



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 12:42 AM GMT

PDB ID : 1RKW
Title : CRYSTAL STRUCTURE OF THE MULTIDRUG BINDING TRANSCRIPTIONAL REPRESSOR QACR BOUND TO PENTAMADINE
Authors : Murray, D.S.; Schumacher, M.A.; Brennan, R.G.
Deposited on : 2003-11-23
Resolution : 2.62 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

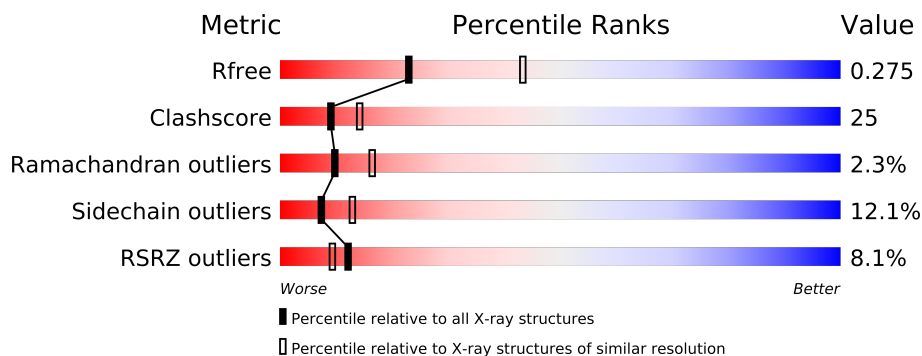
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.62 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}	66092	1940 (2.64-2.60)
Clashscore	79885	2404 (2.64-2.60)
Ramachandran outliers	78287	2360 (2.64-2.60)
Sidechain outliers	78261	2360 (2.64-2.60)
RSRZ outliers	66119	1939 (2.64-2.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	194	
1	B	194	
1	D	194	
1	E	194	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	SO4	A	199	-	X
3	SO4	A	279	-	X
3	SO4	A	579	-	X
3	SO4	B	259	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	SO4	B	299	-	X
3	SO4	D	639	-	X
3	SO4	E	239	-	X
3	SO4	E	899	-	X
3	SO4	E	999	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6403 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Transcriptional regulator qacR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	186	Total	C	N	O	S	0	0	0
			1547	998	252	295	2			
1	D	186	Total	C	N	O	S	0	0	0
			1547	998	252	295	2			
1	A	186	Total	C	N	O	S	0	0	0
			1547	998	252	295	2			
1	E	186	Total	C	N	O	S	0	0	0
			1547	998	252	295	2			

There are 32 discrepancies between the modelled and reference sequences:

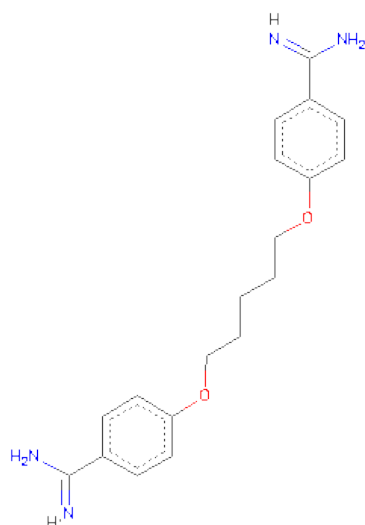
Chain	Residue	Modelled	Actual	Comment	Reference
B	72	ALA	CYS	ENGINEERED	UNP P0A0N4
B	141	SER	CYS	ENGINEERED	UNP P0A0N4
B	189	HIS	-	EXPRESSION TAG	UNP P0A0N4
B	190	HIS	-	EXPRESSION TAG	UNP P0A0N4
B	191	HIS	-	EXPRESSION TAG	UNP P0A0N4
B	192	HIS	-	EXPRESSION TAG	UNP P0A0N4
B	193	HIS	-	EXPRESSION TAG	UNP P0A0N4
B	194	HIS	-	EXPRESSION TAG	UNP P0A0N4
D	72	ALA	CYS	ENGINEERED	UNP P0A0N4
D	141	SER	CYS	ENGINEERED	UNP P0A0N4
D	189	HIS	-	EXPRESSION TAG	UNP P0A0N4
D	190	HIS	-	EXPRESSION TAG	UNP P0A0N4
D	191	HIS	-	EXPRESSION TAG	UNP P0A0N4
D	192	HIS	-	EXPRESSION TAG	UNP P0A0N4
D	193	HIS	-	EXPRESSION TAG	UNP P0A0N4
D	194	HIS	-	EXPRESSION TAG	UNP P0A0N4
A	72	ALA	CYS	ENGINEERED	UNP P0A0N4
A	141	SER	CYS	ENGINEERED	UNP P0A0N4
A	189	HIS	-	EXPRESSION TAG	UNP P0A0N4
A	190	HIS	-	EXPRESSION TAG	UNP P0A0N4
A	191	HIS	-	EXPRESSION TAG	UNP P0A0N4

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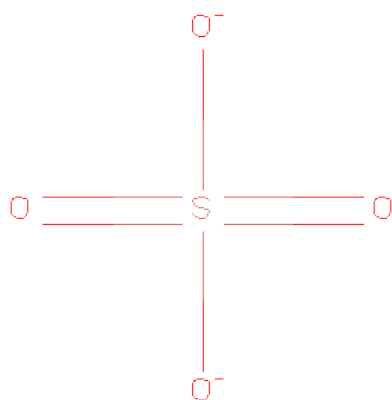
Chain	Residue	Modelled	Actual	Comment	Reference
A	192	HIS	-	EXPRESSION TAG	UNP P0A0N4
A	193	HIS	-	EXPRESSION TAG	UNP P0A0N4
A	194	HIS	-	EXPRESSION TAG	UNP P0A0N4
E	72	ALA	CYS	ENGINEERED	UNP P0A0N4
E	141	SER	CYS	ENGINEERED	UNP P0A0N4
E	189	HIS	-	EXPRESSION TAG	UNP P0A0N4
E	190	HIS	-	EXPRESSION TAG	UNP P0A0N4
E	191	HIS	-	EXPRESSION TAG	UNP P0A0N4
E	192	HIS	-	EXPRESSION TAG	UNP P0A0N4
E	193	HIS	-	EXPRESSION TAG	UNP P0A0N4
E	194	HIS	-	EXPRESSION TAG	UNP P0A0N4

- Molecule 2 is 1,5-BIS(4-AMIDINOPHENOXY)PENTANE (three-letter code: PNT) (formula: C₁₉H₂₄N₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			25	19	4	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

