



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:53 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

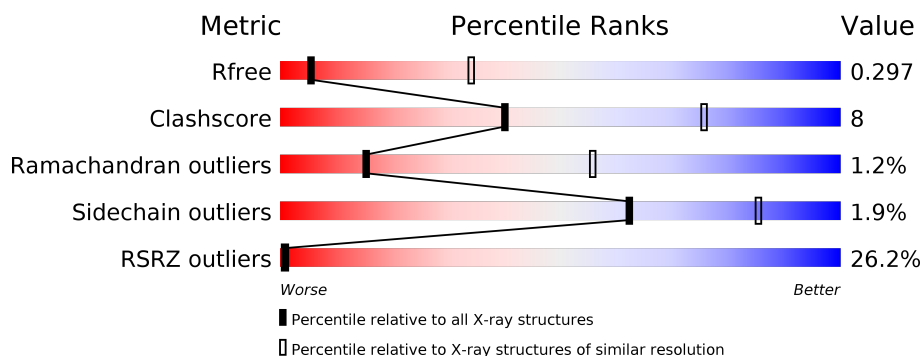
1 Overall quality at a glance

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}	100719	1049 (3.58-3.38)
Clashscore	112137	1096 (3.56-3.40)
Ramachandran outliers	110173	1063 (3.56-3.40)
Sidechain outliers	110143	1064 (3.56-3.40)
RSRZ outliers	101464	1019 (3.56-3.40)

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

Mol	Chain	Length	Quality of chain
1	A	343	
1	B	343	
1	C	343	
1	D	343	
1	E	343	
1	F	343	

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:

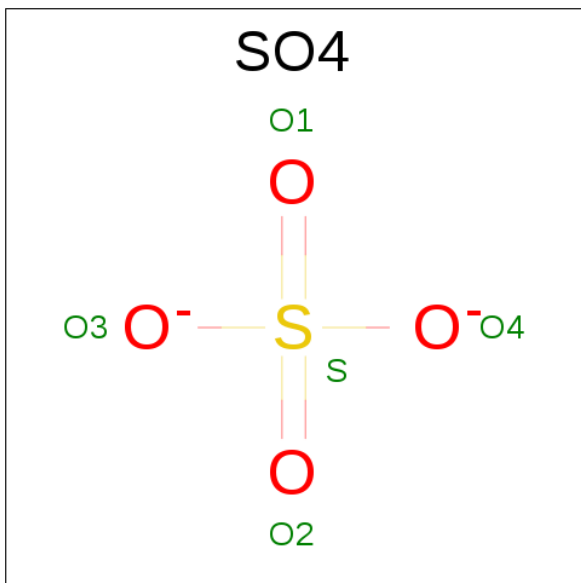
Chain	Residue	Modelled	Actual	Comment	Reference
A	18	GLU	ASP	SEE REMARK 999	UNP Q9K597
A	124	HIS	ARG	SEE REMARK 999	UNP Q9K597
A	271	PHE	SER	SEE REMARK 999	UNP Q9K597
B	18	GLU	ASP	SEE REMARK 999	UNP Q9K597
B	124	HIS	ARG	SEE REMARK 999	UNP Q9K597
B	271	PHE	SER	SEE REMARK 999	UNP Q9K597
C	18	GLU	ASP	SEE 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: O₄S).

