:60:ILE:HB	2.01	0.89
1:C:36:MET:CE	1:C:60:ILE:HB	2.04	0.86
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:A:101:THR:HG23	1:A:219:THR:HG21	1.72	0.72
1:F:268:LEU:HD11	1:F:299:ALA:HB1	1.72	0.71
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:E:36:MET:HE2	1:F:56:TRP:NE1	2.07	0.69
1:A:268:LEU:HD11	1:A:299:ALA:HB1	1.75	0.69
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
1:B:307:MET:HE3	1:C:52:GLY:HA3	1.76	0.67
1:B:18:GLU:HG3	1:B:340:VAL:HG22	1.76	0.67
1:D:56:TRP:NE1	1:F:36:MET:HE2	2.10	0.66
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:GLU:HG3	1:D:340:VAL:HG22	1.80	0.64
1:D:307:MET:HE2	1:D:341:TYR:HD1	1.62	0.64
1:E:268:LEU:HD11	1:E:299:ALA:HB1	1.79	0.64
1:C:247:LEU:HD12	1:C:327:ALA:HB2	1.80	0.64
1:D:36:MET:HE3	1:E:56:TRP:CD2	2.33	0.63
1:B:101:THR:HG23	1:B:219:THR:HG21	1.80	0.63
1:A:56:TRP:NE1	1:C:36:MET:HE2	2.14	0.63
1:F:36:MET:HE1	1:F:60:ILE:HD12	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:F:307:MET:HE2	1:F:341:TYR:HD1	1.62	0.62
1:E:130:THR:CG2	1:E:148:GLN:HE21	2.13	0.62
1:C:107:LEU:HD12	1:C:111:GLY:HA3	1.81	0.62
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:E:36:MET:CE	1:E:60:ILE:HB	2.19	0.61
1:A:36:MET:HE3	1:B:56:TRP:CD2	2.35	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:D:1:ALA:N	1:D:12:ASP:OD1	2.29	0.60
1:D:130:THR:CG2	1:D:148:GLN:HE21	2.14	0.60
1:D:107:LEU:HD12	1:D:111:GLY:HA3	1.83	0.60
1:A:307:MET:HE2	1:A:341:TYR:HD1	1.67	0.59
1:D:268:LEU:HD11	1:D:299:ALA:HB1	1.85	0.59
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:F:36:MET:HE3	1:F:60:ILE:CB	2.15	0.58
1:E:130:THR:HG22	1:E:148:GLN:CG	2.20	0.58
1:E:36:MET:CE	1:F:56:TRP:NE1	2.67	0.57
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:D:209:ILE:CG2	1:D:284:ARG:HD3	2.34	0.57
1:C:209:ILE:CG2	1:C:284:ARG:HD3	2.35	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:A:209:ILE:CG2	1:A:284:ARG:HD3	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:209:ILE:CG2	1:E:284:ARG:HD3	2.36	0.56
1:B:36:MET:HE2	1:B:38:LEU:HB2	1.87	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: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:F:130:THR:CG2	1:F:148:GLN:HG3	2.21	0.55
1:D:130:THR:HG22	1:D:148:GLN:CG	2.25	0.55
1:A:18:GLU:HG3	1:A:340:VAL:HG22	1.87	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:B:307:MET:HE3	1:C:52:GLY:CA	2.36	0.54
1:F:18:GLU:HG3	1:F:340:VAL:HG22	1.89	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:C:36:MET:HE1	1:C:60:ILE:HD12	1.91	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:B:274:TYR:C	1:B:275:LEU:HD12	2.31	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:C:106:VAL:CG2	1:C:259:VAL:HG11	2.41	0.51