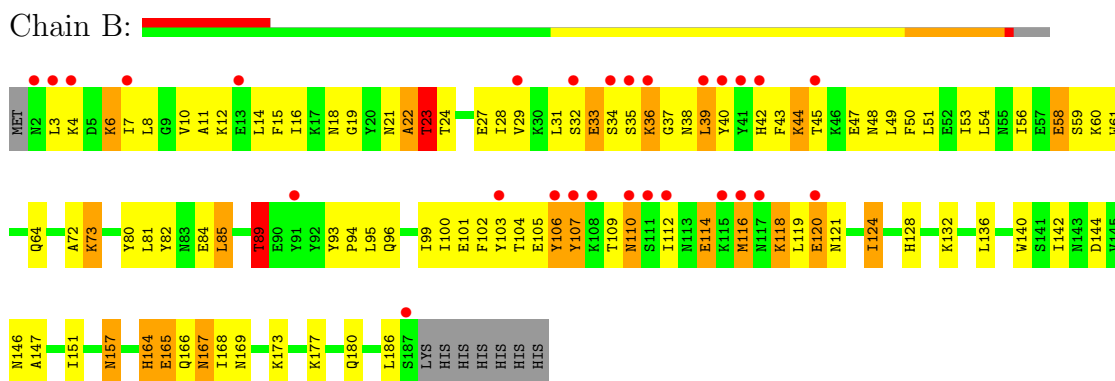
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	35	Total	O	0	0
			35	35		
4	B	10	Total	O	0	0
			10	10		
4	D	12	Total	O	0	0
			12	12		
4	E	23	Total	O	0	0
			23	23		

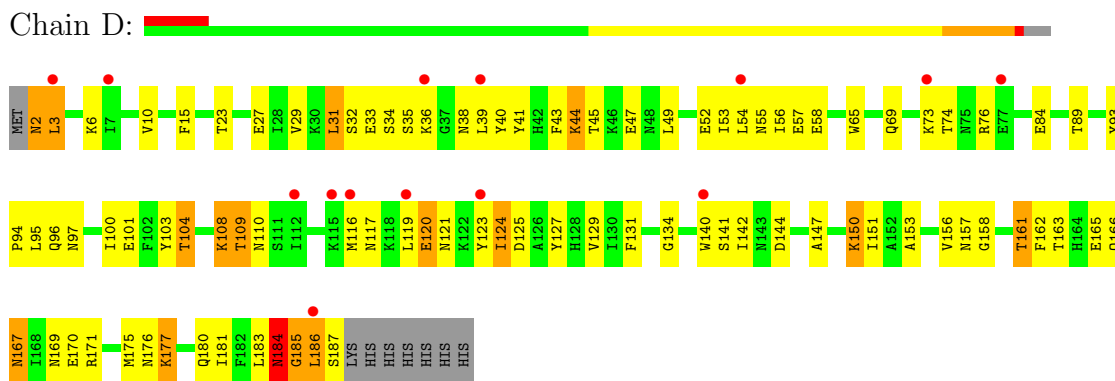
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

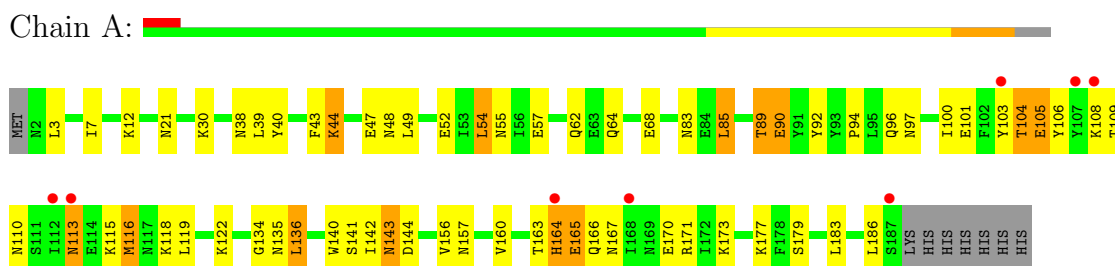
- Molecule 1: Transcriptional regulator qacR



- Molecule 1: Transcriptional regulator qacR

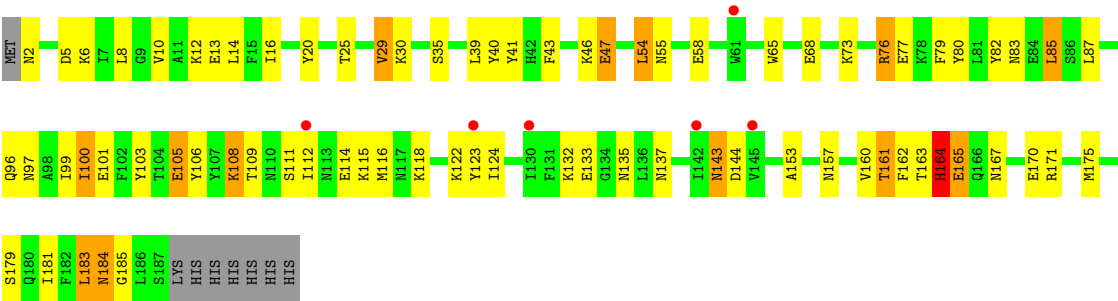


- Molecule 1: Transcriptional regulator qacR



- Molecule 1: Transcriptional regulator qacR





4 Data and refinement statistics

Property	Value	Source
Space group	P 4 ₂ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	172.05Å 172.05Å 94.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	86.03 – 2.62 86.02 – 2.62	Depositor EDS
% Data completeness (in resolution range)	96.0 (86.03-2.62) 96.1 (86.02-2.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 2.62Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.224 , 0.275 0.224 , 0.275	Depositor DCC
R_{free} test set	2082 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	74.3	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 72.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 41350 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6403	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, PNT

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	0.76	0/1578	0.78	0/2126
1	B	0.62	0/1578	0.70	0/2126
1	D	0.60	0/1578	0.72	0/2126
1	E	0.67	0/1578	0.77	0/2126
All	All	0.66	0/6312	0.75	0/8504

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1547	0	1536	63	0
1	B	1547	0	1536	113	1
1	D	1547	0	1536	81	0
1	E	1547	0	1536	75	0
2	A	25	0	23	3	0
3	A	25	0	0	2	0
3	B	15	0	0	1	0
3	D	40	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	30	0	0	2	0
4	A	35	0	0	3	0
4	B	10	0	0	0	0
4	D	12	0	0	1	0
4	E	23	0	0	2	0
All	All	6403	0	6167	313	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 25.