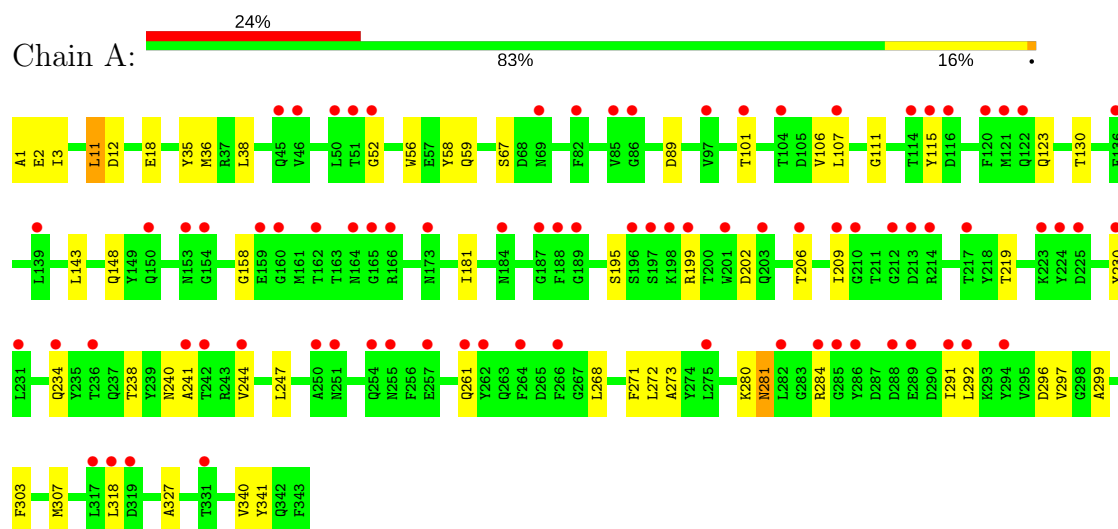


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

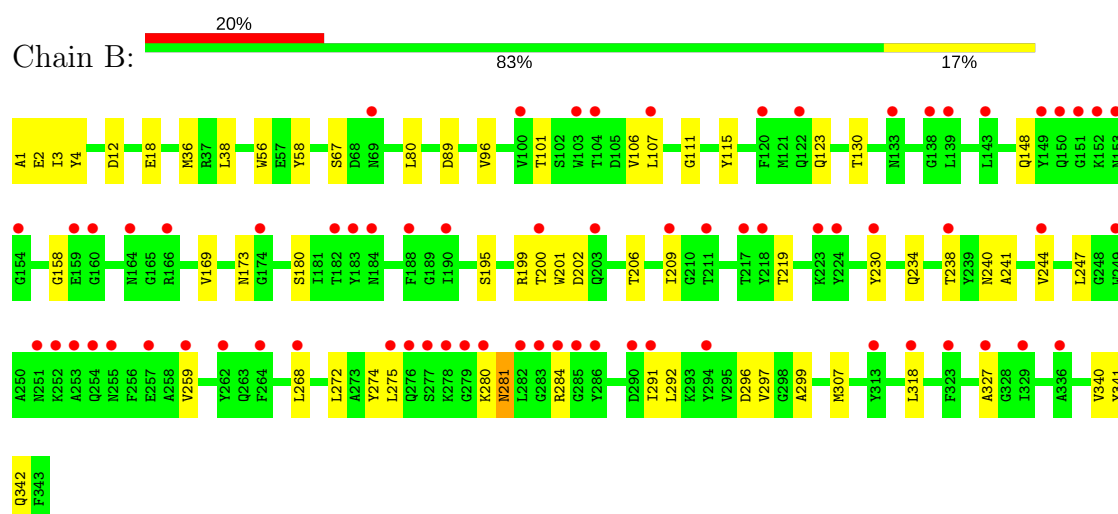
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