1:A:272:LEU:HD13	1:A:297:VAL:HG22	1.93	0.51
1:F:107:LEU:HD12	1:F:111:GLY:HA3	1.92	0.51
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:E:2:GLU:HA	1:E:12:ASP:HA	1.92	0.51
1:A:202:ASP:O	1:A:206:THR:HG23	2.11	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:D:272:LEU:HD13	1:D:297:VAL:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:307:MET:HE2	1:B:341:TYR:HD1	1.77	0.49
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:D:130:THR:HG22	1:D:148:GLN:HE21	1.76	0.49
1:A:199:ARG:NH1	1:A:240:ASN:O	2.45	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:D:56:TRP:CZ2	1:F:36:MET:HE1	2.47	0.49
1:C:2:GLU:HA	1:C:12:ASP:HA	1.94	0.49
1:A:143:LEU:HD11	1:A:181:ILE:HG23	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:A:36:MET:HE2	1:A:38:LEU:HB2	1.95	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:209:ILE:HG23	1:D:284:ARG:HH11	1.79	0.48
1:B:209:ILE:HG23	1:B:284:ARG:HH11	1.79	0.48
1:D:33:LYS:HD3	1:E:163:THR:HG21	1.96	0.48
1:E:36:MET:HE1	1:F:56:TRP:CZ2	2.48	0.47
1:B:106:VAL:HG11	1:B:230:TYR:CE2	2.48	0.47
1:F:209:ILE:HG23	1:F:284:ARG:HH11	1.79	0.47
1:E:36:MET:HE1	1:F:56:TRP:CE2	2.48	0.47
1:E:247:LEU:CD1	1:E:327:ALA:HB2	2.44	0.47
1:E:209:ILE:HG23	1:E:284:ARG:HH11	1.80	0.47
1:B:268:LEU:HD11	1:B:299:ALA:HB1	1.96	0.47
1:E:36:MET:HE1	1:E:60:ILE:HD12	1.97	0.47
1:D:107:LEU:HD13	1:D:296:ASP:OD2	2.14	0.47
1:C:209:ILE:HG23	1:C:284:ARG:HH11	1.80	0.47
1:E:307:MET:HE1	1:E:341:TYR:HB2	1.95	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:56:TRP:CZ2	1:E:58:TYR:HB2	2.50	0.47
1:F:307:MET:HE2	1:F:341:TYR:CD1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:ALA:O	1:B:3:ILE:HG23	2.14	0.47
1:E:33:LYS:HD3	1:F:163:THR:HG21	1.96	0.47
1:C:56:TRP:CZ2	1:C:58:TYR:HB2	2.50	0.46
1:D:1:ALA:O	1:D:3:ILE:HG23	2.15	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:52:GLY:HA3	1:C:307:MET:HE3	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: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:D:36:MET:HE2	1:D:38:LEU:HB2	1.97	0.45
1:A:56:TRP:CZ2	1:A:58:TYR:HB2	2.51	0.45
1:A:3:ILE:HD13	1:B:3:ILE:HD12	1.98	0.45
1:F:272:LEU:HD13	1:F:297:VAL:HG22	1.99	0.45
1:D:56:TRP:NE1	1:F:36:MET:CE	2.78	0.45
1:E:101:THR:HG22	1:E:234:GLN:OE1	2.16	0.45
1:B:36:MET:HE3	1:C:56:TRP:CD2	2.52	0.45
1:F:1:ALA:O	1:F:3:ILE:HG23	2.15	0.45
1:D:130:THR:HG21	1:D:148:GLN:HE21	1.82	0.45
1:C:107:LEU:HD13	1:C:296:ASP:OD2	2.17	0.45
1:E:36:MET:CE	1:F:56:TRP:CE2	3.00	0.45
1:A:307:MET:HE2	1:A:341:TYR:CD1	2.50	0.45