All (313) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:68:GLU:HG2	1:E:85:LEU:HD21	1.35	1.08
1:E:143:ASN:ND2	1:E:144:ASP:H	1.57	1.03
1:D:157:ASN:O	1:D:161:THR:HG23	1.57	1.01
1:B:36:LYS:H	1:B:36:LYS:HD3	1.27	0.97
1:B:96:GLN:HG3	1:B:157:ASN:HD21	1.29	0.96
1:B:56:ILE:HG22	1:B:60:LYS:HD2	1.47	0.96
1:B:6:LYS:HE3	1:B:6:LYS:HA	1.50	0.93
1:A:85:LEU:O	1:A:89:THR:HG23	1.73	0.88
1:E:157:ASN:O	1:E:161:THR:HG23	1.73	0.87
1:D:165:GLU:HB3	1:E:103:TYR:CE1	2.09	0.87
1:B:106:TYR:HB3	1:B:112:ILE:HG13	1.59	0.84
1:B:167:ASN:ND2	1:B:169:ASN:H	1.77	0.82
1:D:142:ILE:HD11	1:D:186:LEU:HD13	1.59	0.81
1:D:101:GLU:HG3	1:E:97:ASN:HD21	1.46	0.80
1:B:167:ASN:HD22	1:B:168:ILE:N	1.79	0.80
1:A:142:ILE:HD11	1:A:186:LEU:HD13	1.63	0.79
1:A:164:HIS:HA	1:A:171:ARG:CZ	2.12	0.78
1:B:18:ASN:HB2	1:B:23:THR:HG22	1.66	0.78
1:B:4:LYS:O	1:B:8:LEU:HD23	1.84	0.78
1:D:6:LYS:HG3	1:D:32:SER:HB2	1.66	0.76
1:B:58:GLU:HG3	1:B:119:LEU:HD21	1.68	0.75
1:B:47:GLU:OE2	1:B:112:ILE:HD11	1.86	0.75
1:B:39:LEU:H	1:B:39:LEU:HD22	1.51	0.75
1:E:143:ASN:HD22	1:E:144:ASP:H	1.35	0.75
1:B:118:LYS:HD2	1:B:121:ASN:HD22	1.51	0.74
1:B:10:VAL:O	1:B:14:LEU:HD13	1.87	0.73
1:A:100:ILE:O	1:A:104:THR:HG23	1.88	0.73
1:B:72:ALA:HA	1:B:73:LYS:HZ1	1.55	0.72
1:E:106:TYR:HB3	1:E:112:ILE:HG21	1.71	0.72
1:A:163:THR:O	1:A:165:GLU:N	2.22	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:44:LYS:H	1:B:48:ASN:HD22	1.37	0.71
1:D:36:LYS:HG3	1:D:40:TYR:CE1	2.25	0.71
1:B:32:SER:O	1:B:33:GLU:HB2	1.89	0.71
1:A:52:GLU:HG2	3:A:579:SO4:O2	1.90	0.71
1:D:185:GLY:HA2	1:E:184:ASN:HB3	1.73	0.71
1:B:104:THR:O	1:B:105:GLU:HG3	1.92	0.70
1:B:6:LYS:O	1:B:10:VAL:HG23	1.93	0.69
1:D:101:GLU:HG3	1:E:97:ASN:ND2	2.07	0.69
1:D:2:ASN:CG	1:D:3:LEU:H	1.96	0.69
1:D:76:ARG:HG3	1:D:183:LEU:HD13	1.75	0.68
1:B:44:LYS:H	1:B:48:ASN:ND2	1.92	0.68
1:A:62:GLN:HG2	4:A:706:HOH:O	1.93	0.67
1:B:36:LYS:HG2	1:B:37:GLY:H	1.59	0.67
1:B:120:GLU:O	1:B:124:ILE:HG23	1.95	0.67
1:B:14:LEU:HD21	1:B:27:GLU:HG2	1.77	0.67
1:A:96:GLN:O	1:A:100:ILE:HG12	1.95	0.66
1:B:73:LYS:H	1:B:73:LYS:HZ2	1.43	0.66
1:D:2:ASN:ND2	1:D:3:LEU:H	1.93	0.66
1:B:39:LEU:N	1:B:39:LEU:HD22	2.10	0.66
1:B:167:ASN:HD21	1:B:169:ASN:H	1.43	0.66
1:D:184:ASN:HB3	1:E:185:GLY:HA2	1.78	0.66
1:E:97:ASN:O	1:E:100:ILE:HG13	1.96	0.66
1:E:105:GLU:HG2	1:E:106:TYR:CD2	2.31	0.65
1:A:64:GLN:NE2	2:A:225:PNT:H3'	2.11	0.65
1:E:106:TYR:HA	1:E:108:LYS:HE2	1.78	0.65
1:B:103:TYR:HD2	1:B:116:MET:SD	2.19	0.65
1:B:24:THR:HG23	1:B:27:GLU:H	1.61	0.64
1:B:28:ILE:HD13	1:B:49:LEU:HD21	1.79	0.64
1:A:109:THR:O	1:A:113:ASN:HB2	1.98	0.64
1:A:12:LYS:HD2	3:A:199:SO4:O3	1.96	0.64
1:B:167:ASN:C	1:B:167:ASN:HD22	2.00	0.64
1:D:54:LEU:HD23	1:D:119:LEU:HD13	1.80	0.64
1:E:165:GLU:OE1	1:E:165:GLU:HA	1.95	0.64
1:D:120:GLU:O	1:D:124:ILE:HG12	1.98	0.64
1:E:105:GLU:O	1:E:105:GLU:HG3	1.98	0.63
1:B:7:ILE:HD13	1:B:32:SER:OG	1.99	0.63
1:D:165:GLU:HB3	1:E:103:TYR:HE1	1.63	0.63
1:E:132:LYS:HD2	3:E:209:SO4:O3	1.99	0.63
1:B:3:LEU:HD21	1:B:34:SER:OG	1.97	0.63
1:B:72:ALA:HA	1:B:73:LYS:NZ	2.13	0.63
1:B:103:TYR:CE2	1:B:116:MET:HG2	2.34	0.62
1:D:2:ASN:ND2	1:D:3:LEU:N	2.47	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:27:GLU:HG3	1:B:31:LEU:HD23	1.81	0.62
1:B:54:LEU:HB3	1:B:119:LEU:HD11	1.80	0.62
1:B:38:ASN:HB2	1:B:39:LEU:HD22	1.81	0.62
1:B:15:PHE:CE1	1:B:50:PHE:HD2	2.16	0.62
1:D:65:TRP:O	1:D:69:GLN:HB3	2.00	0.62