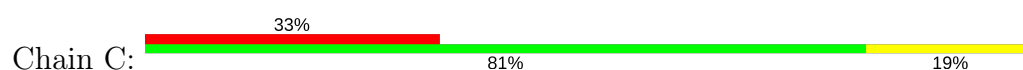
• Molecule 1: OMPC

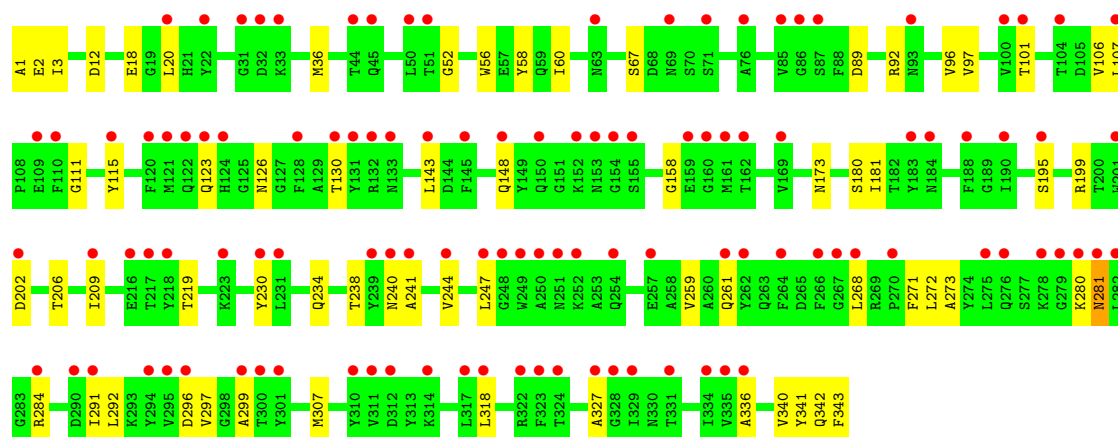


• Molecule 1: OMPC

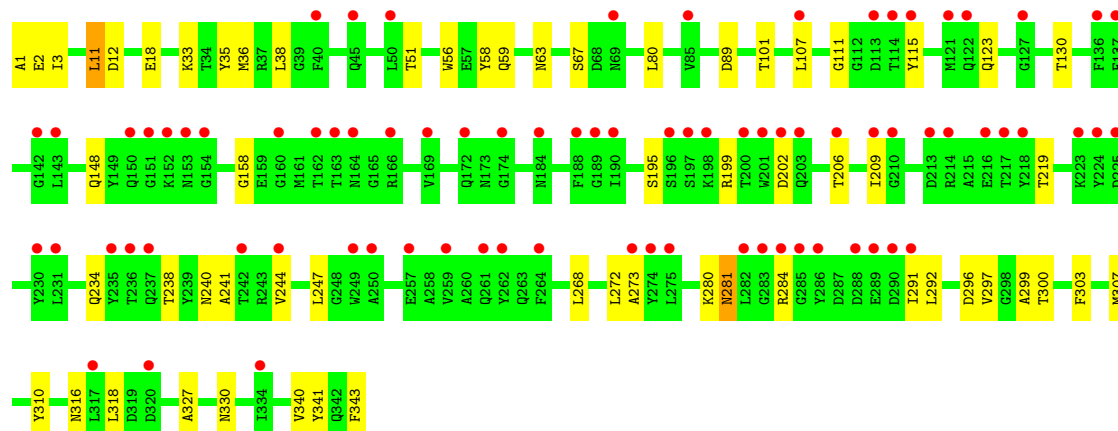
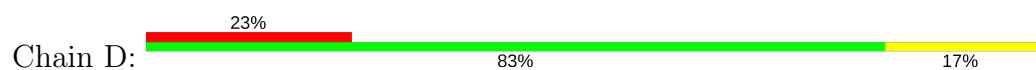


• Molecule 1: OMPC

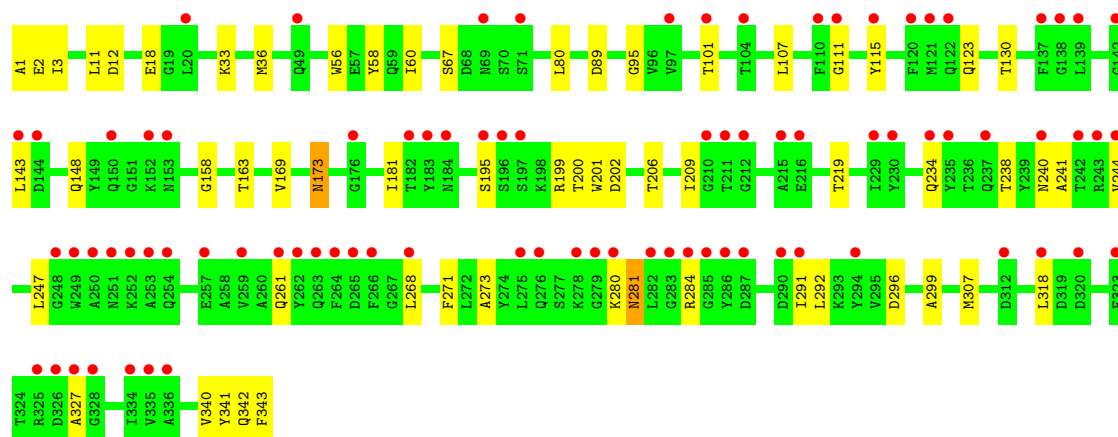
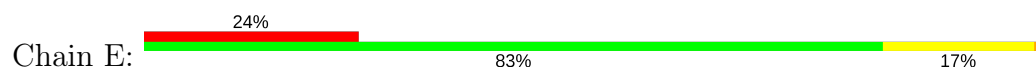