1:A:106:VAL:HG11	1:A:230:TYR:CE2	2.51	0.45
1:B:272:LEU:HD13	1:B:297:VAL:CG2	2.47	0.45
1:B:106:VAL:CG2	1:B:259:VAL:HG11	2.47	0.45
1:D:300:THR:HG23	1:D:310:TYR:HB3	1.99	0.45
1:C:238:THR:HB	1:C:241:ALA:HB3	1.97	0.45
1:D:307:MET:HE2	1:D:341:TYR:CD1	2.46	0.44
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: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:307:MET:CE	1:A:341:TYR:HD1	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:THR:HG22	1:B:234:GLN:OE1	2.18	0.43
1:A:107:LEU:HD13	1:A:296:ASP:OD2	2.18	0.43
1:E:343:PHE:CG	1:F:11:LEU:HD13	2.52	0.43
1:C:107:LEU:HD21	1:C:273:ALA:HB2	2.01	0.43
1:D:280:LYS:O	1:D:281:ASN:C	2.56	0.43
1:F:107:LEU:HD13	1:F:296:ASP:OD2	2.19	0.43
1:D:56:TRP:CZ2	1:D:58:TYR:HB2	2.53	0.43
1:A:268:LEU:CD1	1:A:299:ALA:HB1	2.47	0.43
1:D:36:MET:HE3	1:E:56:TRP:CE3	2.53	0.43
1:C:244:VAL:HG22	1:C:291:ILE:HD13	2.01	0.43
1:C:280:LYS:O	1:C:281:ASN:C	2.56	0.43
1:A:303:PHE:CZ	1:B:80:LEU:HD11	2.54	0.43
1:F:101:THR:HG22	1:F:234:GLN:OE1	2.18	0.43
1:A:107:LEU:HD21	1:A:273:ALA:HB2	2.01	0.43
1:A:280:LYS:O	1:A:281:ASN:C	2.57	0.43
1:D:56:TRP:CE2	1:F:36:MET:CE	3.01	0.43
1:F:244:VAL:HG22	1:F:291:ILE:HD13	2.01	0.42
1:E:238:THR:HB	1:E:241:ALA:HB3	2.00	0.42
1:E:280:LYS:O	1:E:281:ASN:C	2.57	0.42
1:C:20:LEU:HD11	1:C:336:ALA:HB1	2.01	0.42
1:D:268:LEU:CD1	1:D:299:ALA:HB1	2.49	0.42
1:F:280:LYS:O	1:F:281:ASN:C	2.57	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:A:36:MET:HE3	1:B:56:TRP:CE3	2.54	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:N	1:C:12:ASP:OD1	2.49	0.42
1:C:1:ALA:O	1:C:3:ILE:HG23	2.19	0.42
1:A:52:GLY:CA	1:C:307:MET:HE3	2.49	0.42
1:E:292:LEU:HA	1:E:318:LEU:HD11	2.00	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
1:C:96:VAL:HG22	1:C:180:SER:HB3	2.01	0.42
1:B:280:LYS:O	1:B:281:ASN:C	2.58	0.41
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:D:292:LEU:HA	1:D:318:LEU:HD11	2.01	0.41
1:C:307:MET:HE1	1:C:341:TYR:HB2	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:THR:HG22	1:D:234:GLN:OE1	2.20	0.41
1:D:33:LYS:HA	1:D:63:ASN:HD22	1.86	0.41
1:C:261:GLN:HG2	1:C:271:PHE:HB3	2.03	0.41
1:B:238:THR:HB	1:B:241:ALA:HB3	2.02	0.41
1:E:200:THR:HG22	1:E:201:TRP:N	2.36	0.41
1:A:261:GLN:HG2	1:A:271:PHE:HB3	2.03	0.41
1:D:316:ASN:ND2	1:D:330:ASN:O	2.53	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:B:169:VAL:HG21	1:B:206:THR:HG21	2.03	0.41
1:F:106:VAL:HG23	1:F:261:GLN:NE2	2.36	0.41
1:E:244:VAL:HG22	1:E:291:ILE:HD13	2.03	0.41
1:E:1:ALA:N	1:E:12:ASP:OD1	2.50	0.41
1:F:208:LEU:O	1:F:211:THR:HG23	2.22	0.41