1:A:64:GLN:HE21	2:A:225:PNT:H3'	1.65	0.62
1:A:97:ASN:ND2	4:A:727:HOH:O	2.33	0.62
1:E:76:ARG:HD3	1:E:183:LEU:HD23	1.82	0.61
1:E:143:ASN:CG	1:E:144:ASP:H	2.03	0.61
1:B:29:VAL:HG13	1:B:34:SER:O	2.01	0.61
1:B:167:ASN:C	1:B:167:ASN:ND2	2.53	0.61
1:D:38:ASN:O	1:D:41:TYR:HB3	2.00	0.61
1:B:177:LYS:HE2	1:A:144:ASP:OD2	2.02	0.60
1:E:6:LYS:O	1:E:10:VAL:HG23	2.00	0.60
1:B:14:LEU:C	1:B:23:THR:HG21	2.21	0.60
1:B:106:TYR:HB3	1:B:112:ILE:CG1	2.31	0.60
1:B:14:LEU:HB3	1:B:23:THR:HB	1.83	0.60
1:B:103:TYR:CD2	1:B:116:MET:HG2	2.35	0.60
1:B:116:MET:O	1:B:116:MET:HG3	2.01	0.60
1:B:103:TYR:CE1	1:B:107:TYR:HB3	2.37	0.59
1:D:73:LYS:HG3	1:D:74:THR:H	1.66	0.59
1:B:144:ASP:OD1	1:A:177:LYS:HE2	2.02	0.59
1:B:39:LEU:CD2	1:B:39:LEU:H	2.15	0.59
1:D:6:LYS:CG	1:D:32:SER:HB2	2.32	0.59
1:B:112:ILE:C	1:B:114:GLU:H	2.05	0.59
1:A:43:PHE:O	1:A:44:LYS:HB2	2.02	0.59
1:B:107:TYR:H	1:B:107:TYR:HD1	1.48	0.59
1:E:114:GLU:O	1:E:118:LYS:HG3	2.02	0.59
1:E:68:GLU:HG2	1:E:85:LEU:CD2	2.23	0.59
1:B:104:THR:C	1:B:105:GLU:HG3	2.24	0.58
1:B:8:LEU:CD2	1:B:43:PHE:HZ	2.16	0.58
1:A:68:GLU:HG2	1:A:85:LEU:HD21	1.85	0.58
1:D:165:GLU:CB	1:E:103:TYR:CE1	2.84	0.58
1:B:80:TYR:O	1:B:84:GLU:HG3	2.02	0.58
1:A:134:GLY:HA3	1:A:140:TRP:CE2	2.39	0.58
1:D:147:ALA:O	1:D:151:ILE:HG13	2.04	0.58
1:D:54:LEU:O	1:D:58:GLU:HB2	2.03	0.58
1:E:164:HIS:CE1	4:E:1021:HOH:O	2.57	0.57
1:B:58:GLU:HG3	1:B:119:LEU:CD2	2.32	0.57
1:E:157:ASN:O	1:E:161:THR:CG2	2.48	0.57
1:A:144:ASP:OD1	1:A:144:ASP:N	2.36	0.57
1:A:90:GLU:HG2	1:A:160:VAL:CG1	2.35	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:100:ILE:O	1:B:104:THR:HG23	2.04	0.57
1:A:164:HIS:HA	1:A:171:ARG:NH2	2.19	0.57
1:B:44:LYS:N	1:B:48:ASN:HD22	2.01	0.57
1:E:108:LYS:HE3	1:E:108:LYS:H	1.69	0.57
1:B:6:LYS:CA	1:B:6:LYS:HE3	2.30	0.56
1:D:125:ASP:O	1:D:129:VAL:HG23	2.04	0.56
1:B:96:GLN:NE2	1:B:157:ASN:OD1	2.37	0.56
1:B:81:LEU:HG	1:B:85:LEU:HD22	1.87	0.56
1:D:177:LYS:HE3	1:D:180:GLN:OE1	2.05	0.56
1:B:36:LYS:CD	1:B:36:LYS:H	2.07	0.56
1:D:186:LEU:O	1:D:187:SER:HB2	2.06	0.56
1:A:103:TYR:C	1:A:105:GLU:H	2.09	0.56
1:B:21:ASN:O	1:B:22:ALA:O	2.24	0.56
1:B:73:LYS:H	1:B:73:LYS:NZ	2.03	0.56
1:B:19:GLY:O	1:B:23:THR:HG23	2.06	0.55
1:E:164:HIS:HA	1:E:171:ARG:NH1	2.20	0.55
1:D:27:GLU:O	1:D:31:LEU:HB2	2.07	0.55
1:B:119:LEU:O	1:B:119:LEU:HD23	2.06	0.55
1:D:165:GLU:CB	1:E:103:TYR:HE1	2.20	0.54
1:D:185:GLY:HA3	1:E:181:ILE:O	2.06	0.54
1:D:45:THR:HG23	1:D:47:GLU:HG3	1.89	0.54
1:A:164:HIS:C	1:A:171:ARG:NH2	2.61	0.54
1:D:167:ASN:ND2	1:D:169:ASN:H	2.06	0.54
1:E:105:GLU:HG2	1:E:106:TYR:CE2	2.43	0.54
1:E:108:LYS:HE3	1:E:108:LYS:N	2.23	0.54
1:A:135:ASN:OD1	1:A:141:SER:HA	2.08	0.54
1:E:83:ASN:HB3	1:E:175:MET:SD	2.48	0.54
1:A:96:GLN:HE21	1:A:100:ILE:HD11	1.74	0.53
1:D:185:GLY:CA	1:E:184:ASN:HB3	2.37	0.53
1:A:90:GLU:OE2	1:A:96:GLN:HG2	2.08	0.53
1:A:113:ASN:HA	1:A:116:MET:HG3	1.91	0.53
1:D:177:LYS:O	1:D:177:LYS:HD3	2.08	0.53
1:D:184:ASN:O	1:D:186:LEU:N	2.42	0.53
1:A:62:GLN:CG	4:A:706:HOH:O	2.56	0.53
1:E:20:TYR:CZ	1:E:46:LYS:HE2	2.43	0.53
1:B:45:THR:OG1	1:B:47:GLU:HG2	2.09	0.53
1:E:103:TYR:CD2	1:E:116:MET:HG2	2.45	0.52
1:D:186:LEU:O	1:D:187:SER:CB	2.56	0.52
1:B:21:ASN:OD1	1:B:105:GLU:OE2	2.27	0.52
1:D:158:GLY:O	1:D:162:PHE:HD1	1.93	0.52
1:E:73:LYS:HB3	1:E:77:GLU:OE1	2.10	0.52
1:A:83:ASN:ND2	1:A:156:VAL:HG21	2.25	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:96:GLN:NE2	1:D:157:ASN:HD21	2.08	0.52