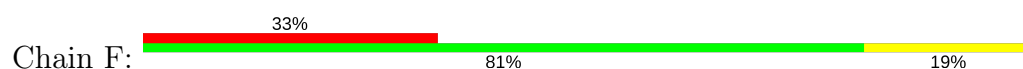
• Molecule 1: OMPC

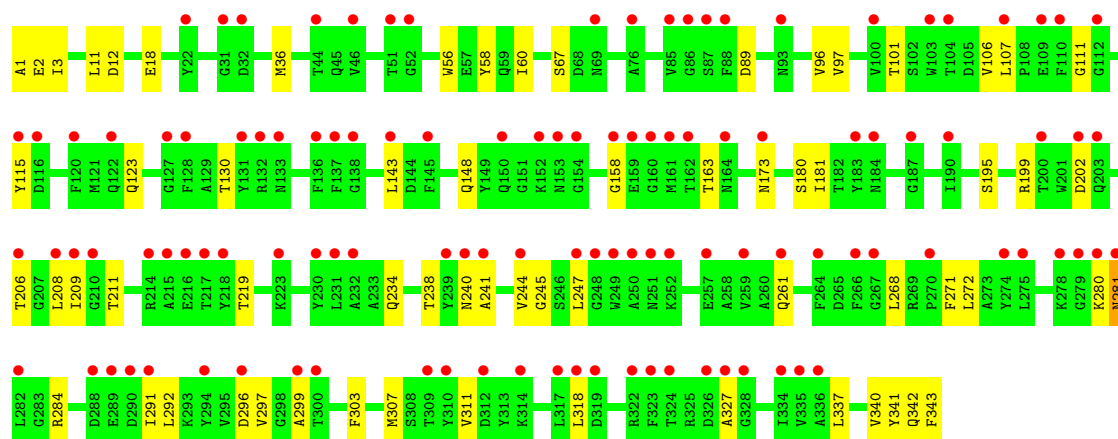


• Molecule 1: OMPC



• 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 (5.31%)	DCC
Wilson B-factor (Å ²)	121.1	Xtriage
Anisotropy	0.541	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 133.0	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	0.88	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	0.39	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: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: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: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: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: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: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: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:B:247:LEU:HD12	1:B:327:ALA:HB2	1.83	0.61
1:A:36:MET:HE3	1:B:56:TRP:CD2	2.35	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: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: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:C:209:ILE:CG2	1:C:284:ARG:HD3	2.35	0.57
1:D:209:ILE:CG2	1:D:284:ARG:HD3	2.34	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: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: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: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
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: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: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: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:D:56:TRP:CZ2	1:F:36:MET:HE1	2.47	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: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: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:E:36:MET:HE1	1:F:56:TRP:CZ2	2.48	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
1:E:36:MET:HE1	1:F:56:TRP:CE2	2.48	0.47
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:36:MET:HE1	1:E:60:ILE:HD12	1.97	0.47
1:E:307:MET:HE1	1:E:341:TYR:HB2	1.95	0.47
1:F:238:THR:HB	1:F:241:ALA:HB3	1.95	0.47
1:F:56:TRP:CZ2	1:F:58:TYR:HB2	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:307:MET:HE2	1:F:341:TYR:CD1	2.47	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:B:36:MET:HE3	1:C:56:TRP:CD2	2.52	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:F:1:ALA:O	1:F:3:ILE:HG23	2.15	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:A:307:MET:HE2	1:A:341:TYR:CD1	2.50	0.45
1:E:36:MET:CE	1:F:56:TRP:CE2	3.00	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
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: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:A:307:MET:CE	1:A:341:TYR:HD1	2.30	0.44
1:D:107:LEU:HD21	1:D:273:ALA:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:C:280:LYS:O	1:C:281:ASN:C	2.56	0.43
1:D:36:MET:HE3	1:E:56:TRP:CE3	2.53	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:F:101:THR:HG22	1:F:234:GLN:OE1	2.18	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:C:20:LEU:HD11	1:C:336:ALA:HB1	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: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:A:52:GLY:CA	1:C:307:MET:HE3	2.49	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: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
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:B:200:THR:HG22	1:B:201:TRP:N	2.35	0.41
1:C:307:MET:HE1	1:C:341:TYR:HB2	2.00	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: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: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:E:200:THR:HG22	1:E:201:TRP:N	2.36	0.41
1:D:316:ASN:ND2	1:D:330:ASN:O	2.53	0.41
1:B:169:VAL:HG21	1:B:206:THR:HG21	2.03	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: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: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:173:ASN:HD22	1:E:173:ASN:C	2.24	0.40
1:E:292:LEU:HD12	1:E:318:LEU:HD11	2.02	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%)	15 56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	341/343 (99%)	307 (90%)	30 (9%)	4 (1%)	15	56
1	C	341/343 (99%)	309 (91%)	28 (8%)	4 (1%)	15	56
1	D	341/343 (99%)	310 (91%)	27 (8%)	4 (1%)	15	56
1	E	341/343 (99%)	310 (91%)	27 (8%)	4 (1%)	15	56
1	F	341/343 (99%)	310 (91%)	27 (8%)	4 (1%)	15	56
All	All	2046/2058 (99%)	1856 (91%)	166 (8%)	24 (1%)	15	56

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%)	71	89
1	B	277/277 (100%)	272 (98%)	5 (2%)	64	86
1	C	277/277 (100%)	271 (98%)	6 (2%)	57	83
1	D	277/277 (100%)	272 (98%)	5 (2%)	64	86
1	E	277/277 (100%)	272 (98%)	5 (2%)	64	86
1	F	277/277 (100%)	271 (98%)	6 (2%)	57	83
All	All	1662/1662 (100%)	1631 (98%)	31 (2%)	62	85