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: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:A:56:TRP:NE1	1:C:36:MET:CE	2.84	0.40
1:E:292:LEU:HD12	1:E:318:LEU:HD11	2.02	0.40
1:E:173:ASN:HD22	1:E:173:ASN:C	2.24	0.40
1:A:1:ALA:N	1:A:12:ASP:OD1	2.49	0.40
1:B:307:MET:HE3	1:C:52:GLY:C	2.42	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 [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	341/343 (99%)	310 (91%)	27 (8%)	4 (1%)	16 61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	341/343 (99%)	307 (90%)	30 (9%)	4 (1%)	16	61
1	C	341/343 (99%)	309 (91%)	28 (8%)	4 (1%)	16	61
1	D	341/343 (99%)	310 (91%)	27 (8%)	4 (1%)	16	61
1	E	341/343 (99%)	310 (91%)	27 (8%)	4 (1%)	16	61
1	F	341/343 (99%)	310 (91%)	27 (8%)	4 (1%)	16	61
All	All	2046/2058 (99%)	1856 (91%)	166 (8%)	24 (1%)	16	61

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
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%)	273 (99%)	4 (1%)	74	90
1	B	277/277 (100%)	272 (98%)	5 (2%)	66	88
1	C	277/277 (100%)	271 (98%)	6 (2%)	60	85
1	D	277/277 (100%)	272 (98%)	5 (2%)	66	88
1	E	277/277 (100%)	272 (98%)	5 (2%)	66	88
1	F	277/277 (100%)	271 (98%)	6 (2%)	60	85
All	All	1662/1662 (100%)	1631 (98%)	31 (2%)	65	87

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	89	ASP
1	A	115	TYR
1	A	195	SER
1	B	89	ASP
1	B	115	TYR
1	B	173	ASN
1	B	195	SER
1	B	342	GLN
1	C	89	ASP
1	C	97	VAL
1	C	115	TYR
1	C	173	ASN
1	C	195	SER
1	C	342	GLN
1	D	11	LEU
1	D	51	THR
1	D	89	ASP
1	D	115	TYR
1	D	195	SER
1	E	89	ASP
1	E	115	TYR
1	E	173	ASN
1	E	195	SER
1	E	342	GLN
1	F	89	ASP
1	F	97	VAL

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Mol	Chain	Res	Type
1	F	115	TYR
1	F	173	ASN
1	F	195	SER
1	F	342	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	119	ASN
1	B	173	ASN
1	D	119	ASN
1	E	150	GLN
1	E	173	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 carbohydrates 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	0.18	0	6,6,6	0.17	0
2	SO4	C	1344	-	4,4,4	0.18	0	6,6,6	0.10	0
2	SO4	D	1344	-	4,4,4	0.14	0	6,6,6	0.19	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
2	SO4	A	1344	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1344	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1344	-	-	0/0/0/0	0/0/0/0

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	343/343 (100%)	1.39	86 (25%) 1 1	19, 49, 77, 95	0
1	B	343/343 (100%)	1.23	72 (20%) 1 1	10, 47, 73, 87	0
1	C	343/343 (100%)	1.68	118 (34%) 0 0	27, 61, 85, 131	0
1	D	343/343 (100%)	1.35	86 (25%) 1 1	20, 50, 74, 87	0
1	E	343/343 (100%)	1.43	85 (24%) 1 1	14, 46, 74, 96	0