1:B:56:ILE:O	1:B:59:SER:HB2	2.10	0.52
1:B:61:TRP:HZ2	1:B:82:TYR:CE1	2.28	0.52
1:B:112:ILE:O	1:B:116:MET:HB3	2.10	0.52
1:E:12:LYS:O	1:E:16:ILE:HG13	2.10	0.52
1:D:144:ASP:HB2	4:D:808:HOH:O	2.10	0.52
1:A:105:GLU:OE1	1:A:106:TYR:CE2	2.63	0.52
1:E:47:GLU:HG3	1:E:112:ILE:HD11	1.91	0.51
1:E:103:TYR:HD2	1:E:116:MET:HG2	1.75	0.51
1:D:171:ARG:HG2	1:D:171:ARG:HH11	1.75	0.51
1:D:45:THR:CG2	1:D:47:GLU:HG3	2.40	0.51
1:B:61:TRP:HE3	1:B:89:THR:HG21	1.75	0.51
1:B:18:ASN:HB2	1:B:23:THR:CG2	2.40	0.51
1:A:21:ASN:ND2	1:A:101:GLU:OE1	2.45	0.51
1:E:132:LYS:O	1:E:135:ASN:HB2	2.12	0.50
1:A:38:ASN:ND2	1:E:13:GLU:CD	2.65	0.50
1:D:134:GLY:HA3	1:D:140:TRP:CZ2	2.46	0.50
1:B:11:ALA:HB3	1:B:53:ILE:HD11	1.93	0.50
1:A:47:GLU:HG2	1:A:106:TYR:CZ	2.47	0.50
1:E:96:GLN:O	1:E:100:ILE:HG12	2.11	0.50
1:B:95:LEU:O	1:B:99:ILE:HG13	2.11	0.50
1:B:118:LYS:HD2	1:B:121:ASN:ND2	2.24	0.49
1:B:61:TRP:CZ2	1:B:82:TYR:CE1	2.99	0.49
1:B:164:HIS:CD2	1:B:164:HIS:O	2.65	0.49
1:E:35:SER:HA	4:E:1000:HOH:O	2.13	0.49
1:A:3:LEU:O	1:A:7:ILE:HG13	2.13	0.49
1:B:112:ILE:C	1:B:114:GLU:N	2.66	0.49
1:E:76:ARG:CD	1:E:183:LEU:HD23	2.43	0.49
1:A:39:LEU:C	1:A:39:LEU:HD23	2.33	0.49
1:D:127:TYR:O	1:D:131:PHE:CD2	2.65	0.49
1:B:36:LYS:N	1:B:36:LYS:HD3	2.11	0.49
1:B:106:TYR:CB	1:B:112:ILE:HG13	2.37	0.49
1:D:2:ASN:CG	1:D:3:LEU:N	2.66	0.49
1:B:110:ASN:ND2	1:B:110:ASN:O	2.46	0.49
1:A:170:GLU:HA	1:A:170:GLU:OE2	2.12	0.49
1:B:132:LYS:O	1:B:136:LEU:HD13	2.13	0.49
1:E:163:THR:O	1:E:171:ARG:HD3	2.13	0.48
1:D:29:VAL:HG11	1:D:35:SER:HA	1.95	0.48
1:E:108:LYS:HE3	1:E:109:THR:H	1.78	0.48
1:A:106:TYR:C	1:A:108:LYS:H	2.16	0.48
1:A:40:TYR:CE1	1:E:6:LYS:HD3	2.48	0.48
1:A:143:ASN:H	1:A:143:ASN:ND2	2.11	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:153:ALA:O	1:E:157:ASN:HB2	2.13	0.48
1:E:41:TYR:CD2	1:E:41:TYR:C	2.85	0.48
1:E:79:PHE:CD2	1:E:183:LEU:HD13	2.48	0.48
1:D:15:PHE:CE2	1:D:23:THR:HB	2.49	0.48
1:A:164:HIS:HA	1:A:171:ARG:NH1	2.28	0.48
1:A:40:TYR:CZ	1:E:6:LYS:HD3	2.49	0.48
1:A:90:GLU:HG2	1:A:160:VAL:HG11	1.95	0.48
1:E:106:TYR:CB	1:E:112:ILE:HG21	2.40	0.48
1:B:56:ILE:O	1:B:60:LYS:HG3	2.14	0.48
1:A:163:THR:O	1:A:166:GLN:HG3	2.13	0.48
1:D:27:GLU:HG2	1:D:31:LEU:HD22	1.95	0.48
1:E:143:ASN:HD22	1:E:144:ASP:N	2.09	0.47
1:A:165:GLU:O	1:A:166:GLN:HG2	2.14	0.47
1:E:54:LEU:HD11	1:E:99:ILE:HG12	1.95	0.47
1:D:150:LYS:HE3	1:D:150:LYS:HB2	1.56	0.47
1:A:49:LEU:HD23	1:A:49:LEU:O	2.14	0.47
1:A:96:GLN:HE21	1:A:100:ILE:CD1	2.27	0.47
1:B:106:TYR:HB3	1:B:112:ILE:HG21	1.96	0.47
1:B:54:LEU:HB3	1:B:119:LEU:CD1	2.45	0.47
1:D:40:TYR:O	1:D:44:LYS:HA	2.14	0.47
1:D:103:TYR:HE1	1:E:165:GLU:HG2	1.79	0.47
1:A:92:TYR:O	1:A:94:PRO:HD3	2.15	0.47
1:B:58:GLU:CG	1:B:119:LEU:HD21	2.42	0.47
1:E:2:ASN:HB2	1:E:5:ASP:HB2	1.97	0.47
1:A:134:GLY:HA3	1:A:140:TRP:CZ2	2.50	0.47
1:D:177:LYS:O	1:D:181:ILE:HG13	2.15	0.47
1:A:57:GLU:OE1	2:A:225:PNT:H6'	2.15	0.46
1:E:39:LEU:C	1:E:39:LEU:HD23	2.35	0.46
1:A:165:GLU:N	1:A:165:GLU:CD	2.69	0.46
1:B:106:TYR:O	1:B:112:ILE:HB	2.15	0.46
1:A:109:THR:HG22	1:A:110:ASN:N	2.30	0.46
1:A:179:SER:O	1:A:183:LEU:HB2	2.15	0.46
1:E:133:GLU:O	1:E:137:ASN:ND2	2.46	0.46
1:D:101:GLU:OE2	1:E:101:GLU:OE2	2.33	0.46
1:B:96:GLN:O	1:B:100:ILE:HG13	2.15	0.46
1:E:76:ARG:NH1	1:E:80:TYR:OH	2.48	0.46
1:B:102:PHE:CZ	1:B:112:ILE:HD12	2.51	0.46
1:D:163:THR:O	1:D:171:ARG:HD2	2.16	0.46