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	0.15	0	6,6,6	0.13	0
2	SO4	C	1344	-	4,4,4	0.17	0	6,6,6	0.16	0
2	SO4	D	1344	-	4,4,4	0.18	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, 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%)	1.33	81 (23%)  	19, 49, 77, 95	0
1	B	343/343 (100%)	1.18	69 (20%)  	10, 47, 73, 87	0
1	C	343/343 (100%)	1.62	112 (32%)  	27, 61, 85, 131	0
1	D	343/343 (100%)	1.30	80 (23%)  	20, 50, 74, 87	0
1	E	343/343 (100%)	1.37	84 (24%)  	14, 46, 74, 96	0
1	F	343/343 (100%)	1.79	114 (33%)  	30, 61, 84, 115	0
All	All	2058/2058 (100%)	1.43	540 (26%)  	10, 53, 80, 131	0

All (540) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	160	GLY	21.2
1	C	290	ASP	15.5
1	F	86	GLY	13.4
1	F	319	ASP	12.0
1	C	160	GLY	10.2
1	F	87	SER	9.7
1	F	159	GLU	9.6
1	F	250	ALA	9.5
1	C	159	GLU	9.3
1	F	318	LEU	8.6
1	A	224	TYR	8.2
1	C	291	ILE	8.2
1	F	249	TRP	7.7
1	F	323	PHE	7.5
1	F	280	LYS	7.3
1	F	131	TYR	7.0
1	C	249	TRP	6.6
1	C	122	GLN	6.5
1	C	328	GLY	6.5

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Mol	Chain	Res	Type	RSRZ
1	E	262	TYR	6.5
1	F	279	GLY	6.5
1	A	122	GLN	6.5
1	F	31	GLY	6.4
1	D	203	GLN	6.2
1	E	196	SER	6.2
1	E	285	GLY	6.2
1	F	289	GLU	6.2
1	F	161	MET	5.9
1	F	247	LEU	5.8
1	F	336	ALA	5.8
1	A	188	PHE	5.7
1	F	296	ASP	5.7
1	C	217	THR	5.6
1	F	52	GLY	5.6
1	E	280	LYS	5.6
1	E	291	ILE	5.6
1	F	162	THR	5.6
1	C	86	GLY	5.6
1	F	278	LYS	5.5
1	C	318	LEU	5.5
1	B	285	GLY	5.5
1	C	162	THR	5.4
1	F	334	ILE	5.4
1	C	154	GLY	5.4
1	D	242	THR	5.3
1	D	122	GLN	5.3
1	E	290	ASP	5.3
1	D	184	ASN	5.3
1	F	120	PHE	5.2
1	B	160	GLY	5.2
1	C	280	LYS	5.2
1	E	182	THR	5.2
1	C	247	LEU	5.2
1	F	240	ASN	5.1
1	A	210	GLY	5.1
1	C	110	PHE	5.1
1	E	252	LYS	5.1
1	D	213	ASP	5.1
1	D	286	TYR	5.0
1	F	312	ASP	4.9
1	D	164	ASN	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	184	ASN	4.9
1	A	164	ASN	4.8
1	A	319	ASP	4.8
1	D	153	ASN	4.8
1	F	154	GLY	4.8
1	E	197	SER	4.8
1	A	187	GLY	4.7
1	A	160	GLY	4.7
1	F	275	LEU	4.6
1	F	281	ASN	4.6
1	A	52	GLY	4.6
1	D	154	GLY	4.6
1	C	85	VAL	4.6
1	C	317	LEU	4.6
1	A	154	GLY	4.6
1	C	278	LYS	4.6
1	A	203	GLN	4.5
1	F	282	LEU	4.5
1	A	251	ASN	4.5
1	C	327	ALA	4.5
1	F	122	GLN	4.5
1	F	291	ILE	4.5
1	F	46	VAL	4.5
1	E	212	GLY	4.4
1	C	294	TYR	4.4
1	C	266	PHE	4.4
1	E	275	LEU	4.4
1	A	214	ARG	4.4
1	E	122	GLN	4.4
1	A	197	SER	4.4
1	C	336	ALA	4.4
1	E	278	LYS	4.4
1	F	290	ASP	4.3
1	C	101	THR	4.3
1	D	285	GLY	4.3
1	A	121	MET	4.3
1	B	139	LEU	4.3
1	D	209	ILE	4.2
1	F	136	PHE	4.2
1	D	283	GLY	4.2
1	E	326	ASP	4.2
1	C	104	THR	4.2