1	F	343/343 (100%)	1.85	115 (33%) 0 0	30, 61, 84, 115	0
All	All	2058/2058 (100%)	1.49	562 (27%) 1 1	10, 53, 80, 131	0

All (562) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	160	GLY	21.7
1	C	290	ASP	15.8
1	F	86	GLY	13.7
1	F	319	ASP	12.3
1	C	160	GLY	10.5
1	F	87	SER	10.0
1	F	159	GLU	9.8
1	F	250	ALA	9.8
1	C	159	GLU	9.5
1	F	318	LEU	8.8
1	A	224	TYR	8.6
1	C	291	ILE	8.3
1	F	249	TRP	8.0
1	F	323	PHE	7.7
1	F	280	LYS	7.5
1	F	131	TYR	7.3
1	C	249	TRP	6.9
1	E	262	TYR	6.7
1	C	328	GLY	6.7

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Mol	Chain	Res	Type	RSRZ
1	C	122	GLN	6.7
1	F	279	GLY	6.6
1	A	122	GLN	6.6
1	F	31	GLY	6.5
1	E	196	SER	6.4
1	D	203	GLN	6.4
1	E	285	GLY	6.3
1	F	289	GLU	6.3
1	F	161	MET	6.1
1	F	247	LEU	5.9
1	F	336	ALA	5.9
1	A	188	PHE	5.9
1	F	296	ASP	5.8
1	C	217	THR	5.8
1	F	52	GLY	5.8
1	E	280	LYS	5.8
1	F	162	THR	5.7
1	C	86	GLY	5.7
1	E	291	ILE	5.7
1	C	318	LEU	5.6
1	F	278	LYS	5.6
1	B	285	GLY	5.6
1	C	162	THR	5.6
1	C	154	GLY	5.5
1	F	334	ILE	5.5
1	D	242	THR	5.5
1	D	122	GLN	5.4
1	E	290	ASP	5.4
1	F	120	PHE	5.4
1	B	160	GLY	5.4
1	D	184	ASN	5.4
1	C	280	LYS	5.4
1	E	182	THR	5.3
1	C	247	LEU	5.3
1	C	110	PHE	5.3
1	A	210	GLY	5.3
1	F	240	ASN	5.2
1	E	252	LYS	5.2
1	D	286	TYR	5.2
1	D	213	ASP	5.2
1	F	312	ASP	5.0
1	D	164	ASN	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	184	ASN	5.0
1	A	319	ASP	4.9
1	F	154	GLY	4.9
1	A	164	ASN	4.9
1	E	197	SER	4.9
1	D	153	ASN	4.9
1	A	187	GLY	4.9
1	A	160	GLY	4.8
1	F	275	LEU	4.8
1	A	52	GLY	4.8
1	D	154	GLY	4.7
1	F	281	ASN	4.7
1	C	317	LEU	4.7
1	A	154	GLY	4.7
1	C	85	VAL	4.7
1	C	278	LYS	4.7
1	F	282	LEU	4.7
1	A	203	GLN	4.6
1	C	294	TYR	4.6
1	C	327	ALA	4.6
1	A	251	ASN	4.6
1	F	122	GLN	4.6
1	F	291	ILE	4.6
1	E	212	GLY	4.6
1	F	46	VAL	4.6
1	A	214	ARG	4.6
1	C	266	PHE	4.6
1	E	275	LEU	4.6
1	A	197	SER	4.5
1	E	122	GLN	4.5
1	E	278	LYS	4.5
1	C	336	ALA	4.5
1	A	121	MET	4.5
1	F	290	ASP	4.4
1	C	101	THR	4.4
1	D	285	GLY	4.4
1	B	139	LEU	4.4
1	F	136	PHE	4.4
1	D	283	GLY	4.3
1	D	209	ILE	4.3
1	E	326	ASP	4.3
1	C	104	THR	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	327	ALA	4.3
1	E	253	ALA	4.3
1	F	209	ILE	4.3
1	D	150	GLN	4.3
1	C	183	TYR	4.3
1	C	143	LEU	4.3
1	A	285	GLY	4.2
1	C	133	ASN	4.2
1	A	50	LEU	4.2
1	D	275	LEU	4.2
1	B	318	LEU	4.2
1	F	217	THR	4.2
1	C	251	ASN	4.1
1	E	120	PHE	4.1
1	B	100	VAL	4.1
1	F	324	THR	4.1
1	C	132	ARG	4.1
1	B	280	LYS	4.1
1	C	334	ILE	4.1
1	C	244	VAL	4.1
1	D	261	GLN	4.1
1	A	184	ASN	4.1
1	B	122	GLN	4.1
1	A	159	GLU	4.1
1	B	279	GLY	4.1
1	B	253	ALA	4.1
1	C	312	ASP	4.0
1	C	323	PHE	4.0
1	E	264	PHE	4.0
1	C	87	SER	4.0