1:A:103:TYR:O	1:A:105:GLU:N	2.48	0.46
1:D:49:LEU:O	1:D:53:ILE:HG13	2.16	0.46
1:E:111:SER:O	1:E:115:LYS:HG3	2.16	0.46
1:E:29:VAL:HG21	1:E:35:SER:C	2.37	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:54:LEU:HB3	1:A:119:LEU:HD21	1.98	0.45
1:B:167:ASN:ND2	1:B:168:ILE:N	2.57	0.45
1:A:52:GLU:OE1	1:A:52:GLU:HA	2.16	0.45
1:A:103:TYR:C	1:A:105:GLU:N	2.68	0.45
1:B:107:TYR:CD1	1:B:107:TYR:N	2.84	0.45
1:D:100:ILE:O	1:D:104:THR:HG23	2.16	0.45
1:B:12:LYS:HD2	3:B:299:SO4:O1	2.17	0.45
1:D:10:VAL:HG21	1:D:32:SER:HB3	1.99	0.45
1:D:43:PHE:O	1:D:44:LYS:HB2	2.16	0.45
1:B:14:LEU:HB3	1:B:23:THR:CB	2.46	0.45
1:B:165:GLU:OE1	1:B:166:GLN:OE1	2.35	0.45
1:B:37:GLY:O	1:B:38:ASN:C	2.54	0.44
1:D:177:LYS:C	1:D:177:LYS:HD3	2.37	0.44
1:A:49:LEU:C	1:A:49:LEU:HD23	2.38	0.44
1:A:136:LEU:N	1:A:136:LEU:CD1	2.80	0.44
1:B:14:LEU:HB3	1:B:23:THR:CG2	2.47	0.44
1:B:118:LYS:O	1:B:118:LYS:HD2	2.18	0.44
1:E:40:TYR:O	1:E:43:PHE:O	2.36	0.44
1:B:36:LYS:HG2	1:B:37:GLY:N	2.27	0.44
1:D:55:ASN:OD1	1:D:119:LEU:HD21	2.18	0.44
1:D:177:LYS:CE	1:D:180:GLN:OE1	2.66	0.44
1:E:12:LYS:HD2	3:E:899:SO4:O3	2.18	0.44
1:D:39:LEU:HD23	1:D:39:LEU:C	2.38	0.44
1:D:117:ASN:O	1:D:121:ASN:ND2	2.51	0.44
1:A:165:GLU:H	1:A:165:GLU:CD	2.22	0.43
1:A:55:ASN:HD22	1:A:122:LYS:NZ	2.16	0.43
1:B:142:ILE:HD11	1:B:186:LEU:HD13	1.99	0.43
1:B:21:ASN:ND2	1:B:101:GLU:CG	2.82	0.43
1:D:29:VAL:HG13	1:D:34:SER:C	2.39	0.43
1:D:84:GLU:CD	1:D:176:ASN:HD21	2.21	0.43
1:B:40:TYR:HA	1:B:43:PHE:O	2.18	0.43
1:B:28:ILE:HD13	1:B:49:LEU:CD2	2.47	0.43
1:A:103:TYR:CZ	1:A:116:MET:HE2	2.54	0.43
1:D:73:LYS:HG3	1:D:74:THR:N	2.32	0.43
1:D:166:GLN:HG2	1:D:166:GLN:H	1.55	0.43
1:D:96:GLN:HG3	1:E:162:PHE:CE2	2.53	0.43
1:D:96:GLN:HG3	1:E:162:PHE:HE2	1.84	0.43
1:D:3:LEU:HD13	1:D:3:LEU:O	2.19	0.43
1:B:147:ALA:O	1:B:151:ILE:HG13	2.19	0.42
1:B:3:LEU:C	1:B:3:LEU:HD13	2.39	0.42
1:E:179:SER:O	1:E:183:LEU:HB2	2.19	0.42
1:D:127:TYR:CE2	1:D:153:ALA:HA	2.53	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:93:TYR:N	1:D:94:PRO:CD	2.82	0.42
1:D:57:GLU:HG3	1:D:95:LEU:HD12	2.01	0.42
1:D:156:VAL:HG13	1:D:175:MET:CE	2.49	0.42
1:D:108:LYS:O	1:D:110:ASN:N	2.52	0.42
1:B:14:LEU:CD2	1:B:27:GLU:HG2	2.46	0.42
1:B:93:TYR:N	1:B:94:PRO:CD	2.82	0.42
1:D:52:GLU:O	1:D:56:ILE:HG12	2.20	0.42
1:D:142:ILE:CD1	1:D:186:LEU:HD13	2.41	0.42
1:D:57:GLU:HG3	1:D:95:LEU:CD1	2.49	0.42
1:E:122:LYS:C	1:E:124:ILE:H	2.22	0.42
1:E:65:TRP:CH2	1:E:82:TYR:HB2	2.55	0.41
1:D:36:LYS:HG3	1:D:40:TYR:CD1	2.55	0.41
1:D:183:LEU:HA	1:D:183:LEU:HD23	1.88	0.41
1:A:134:GLY:HA3	1:A:140:TRP:NE1	2.35	0.41
1:A:142:ILE:CD1	1:A:186:LEU:HD13	2.42	0.41
1:B:114:GLU:C	1:B:114:GLU:OE1	2.59	0.41
1:E:108:LYS:CE	1:E:108:LYS:H	2.34	0.41
1:B:15:PHE:CD1	1:B:50:PHE:HD2	2.38	0.41
1:B:35:SER:HB3	1:B:38:ASN:OD1	2.20	0.41
1:D:6:LYS:O	1:D:10:VAL:HG23	2.21	0.41
1:B:16:ILE:HG13	1:B:95:LEU:CD2	2.51	0.41
1:E:122:LYS:C	1:E:124:ILE:N	2.74	0.41
1:E:8:LEU:HA	1:E:8:LEU:HD23	1.91	0.41
1:B:45:THR:H	1:B:48:ASN:HB2	1.85	0.41
1:E:14:LEU:HD23	1:E:14:LEU:HA	1.88	0.41
1:E:87:LEU:HD23	1:E:160:VAL:HG22	2.03	0.41
1:D:123:TYR:OH	1:D:157:ASN:HB2	2.21	0.40
1:D:127:TYR:O	1:D:131:PHE:HD2	2.03	0.40
1:B:8:LEU:CD2	1:B:43:PHE:CZ	3.01	0.40
1:E:108:LYS:HE3	1:E:108:LYS:CA	2.52	0.40
1:B:144:ASP:OD2	1:B:144:ASP:N	2.53	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:42:HIS:CE1	1:B:42:HIS:CE1[8_445]	2.08	0.12