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Mol	Chain	Res	Type	RSRZ
1	F	209	ILE	4.2
1	B	327	ALA	4.2
1	E	253	ALA	4.2
1	D	150	GLN	4.2
1	C	133	ASN	4.2
1	A	285	GLY	4.1
1	C	143	LEU	4.1
1	A	50	LEU	4.1
1	C	183	TYR	4.1
1	C	251	ASN	4.1
1	D	275	LEU	4.1
1	B	318	LEU	4.0
1	F	217	THR	4.0
1	C	334	ILE	4.0
1	B	100	VAL	4.0
1	E	120	PHE	4.0
1	D	261	GLN	4.0
1	F	324	THR	4.0
1	A	184	ASN	4.0
1	B	280	LYS	4.0
1	C	244	VAL	4.0
1	B	122	GLN	4.0
1	A	159	GLU	4.0
1	C	132	ARG	4.0
1	B	253	ALA	4.0
1	B	279	GLY	3.9
1	C	312	ASP	3.9
1	C	323	PHE	3.9
1	E	264	PHE	3.9
1	A	291	ILE	3.9
1	D	291	ILE	3.9
1	E	216	GLU	3.9
1	F	241	ALA	3.9
1	C	87	SER	3.9
1	E	279	GLY	3.8
1	A	286	TYR	3.8
1	A	162	THR	3.8
1	E	143	LEU	3.8
1	A	85	VAL	3.7
1	C	252	LYS	3.7
1	D	214	ARG	3.7
1	A	318	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	212	GLY	3.7
1	F	103	TRP	3.7
1	A	284	ARG	3.7
1	F	143	LEU	3.7
1	B	294	TYR	3.7
1	D	218	TYR	3.7
1	D	206	THR	3.7
1	F	261	GLN	3.7
1	C	248	GLY	3.6
1	F	104	THR	3.6
1	F	251	ASN	3.6
1	B	278	LYS	3.6
1	F	216	GLU	3.6
1	E	294	TYR	3.6
1	B	275	LEU	3.6
1	C	240	ASN	3.6
1	C	282	LEU	3.6
1	D	249	TRP	3.6
1	E	251	ASN	3.6
1	C	262	TYR	3.6
1	D	160	GLY	3.6
1	A	289	GLU	3.6
1	C	121	MET	3.6
1	E	249	TRP	3.6
1	E	121	MET	3.5
1	B	291	ILE	3.5
1	B	251	ASN	3.5
1	A	261	GLN	3.5
1	B	255	ASN	3.5
1	D	290	ASP	3.5
1	B	282	LEU	3.5
1	D	237	GLN	3.5
1	F	299	ALA	3.5
1	D	230	TYR	3.5
1	E	242	THR	3.5
1	F	335	VAL	3.5
1	E	183	TYR	3.4
1	F	314	LYS	3.4
1	B	182	THR	3.4
1	C	123	GLN	3.4
1	F	317	LEU	3.4
1	C	184	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	322	ARG	3.4
1	F	85	VAL	3.4
1	C	209	ILE	3.4
1	E	250	ALA	3.4
1	C	45	GLN	3.4
1	C	51	THR	3.4
1	A	225	ASP	3.4
1	C	131	TYR	3.4
1	C	190	ILE	3.4
1	C	296	ASP	3.4
1	D	201	TRP	3.4
1	B	69	ASN	3.4
1	F	183	TYR	3.3
1	E	138	GLY	3.3
1	C	216	GLU	3.3
1	E	263	GLN	3.3
1	E	282	LEU	3.3
1	B	276	GLN	3.3
1	D	198	LYS	3.3
1	D	136	PHE	3.3
1	B	329	ILE	3.3
1	D	197	SER	3.3
1	C	254	GLN	3.3
1	A	104	THR	3.3
1	F	266	PHE	3.3
1	A	209	ILE	3.3
1	C	300	THR	3.3
1	A	189	GLY	3.3
1	E	254	GLN	3.3
1	A	213	ASP	3.2
1	B	284	ARG	3.2
1	E	276	GLN	3.2
1	B	138	GLY	3.2
1	A	198	LYS	3.2
1	E	237	GLN	3.2
1	B	286	TYR	3.2
1	C	188	PHE	3.2
1	C	152	LYS	3.2
1	E	110	PHE	3.2
1	F	93	ASN	3.2
1	C	275	LEU	3.2
1	F	110	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	159	GLU	3.2
1	F	133	ASN	3.2
1	A	150	GLN	3.2
1	C	115	TYR	3.2
1	D	217	THR	3.1
1	B	244	VAL	3.1
1	E	184	ASN	3.1
1	C	201	TRP	3.1
1	D	224	TYR	3.1
1	C	261	GLN	3.1
1	E	104	THR	3.1
1	E	320	ASP	3.1
1	C	250	ALA	3.1
1	D	188	PHE	3.1
1	D	244	VAL	3.1
1	D	282	LEU	3.1
1	A	166	ARG	3.1
1	B	153	ASN	3.1
1	F	153	ASN	3.1