1	F	241	ALA	4.0
1	E	216	GLU	4.0
1	A	286	TYR	4.0
1	A	291	ILE	4.0
1	D	291	ILE	4.0
1	E	279	GLY	4.0
1	A	162	THR	3.9
1	E	143	LEU	3.9
1	D	214	ARG	3.9
1	A	85	VAL	3.8
1	B	294	TYR	3.8
1	C	252	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	318	LEU	3.8
1	D	218	TYR	3.8
1	F	103	TRP	3.8
1	A	284	ARG	3.8
1	A	212	GLY	3.8
1	F	143	LEU	3.8
1	D	206	THR	3.8
1	F	104	THR	3.8
1	C	248	GLY	3.8
1	E	294	TYR	3.8
1	C	262	TYR	3.7
1	F	261	GLN	3.7
1	B	278	LYS	3.7
1	D	249	TRP	3.7
1	C	121	MET	3.7
1	F	251	ASN	3.7
1	B	275	LEU	3.7
1	C	282	LEU	3.7
1	E	121	MET	3.7
1	E	249	TRP	3.7
1	F	216	GLU	3.7
1	D	160	GLY	3.7
1	A	289	GLU	3.7
1	C	240	ASN	3.7
1	E	251	ASN	3.7
1	D	230	TYR	3.6
1	B	282	LEU	3.6
1	B	291	ILE	3.6
1	E	183	TYR	3.6
1	A	261	GLN	3.6
1	B	251	ASN	3.6
1	D	290	ASP	3.6
1	B	255	ASN	3.6
1	E	242	THR	3.6
1	F	299	ALA	3.6
1	D	237	GLN	3.6
1	F	335	VAL	3.6
1	F	314	LYS	3.5
1	C	322	ARG	3.5
1	B	182	THR	3.5
1	F	317	LEU	3.5
1	C	131	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	183	TYR	3.5
1	C	123	GLN	3.5
1	F	85	VAL	3.5
1	D	201	TRP	3.5
1	C	51	THR	3.5
1	C	184	ASN	3.5
1	E	250	ALA	3.5
1	C	209	ILE	3.5
1	C	45	GLN	3.5
1	A	225	ASP	3.5
1	C	296	ASP	3.4
1	E	138	GLY	3.4
1	C	190	ILE	3.4
1	B	69	ASN	3.4
1	E	282	LEU	3.4
1	C	216	GLU	3.4
1	D	136	PHE	3.4
1	D	198	LYS	3.4
1	D	197	SER	3.4
1	E	263	GLN	3.4
1	F	266	PHE	3.4
1	A	104	THR	3.4
1	B	276	GLN	3.4
1	B	329	ILE	3.4
1	C	300	THR	3.4
1	B	284	ARG	3.4
1	A	189	GLY	3.4
1	C	254	GLN	3.4
1	A	209	ILE	3.3
1	B	286	TYR	3.3
1	E	254	GLN	3.3
1	A	213	ASP	3.3
1	B	138	GLY	3.3
1	A	198	LYS	3.3
1	E	276	GLN	3.3
1	C	188	PHE	3.3
1	C	115	TYR	3.3
1	E	110	PHE	3.3
1	C	152	LYS	3.3
1	E	237	GLN	3.3
1	F	110	PHE	3.3
1	C	275	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	224	TYR	3.3
1	C	201	TRP	3.2
1	B	159	GLU	3.2
1	F	93	ASN	3.2
1	D	217	THR	3.2
1	A	150	GLN	3.2
1	B	244	VAL	3.2
1	F	133	ASN	3.2
1	E	184	ASN	3.2
1	A	166	ARG	3.2
1	E	104	THR	3.2
1	D	188	PHE	3.2
1	F	115	TYR	3.2
1	E	320	ASP	3.2
1	C	261	GLN	3.2
1	D	282	LEU	3.2
1	D	244	VAL	3.2
1	C	250	ALA	3.2
1	F	187	GLY	3.2
1	F	210	GLY	3.2
1	F	252	LYS	3.2
1	E	211	THR	3.1
1	F	132	ARG	3.1
1	B	277	SER	3.1
1	B	257	GLU	3.1
1	B	153	ASN	3.1
1	F	153	ASN	3.1
1	C	155	SER	3.1
1	B	103	TRP	3.1
1	D	189	GLY	3.1
1	E	283	GLY	3.1
1	C	223	LYS	3.1
1	F	32	ASP	3.1
1	F	223	LYS	3.1
1	F	328	GLY	3.1
1	B	188	PHE	3.1
1	B	252	LYS	3.1
1	B	323	PHE	3.1
1	E	69	ASN	3.1
1	E	244	VAL	3.1
1	F	300	THR	3.1
1	D	196	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	322	ARG	3.1
1	C	268	LEU	3.0
1	F	184	ASN	3.0
1	A	242	THR	3.0
1	F	44	THR	3.0
1	E	20	LEU	3.0
1	A	114	THR	3.0
1	B	217	THR	3.0