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	184/194 (95%)	172 (94%)	10 (5%)	2 (1%)	21	41
1	B	184/194 (95%)	150 (82%)	27 (15%)	7 (4%)	5	6
1	D	184/194 (95%)	153 (83%)	25 (14%)	6 (3%)	6	9
1	E	184/194 (95%)	169 (92%)	13 (7%)	2 (1%)	21	41
All	All	736/776 (95%)	644 (88%)	75 (10%)	17 (2%)	10	16

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	22	ALA
1	A	164	HIS
1	E	143	ASN
1	B	44	LYS
1	B	106	TYR
1	D	109	THR
1	D	185	GLY
1	A	104	THR
1	E	164	HIS
1	B	23	THR
1	B	33	GLU
1	B	164	HIS
1	D	44	LYS
1	B	89	THR
1	D	33	GLU
1	D	184	ASN
1	D	186	LEU

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	169/177 (96%)	151 (89%)	18 (11%)	10	17
1	B	169/177 (96%)	143 (85%)	26 (15%)	4	6
1	D	169/177 (96%)	151 (89%)	18 (11%)	10	17
1	E	169/177 (96%)	149 (88%)	20 (12%)	8	14
All	All	676/708 (96%)	594 (88%)	82 (12%)	7	13

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	6	LYS
1	B	23	THR
1	B	36	LYS
1	B	39	LEU
1	B	51	LEU
1	B	58	GLU
1	B	64	GLN
1	B	73	LYS
1	B	85	LEU
1	B	89	THR
1	B	107	TYR
1	B	109	THR
1	B	110	ASN
1	B	114	GLU
1	B	116	MET
1	B	118	LYS
1	B	120	GLU
1	B	124	ILE
1	B	128	HIS
1	B	140	TRP
1	B	146	ASN
1	B	157	ASN
1	B	165	GLU
1	B	167	ASN
1	B	173	LYS
1	B	180	GLN
1	D	2	ASN
1	D	3	LEU
1	D	31	LEU
1	D	89	THR
1	D	97	ASN
1	D	104	THR
1	D	108	LYS

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Mol	Chain	Res	Type
1	D	109	THR
1	D	116	MET
1	D	120	GLU
1	D	124	ILE
1	D	141	SER
1	D	150	LYS
1	D	161	THR
1	D	167	ASN
1	D	170	GLU
1	D	177	LYS
1	D	184	ASN
1	A	30	LYS
1	A	44	LYS
1	A	48	ASN
1	A	54	LEU
1	A	85	LEU
1	A	89	THR
1	A	90	GLU
1	A	105	GLU
1	A	113	ASN
1	A	115	LYS
1	A	116	MET
1	A	118	LYS
1	A	136	LEU
1	A	143	ASN
1	A	157	ASN
1	A	165	GLU
1	A	167	ASN
1	A	173	LYS
1	E	25	THR
1	E	29	VAL
1	E	30	LYS
1	E	47	GLU
1	E	54	LEU
1	E	55	ASN
1	E	58	GLU
1	E	76	ARG
1	E	85	LEU
1	E	100	ILE
1	E	105	GLU
1	E	108	LYS
1	E	123	TYR

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Mol	Chain	Res	Type
1	E	161	THR
1	E	164	HIS
1	E	165	GLU
1	E	167	ASN
1	E	170	GLU
1	E	183	LEU
1	E	184	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	21	ASN
1	B	48	ASN
1	B	83	ASN
1	B	96	GLN
1	B	97	ASN
1	B	110	ASN
1	B	121	ASN
1	B	154	ASN
1	B	157	ASN
1	B	164	HIS
1	B	167	ASN
1	D	2	ASN
1	D	18	ASN
1	D	75	ASN
1	D	83	ASN
1	D	96	GLN
1	D	121	ASN
1	D	143	ASN
1	D	154	ASN
1	D	167	ASN
1	D	176	ASN
1	A	21	ASN
1	A	38	ASN
1	A	55	ASN
1	A	64	GLN
1	A	69	GLN
1	A	83	ASN
1	A	96	GLN
1	A	113	ASN
1	A	121	ASN
1	A	143	ASN

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Mol	Chain	Res	Type
1	A	164	HIS
1	A	166	GLN
1	A	180	GLN
1	A	184	ASN
1	E	18	ASN
1	E	62	GLN
1	E	83	ASN
1	E	96	GLN
1	E	97	ASN
1	E	121	ASN
1	E	143	ASN
1	E	184	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