1	F	187	GLY	3.1
1	F	210	GLY	3.1
1	F	252	LYS	3.1
1	F	115	TYR	3.0
1	B	257	GLU	3.0
1	E	211	THR	3.0
1	B	277	SER	3.0
1	C	155	SER	3.0
1	F	32	ASP	3.0
1	F	132	ARG	3.0
1	D	189	GLY	3.0
1	E	283	GLY	3.0
1	C	223	LYS	3.0
1	E	69	ASN	3.0
1	F	223	LYS	3.0
1	B	103	TRP	3.0
1	F	328	GLY	3.0
1	E	244	VAL	3.0
1	B	252	LYS	3.0
1	F	300	THR	3.0
1	B	188	PHE	3.0
1	B	323	PHE	3.0
1	D	196	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	184	ASN	3.0
1	C	268	LEU	2.9
1	F	322	ARG	2.9
1	A	242	THR	2.9
1	F	44	THR	2.9
1	E	20	LEU	2.9
1	E	240	ASN	2.9
1	A	114	THR	2.9
1	B	217	THR	2.9
1	D	162	THR	2.9
1	A	275	LEU	2.9
1	F	100	VAL	2.9
1	F	259	VAL	2.9
1	F	51	THR	2.9
1	A	86	GLY	2.9
1	D	210	GLY	2.9
1	D	114	THR	2.9
1	C	69	ASN	2.9
1	C	329	ILE	2.9
1	F	145	PHE	2.9
1	D	137	PHE	2.8
1	C	128	PHE	2.8
1	A	254	GLN	2.8
1	C	150	GLN	2.8
1	A	139	LEU	2.8
1	E	49	GLN	2.8
1	C	299	ALA	2.8
1	A	46	VAL	2.8
1	E	229	ILE	2.8
1	F	232	ALA	2.8
1	D	320	ASP	2.8
1	C	230	TYR	2.8
1	C	311	VAL	2.8
1	E	234	GLN	2.7
1	B	290	ASP	2.7
1	A	250	ALA	2.7
1	F	127	GLY	2.7
1	D	274	TYR	2.7
1	F	150	GLN	2.7
1	D	169	VAL	2.7
1	C	63	ASN	2.7
1	D	190	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	257	GLU	2.7
1	C	76	ALA	2.7
1	D	273	ALA	2.7
1	A	82	PHE	2.7
1	B	262	TYR	2.7
1	D	289	GLU	2.7
1	F	294	TYR	2.7
1	A	201	TRP	2.7
1	C	281	ASN	2.7
1	A	51	THR	2.7
1	F	215	ALA	2.7
1	D	163	THR	2.7
1	C	31	GLY	2.7
1	C	257	GLU	2.7
1	E	101	THR	2.6
1	A	97	VAL	2.6
1	D	151	GLY	2.6
1	E	215	ALA	2.6
1	F	137	PHE	2.6
1	A	244	VAL	2.6
1	C	264	PHE	2.6
1	E	265	ASP	2.6
1	F	76	ALA	2.6
1	A	223	LYS	2.6
1	B	223	LYS	2.6
1	F	264	PHE	2.6
1	F	257	GLU	2.6
1	D	223	LYS	2.6
1	F	248	GLY	2.6
1	C	20	LEU	2.6
1	E	261	GLN	2.6
1	E	235	TYR	2.6
1	F	88	PHE	2.6
1	F	310	TYR	2.6
1	F	109	GLU	2.6
1	D	200	THR	2.6
1	E	286	TYR	2.6
1	E	284	ARG	2.6
1	A	231	LEU	2.6
1	C	107	LEU	2.6
1	F	200	THR	2.6
1	B	183	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	284	ARG	2.5
1	A	288	ASP	2.5
1	C	32	ASP	2.5
1	E	115	TYR	2.5
1	E	336	ALA	2.5
1	F	203	GLN	2.5
1	C	295	VAL	2.5
1	E	268	LEU	2.5
1	B	152	LYS	2.5
1	C	93	ASN	2.5
1	E	137	PHE	2.5
1	D	69	ASN	2.5
1	D	121	MET	2.5
1	D	284	ARG	2.5
1	B	143	LEU	2.5
1	A	264	PHE	2.5
1	D	142	GLY	2.5
1	A	217	THR	2.5
1	B	151	GLY	2.5
1	E	195	SER	2.5
1	B	211	THR	2.5
1	C	130	THR	2.5
1	D	235	TYR	2.5
1	F	239	TYR	2.5
1	E	312	ASP	2.5
1	A	255	ASN	2.5
1	A	331	THR	2.5
1	D	166	ARG	2.4
1	C	231	LEU	2.4
1	A	120	PHE	2.4
1	A	230	TYR	2.4
1	C	331	THR	2.4
1	D	172	GLN	2.4
1	F	326	ASP	2.4
1	B	336	ALA	2.4
1	C	241	ALA	2.4
1	B	164	ASN	2.4
1	C	161	MET	2.4
1	D	174	GLY	2.4
1	C	310	TYR	2.4
1	C	324	THR	2.4
1	F	116	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	216	GLU	2.4