1	D	162	THR	3.0
1	A	275	LEU	3.0
1	F	51	THR	3.0
1	F	100	VAL	3.0
1	F	259	VAL	3.0
1	E	240	ASN	3.0
1	A	86	GLY	3.0
1	D	210	GLY	3.0
1	D	114	THR	3.0
1	F	145	PHE	3.0
1	D	137	PHE	2.9
1	C	128	PHE	2.9
1	C	69	ASN	2.9
1	C	329	ILE	2.9
1	A	254	GLN	2.9
1	C	150	GLN	2.9
1	A	139	LEU	2.9
1	C	230	TYR	2.9
1	C	299	ALA	2.9
1	E	49	GLN	2.9
1	A	46	VAL	2.9
1	D	274	TYR	2.9
1	D	320	ASP	2.8
1	F	232	ALA	2.8
1	C	311	VAL	2.8
1	E	229	ILE	2.8
1	E	234	GLN	2.8
1	F	127	GLY	2.8
1	B	290	ASP	2.8
1	B	262	TYR	2.8
1	F	294	TYR	2.8
1	A	250	ALA	2.8
1	D	169	VAL	2.8
1	F	150	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	82	PHE	2.8
1	A	201	TRP	2.8
1	C	63	ASN	2.8
1	A	257	GLU	2.8
1	C	76	ALA	2.8
1	D	273	ALA	2.8
1	A	51	THR	2.8
1	D	190	ILE	2.8
1	D	289	GLU	2.8
1	D	163	THR	2.7
1	C	31	GLY	2.7
1	E	101	THR	2.7
1	F	215	ALA	2.7
1	C	281	ASN	2.7
1	D	151	GLY	2.7
1	F	137	PHE	2.7
1	C	257	GLU	2.7
1	A	97	VAL	2.7
1	C	264	PHE	2.7
1	A	244	VAL	2.7
1	E	215	ALA	2.7
1	E	235	TYR	2.7
1	A	223	LYS	2.7
1	B	223	LYS	2.7
1	E	265	ASP	2.7
1	F	264	PHE	2.7
1	F	310	TYR	2.7
1	F	76	ALA	2.7
1	D	223	LYS	2.7
1	E	286	TYR	2.7
1	F	257	GLU	2.7
1	C	20	LEU	2.7
1	F	248	GLY	2.7
1	B	183	TYR	2.7
1	F	88	PHE	2.7
1	E	284	ARG	2.7
1	D	200	THR	2.7
1	E	115	TYR	2.7
1	C	284	ARG	2.7
1	E	261	GLN	2.7
1	F	109	GLU	2.6
1	A	231	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	107	LEU	2.6
1	F	200	THR	2.6
1	D	121	MET	2.6
1	A	288	ASP	2.6
1	C	32	ASP	2.6
1	D	284	ARG	2.6
1	E	137	PHE	2.6
1	E	268	LEU	2.6
1	B	152	LYS	2.6
1	C	295	VAL	2.6
1	E	336	ALA	2.6
1	F	203	GLN	2.6
1	A	264	PHE	2.6
1	B	143	LEU	2.6
1	C	93	ASN	2.6
1	A	217	THR	2.6
1	D	142	GLY	2.6
1	D	235	TYR	2.6
1	F	239	TYR	2.6
1	D	69	ASN	2.6
1	B	151	GLY	2.6
1	B	211	THR	2.6
1	E	195	SER	2.6
1	C	130	THR	2.6
1	D	166	ARG	2.5
1	A	230	TYR	2.5
1	A	331	THR	2.5
1	E	312	ASP	2.5
1	C	310	TYR	2.5
1	C	231	LEU	2.5
1	C	161	MET	2.5
1	A	255	ASN	2.5
1	A	120	PHE	2.5
1	C	331	THR	2.5
1	B	224	TYR	2.5
1	C	301	TYR	2.5
1	F	326	ASP	2.5
1	D	174	GLY	2.5
1	B	336	ALA	2.5
1	C	241	ALA	2.5
1	C	324	THR	2.5
1	B	313	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	172	GLN	2.5
1	E	230	TYR	2.5
1	C	218	TYR	2.5
1	F	116	ASP	2.5
1	F	230	TYR	2.5
1	B	164	ASN	2.5
1	D	216	GLU	2.5
1	A	136	PHE	2.5
1	F	128	PHE	2.5
1	C	314	LYS	2.5
1	A	317	LEU	2.5
1	C	267	GLY	2.4
1	E	144	ASP	2.4
1	E	139	LEU	2.4
1	B	150	GLN	2.4
1	D	85	VAL	2.4
1	F	202	ASP	2.4
1	F	309	THR	2.4
1	B	107	LEU	2.4
1	C	239	TYR	2.4
1	B	238	THR	2.4
1	F	327	ALA	2.4
1	C	279	GLY	2.4
1	D	257	GLU	2.4
1	A	107	LEU	2.4
1	E	97	VAL	2.4
1	B	149	TYR	2.4
1	A	153	ASN	2.4
1	E	266	PHE	2.4
1	D	152	LYS	2.4
1	A	115	TYR	2.4