23 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	$\# Z > 2$
3	SO4	A	199	-	4,4,4	0.17	0	6,6,6	0.17	0
2	PNT	A	225	-	26,26,26	3.57	8 (30%)	33,33,33	1.59	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	279	-	4,4,4	0.17	0	6,6,6	0.08	0
3	SO4	A	399	-	4,4,4	0.24	0	6,6,6	0.13	0
3	SO4	A	579	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	A	699	-	4,4,4	0.25	0	6,6,6	0.15	0
3	SO4	B	259	-	4,4,4	0.21	0	6,6,6	0.26	0
3	SO4	B	269	-	4,4,4	0.23	0	6,6,6	0.11	0
3	SO4	B	299	-	4,4,4	0.21	0	6,6,6	0.08	0
3	SO4	D	219	-	4,4,4	0.27	0	6,6,6	0.07	0
3	SO4	D	229	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	D	289	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	D	499	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	D	539	-	4,4,4	0.26	0	6,6,6	0.07	0
3	SO4	D	639	-	4,4,4	0.27	0	6,6,6	0.10	0
3	SO4	D	779	-	4,4,4	0.21	0	6,6,6	0.12	0
3	SO4	D	799	-	4,4,4	0.31	0	6,6,6	0.14	0
3	SO4	E	209	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	E	239	-	4,4,4	0.28	0	6,6,6	0.24	0
3	SO4	E	249	-	4,4,4	0.26	0	6,6,6	0.09	0
3	SO4	E	599	-	4,4,4	0.28	0	6,6,6	0.13	0
3	SO4	E	899	-	4,4,4	0.12	0	6,6,6	0.12	0
3	SO4	E	999	-	4,4,4	0.25	0	6,6,6	0.11	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
3	SO4	A	199	-	-	0/0/0/0	0/0/0/0
2	PNT	A	225	-	-	0/18/18/18	0/2/2/2
3	SO4	A	279	-	-	0/0/0/0	0/0/0/0
3	SO4	A	399	-	-	0/0/0/0	0/0/0/0
3	SO4	A	579	-	-	0/0/0/0	0/0/0/0
3	SO4	A	699	-	-	0/0/0/0	0/0/0/0
3	SO4	B	259	-	-	0/0/0/0	0/0/0/0
3	SO4	B	269	-	-	0/0/0/0	0/0/0/0
3	SO4	B	299	-	-	0/0/0/0	0/0/0/0
3	SO4	D	219	-	-	0/0/0/0	0/0/0/0
3	SO4	D	229	-	-	0/0/0/0	0/0/0/0
3	SO4	D	289	-	-	0/0/0/0	0/0/0/0
3	SO4	D	499	-	-	0/0/0/0	0/0/0/0
3	SO4	D	539	-	-	0/0/0/0	0/0/0/0
3	SO4	D	639	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	D	779	-	-	0/0/0/0	0/0/0/0
3	SO4	D	799	-	-	0/0/0/0	0/0/0/0
3	SO4	E	209	-	-	0/0/0/0	0/0/0/0
3	SO4	E	239	-	-	0/0/0/0	0/0/0/0
3	SO4	E	249	-	-	0/0/0/0	0/0/0/0
3	SO4	E	599	-	-	0/0/0/0	0/0/0/0
3	SO4	E	899	-	-	0/0/0/0	0/0/0/0
3	SO4	E	999	-	-	0/0/0/0	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	225	PNT	C4-C9	-12.38	1.36	1.49
2	A	225	PNT	C4'-C9'	-9.92	1.39	1.49
2	A	225	PNT	C3-C4	3.72	1.45	1.39
2	A	225	PNT	C9'-N2'	3.60	1.41	1.34
2	A	225	PNT	C9'-N1'	3.01	1.36	1.27
2	A	225	PNT	C3'-C4'	2.85	1.44	1.39
2	A	225	PNT	C6-C1	2.76	1.44	1.38
2	A	225	PNT	C6'-C1'	2.11	1.43	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	225	PNT	O1-C7-C8	-4.21	91.88	108.42
2	A	225	PNT	C10-C8-C7	-3.72	95.57	113.58
2	A	225	PNT	C7'-O1'-C1'	-3.11	110.03	117.94
2	A	225	PNT	C4'-C9'-N2'	2.86	122.51	117.99
2	A	225	PNT	C4-C9-N2	2.52	121.96	117.99
2	A	225	PNT	C10-C8'-C7'	-2.14	103.20	113.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	186/194 (95%)	0.70	8 (4%) 34 30	41, 59, 107, 126	0
1	B	186/194 (95%)	1.14	28 (15%) 3 2	46, 84, 165, 175	0
1	D	186/194 (95%)	0.71	14 (7%) 14 11	53, 84, 115, 127	0
1	E	186/194 (95%)	0.65	6 (3%) 45 42	46, 70, 104, 118	0
All	All	744/776 (95%)	0.80	56 (7%) 12 11	41, 72, 126, 175	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	112	ILE	11.5
1	B	34	SER	8.9
1	B	108	LYS	8.0
1	B	41	TYR	6.5
1	B	40	TYR	5.1
1	B	39	LEU	5.0
1	B	42	HIS	4.7
1	A	187	SER	4.4
1	B	103	TYR	4.3
1	B	110	ASN	3.8
1	B	107	TYR	3.7
1	B	117	ASN	3.4
1	A	164	HIS	3.3
1	B	116	MET	3.2
1	A	112	ILE	3.2
1	B	187	SER	3.2
1	D	3	LEU	3.0
1	A	113	ASN	3.0
1	E	123	TYR	3.0
1	D	186	LEU	2.9
1	E	142	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	36	LYS	2.9
1	B	35	SER	2.8
1	D	112	ILE	2.8
1	B	115	LYS	2.7
1	A	107	TYR	2.6
1	B	111	SER	2.6
1	D	36	LYS	2.6
1	B	120	GLU	2.6
1	B	32	SER	2.5
1	B	7	ILE	2.5
1	B	4	LYS	2.4
1	B	3	LEU	2.4
1	D	73	LYS	2.4
1	B	13	GLU	2.4
1	B	106	TYR	2.4
1	B	29	VAL	2.3
1	E	145	VAL	2.3
1	D	115	LYS	2.3
1	E	130	ILE	2.3
1	A	103	TYR	2.3
1	E	61	TRP	2.2
1	D	123	TYR	2.2
1	D	116	MET	2.1
1	B	91	TYR	2.1
1	A	168	ILE	2.1
1	D	119	LEU	2.1
1	D	77	GLU	2.1
1	B	2	ASN	2.1
1	D	7	ILE	2.1
1	D	39	LEU	2.1
1	B	45	THR	2.1
1	D	140	TRP	2.1
1	E	112	ILE	2.1
1	D	54	LEU	2.0
1	A	108	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	SO4	A	579	5/5	0.46	18.24	188,188,189,189	0
3	SO4	E	899	5/5	0.49	16.20	182,185,186,186	0
3	SO4	E	999	5/5	0.35	13.58	134,135,137,137	0
3	SO4	B	299	5/5	0.57	8.30	198,199,199,199	0
3	SO4	D	639	5/5	0.49	7.70	198,199,199,200	0
3	SO4	A	199	5/5	0.45	6.64	142,143,146,146	0
3	SO4	B	259	5/5	0.40	4.23	142,144,145,146	0
3	SO4	A	279	5/5	0.30	3.79	150,152,155,155	0
3	SO4	E	239	5/5	0.33	2.09	123,125,129,132	0
2	PNT	A	225	25/25	0.27	1.06	58,68,85,98	0
3	SO4	D	289	5/5	0.31	0.82	172,173,173,174	0
3	SO4	E	249	5/5	0.23	0.78	181,182,182,183	0
3	SO4	A	399	5/5	0.21	0.64	140,142,142,144	0
3	SO4	D	229	5/5	0.27	0.07	185,186,186,186	0
3	SO4	B	269	5/5	0.21	-0.41	179,179,180,181	0
3	SO4	A	699	5/5	0.19	-0.64	117,120,126,127	0
3	SO4	E	209	5/5	0.18	-0.72	171,171,172,172	0
3	SO4	D	539	5/5	0.17	-1.03	186,186,187,187	0
3	SO4	D	219	5/5	0.14	-1.37	155,155,156,156	0
3	SO4	D	799	5/5	0.19	-1.41	148,149,149,150	0
3	SO4	E	599	5/5	0.17	-1.77	136,138,139,139	0
3	SO4	D	499	5/5	0.16	-1.94	166,166,167,167	0
3	SO4	D	779	5/5	0.21	-3.75	173,173,174,174	0

6.5 Other polymers ⓘ

There are no such residues in this entry.