1	B	224	TYR	2.4
1	C	301	TYR	2.4
1	B	150	GLN	2.4
1	C	314	LYS	2.4
1	A	136	PHE	2.4
1	F	128	PHE	2.4
1	B	313	TYR	2.4
1	E	230	TYR	2.4
1	E	144	ASP	2.4
1	A	317	LEU	2.4
1	C	267	GLY	2.4
1	C	218	TYR	2.4
1	F	230	TYR	2.4
1	E	139	LEU	2.4
1	F	202	ASP	2.4
1	D	85	VAL	2.4
1	F	309	THR	2.4
1	F	327	ALA	2.3
1	B	107	LEU	2.3
1	D	257	GLU	2.3
1	A	153	ASN	2.3
1	B	238	THR	2.3
1	C	279	GLY	2.3
1	E	97	VAL	2.3
1	A	107	LEU	2.3
1	C	239	TYR	2.3
1	D	152	LYS	2.3
1	E	266	PHE	2.3
1	D	107	LEU	2.3
1	F	69	ASN	2.3
1	C	202	ASP	2.3
1	C	335	VAL	2.3
1	E	323	PHE	2.3
1	A	173	ASN	2.3
1	A	266	PHE	2.3
1	B	149	TYR	2.3
1	B	268	LEU	2.3
1	D	50	LEU	2.3
1	A	234	GLN	2.3
1	C	145	PHE	2.3
1	A	115	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	133	ASN	2.3
1	B	230	TYR	2.3
1	C	109	GLU	2.2
1	A	69	ASN	2.2
1	D	317	LEU	2.2
1	C	270	PRO	2.2
1	A	294	TYR	2.2
1	B	166	ARG	2.2
1	A	262	TYR	2.2
1	A	116	ASP	2.2
1	F	206	THR	2.2
1	F	231	LEU	2.2
1	A	165	GLY	2.2
1	B	218	TYR	2.2
1	D	259	VAL	2.2
1	D	250	ALA	2.2
1	C	44	THR	2.2
1	C	124	HIS	2.2
1	E	335	VAL	2.2
1	D	127	GLY	2.2
1	E	328	GLY	2.2
1	D	262	TYR	2.2
1	F	208	LEU	2.2
1	A	101	THR	2.2
1	E	210	GLY	2.2
1	F	218	TYR	2.2
1	E	318	LEU	2.2
1	B	249	TRP	2.2
1	E	111	GLY	2.2
1	E	152	LYS	2.2
1	B	283	GLY	2.2
1	C	33	LYS	2.2
1	F	214	ARG	2.2
1	C	120	PHE	2.1
1	C	148	GLN	2.1
1	E	248	GLY	2.1
1	F	112	GLY	2.1
1	F	267	GLY	2.1
1	E	327	ALA	2.1
1	E	142	GLY	2.1
1	F	138	GLY	2.1
1	A	241	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	150	GLN	2.1
1	F	270	PRO	2.1
1	A	206	THR	2.1
1	A	282	LEU	2.1
1	E	334	ILE	2.1
1	D	231	LEU	2.1
1	F	152	LYS	2.1
1	B	264	PHE	2.1
1	C	22	TYR	2.1
1	F	288	ASP	2.1
1	C	169	VAL	2.1
1	B	154	GLY	2.1
1	C	153	ASN	2.1
1	C	276	GLN	2.1
1	D	143	LEU	2.1
1	C	195	SER	2.1
1	D	115	TYR	2.1
1	E	71	SER	2.1
1	F	22	TYR	2.1
1	B	254	GLN	2.1
1	F	107	LEU	2.1
1	D	264	PHE	2.1
1	F	173	ASN	2.1
1	B	259	VAL	2.1
1	E	259	VAL	2.1
1	A	196	SER	2.1
1	F	274	TYR	2.1
1	C	50	LEU	2.1
1	F	190	ILE	2.1
1	F	158	GLY	2.1
1	D	40	PHE	2.0
1	D	113	ASP	2.0
1	D	225	ASP	2.0
1	B	190	ILE	2.0
1	D	236	THR	2.0
1	B	120	PHE	2.0
1	E	257	GLU	2.0
1	E	287	ASP	2.0
1	C	100	VAL	2.0
1	F	244	VAL	2.0
1	B	104	THR	2.0
1	B	200	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	176	GLY	2.0
1	A	199	ARG	2.0
1	B	209	ILE	2.0
1	D	334	ILE	2.0
1	E	325	ARG	2.0
1	E	153	ASN	2.0
1	F	164	ASN	2.0
1	B	203	GLN	2.0
1	C	71	SER	2.0
1	D	202	ASP	2.0
1	D	288	ASP	2.0
1	E	243	ARG	2.0
1	B	174	GLY	2.0
1	A	236	THR	2.0
1	A	45	GLN	2.0
1	D	45	GLN	2.0
1	A	292	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	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.