1	D	107	LEU	2.4
1	E	323	PHE	2.4
1	A	266	PHE	2.4
1	B	230	TYR	2.4
1	C	202	ASP	2.4
1	C	335	VAL	2.4
1	A	294	TYR	2.4
1	B	268	LEU	2.4
1	C	145	PHE	2.4
1	D	50	LEU	2.4
1	F	69	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	173	ASN	2.3
1	A	234	GLN	2.3
1	A	262	TYR	2.3
1	B	166	ARG	2.3
1	C	270	PRO	2.3
1	D	317	LEU	2.3
1	C	109	GLU	2.3
1	B	133	ASN	2.3
1	B	218	TYR	2.3
1	A	69	ASN	2.3
1	D	262	TYR	2.3
1	F	206	THR	2.3
1	F	231	LEU	2.3
1	A	116	ASP	2.3
1	F	218	TYR	2.3
1	A	165	GLY	2.3
1	C	44	THR	2.3
1	D	259	VAL	2.3
1	D	127	GLY	2.3
1	E	328	GLY	2.3
1	A	101	THR	2.3
1	B	249	TRP	2.3
1	F	208	LEU	2.3
1	D	250	ALA	2.3
1	E	335	VAL	2.3
1	F	214	ARG	2.3
1	E	210	GLY	2.3
1	E	318	LEU	2.3
1	E	111	GLY	2.2
1	C	124	HIS	2.2
1	E	152	LYS	2.2
1	B	283	GLY	2.2
1	C	33	LYS	2.2
1	C	120	PHE	2.2
1	E	248	GLY	2.2
1	F	112	GLY	2.2
1	F	267	GLY	2.2
1	E	142	GLY	2.2
1	F	138	GLY	2.2
1	C	148	GLN	2.2
1	F	270	PRO	2.2
1	E	327	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	206	THR	2.2
1	C	22	TYR	2.2
1	A	241	ALA	2.2
1	A	282	LEU	2.2
1	D	115	TYR	2.2
1	F	22	TYR	2.2
1	E	150	GLN	2.2
1	D	231	LEU	2.2
1	F	152	LYS	2.2
1	B	264	PHE	2.2
1	D	143	LEU	2.2
1	B	154	GLY	2.2
1	F	288	ASP	2.2
1	C	169	VAL	2.2
1	E	334	ILE	2.2
1	F	274	TYR	2.2
1	C	195	SER	2.2
1	D	264	PHE	2.2
1	E	71	SER	2.2
1	F	107	LEU	2.2
1	C	276	GLN	2.1
1	B	259	VAL	2.1
1	C	153	ASN	2.1
1	E	259	VAL	2.1
1	B	254	GLN	2.1
1	A	196	SER	2.1
1	F	173	ASN	2.1
1	C	50	LEU	2.1
1	D	40	PHE	2.1
1	F	158	GLY	2.1
1	A	199	ARG	2.1
1	D	236	THR	2.1
1	E	325	ARG	2.1
1	B	120	PHE	2.1
1	D	113	ASP	2.1
1	D	225	ASP	2.1
1	F	190	ILE	2.1
1	E	243	ARG	2.1
1	B	104	THR	2.1
1	B	200	THR	2.1
1	E	287	ASP	2.1
1	E	176	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	100	VAL	2.1
1	E	257	GLU	2.1
1	F	244	VAL	2.1
1	B	190	ILE	2.1
1	C	224	TYR	2.1
1	B	174	GLY	2.1
1	C	71	SER	2.1
1	A	236	THR	2.1
1	D	202	ASP	2.1
1	D	288	ASP	2.1
1	A	292	LEU	2.1
1	A	117	SER	2.1
1	A	12	ASP	2.1
1	B	203	GLN	2.1
1	B	209	ILE	2.1
1	D	319	ASP	2.1
1	D	334	ILE	2.1
1	E	153	ASN	2.1
1	F	164	ASN	2.1
1	D	120	PHE	2.1
1	A	259	VAL	2.1
1	B	258	ALA	2.1
1	A	45	GLN	2.1
1	D	45	GLN	2.1
1	C	309	THR	2.1
1	B	127	GLY	2.1
1	D	97	VAL	2.1
1	C	174	GLY	2.0
1	C	134	THR	2.0
1	D	34	THR	2.0
1	B	250	ALA	2.0
1	A	329	ILE	2.0
1	E	241	ALA	2.0
1	F	148	GLN	2.0
1	A	99	ASP	2.0
1	C	97	VAL	2.0
1	D	306	ASN	2.0
1	C	137	PHE	2.0
1	D	318	LEU	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	A	1344	5/5	0.82	0.52	2.06	170,179,185,186	0
2	SO4	D	1344	5/5	0.75	0.46	1.46	148,169,201,210	0
2	SO4	C	1344	5/5	0.69	0.43	0.63	190,214,217,225	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.