



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:02 PM GMT

PDB ID : 3VVZ
Title : Crystal Structure of The Rhodamine 6G-Bound Form of RamR (Transcriptional Regulator of TetR Family) from Salmonella Typhimurium
Authors : Sakurai, K.; Nikaido, E.; Nakashima, R.; Yamasaki, S.; Yamaguchi, A.; Nishino, K.
Deposited on : 2012-07-30
Resolution : 2.51 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 (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

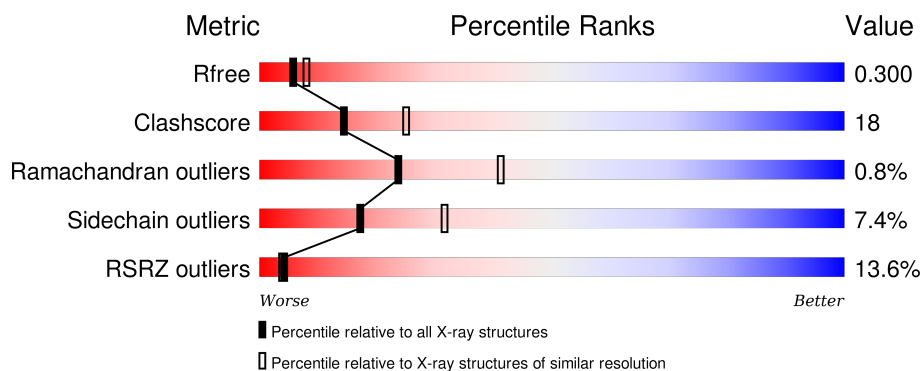
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	194	<div> <div>6%</div> <div>62%</div> <div>27%</div> <div>5%</div> <div>5%</div> </div>
1	B	194	<div> <div>25%</div> <div>52%</div> <div>36%</div> <div>7%</div> <div>5%</div> </div>
1	C	194	<div> <div>8%</div> <div>59%</div> <div>32%</div> <div>•</div> <div>5%</div> </div>
1	D	194	<div> <div>13%</div> <div>65%</div> <div>28%</div> <div>•</div> <div>5%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6038 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.

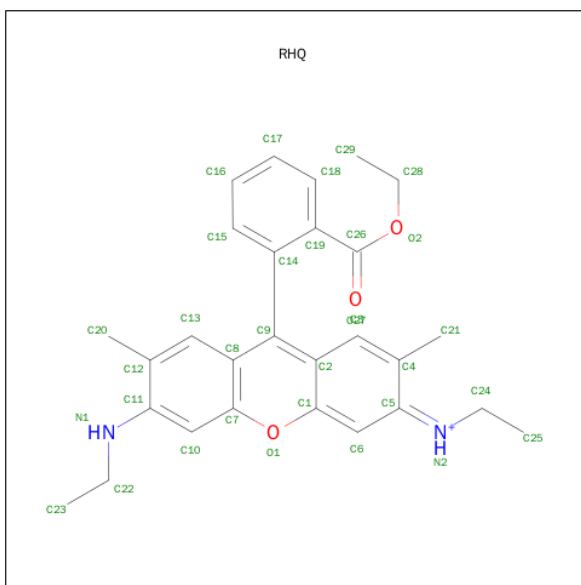
- Molecule 1 is a protein called Putative regulatory protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	184	Total	C	N	O	S	0	0	0
			1462	922	258	271	11			
1	B	184	Total	C	N	O	S	0	0	0
			1462	922	258	271	11			
1	C	184	Total	C	N	O	S	0	0	0
			1462	922	258	271	11			
1	D	184	Total	C	N	O	S	0	0	0
			1462	922	258	271	11			

There are 8 discrepancies between the modelled and reference sequences:

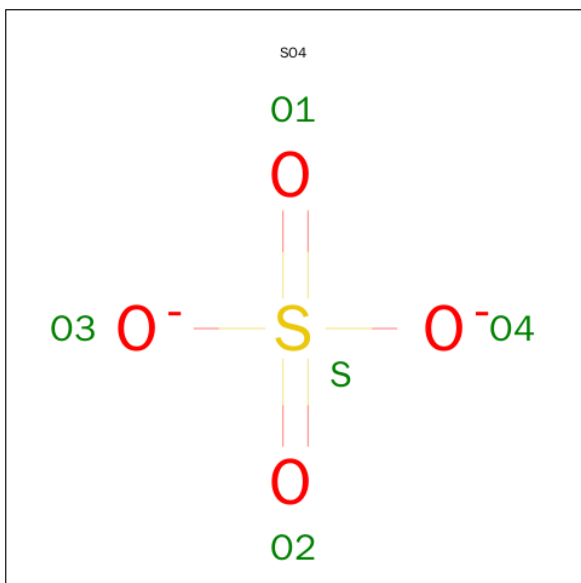
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP D0ZP76
A	1	VAL	-	EXPRESSION TAG	UNP D0ZP76
B	0	MET	-	EXPRESSION TAG	UNP D0ZP76
B	1	VAL	-	EXPRESSION TAG	UNP D0ZP76
C	0	MET	-	EXPRESSION TAG	UNP D0ZP76
C	1	VAL	-	EXPRESSION TAG	UNP D0ZP76
D	0	MET	-	EXPRESSION TAG	UNP D0ZP76
D	1	VAL	-	EXPRESSION TAG	UNP D0ZP76

- Molecule 2 is RHODAMINE 6G (three-letter code: RHQ) (formula: C₂₈H₃₁N₂O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			33	28	2	3		
2	B	1	Total	C	N	O	0	0
			33	28	2	3		
2	C	1	Total	C	N	O	0	0
			33	28	2	3		
2	D	1	Total	C	N	O	0	0
			33	28	2	3		

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



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

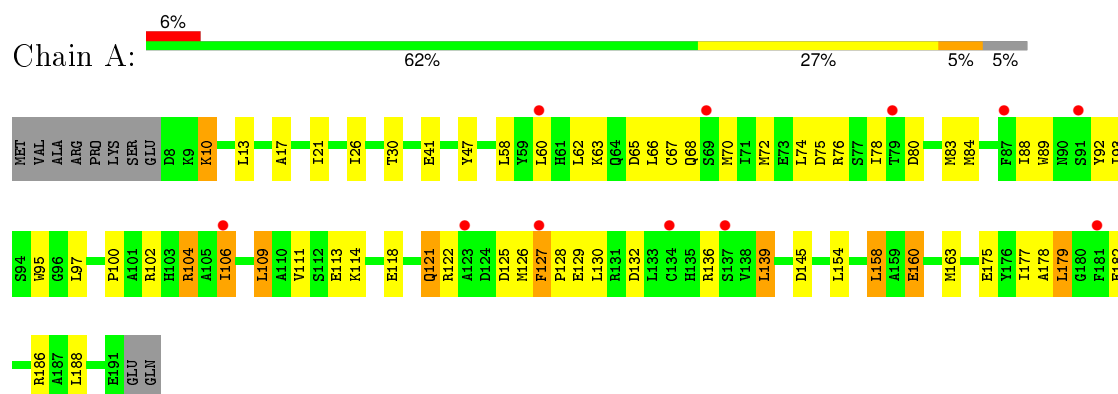
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	13	Total O 13 13	0	0
4	B	8	Total O 8 8	0	0
4	C	8	Total O 8 8	0	0
4	D	9	Total O 9 9	0	0

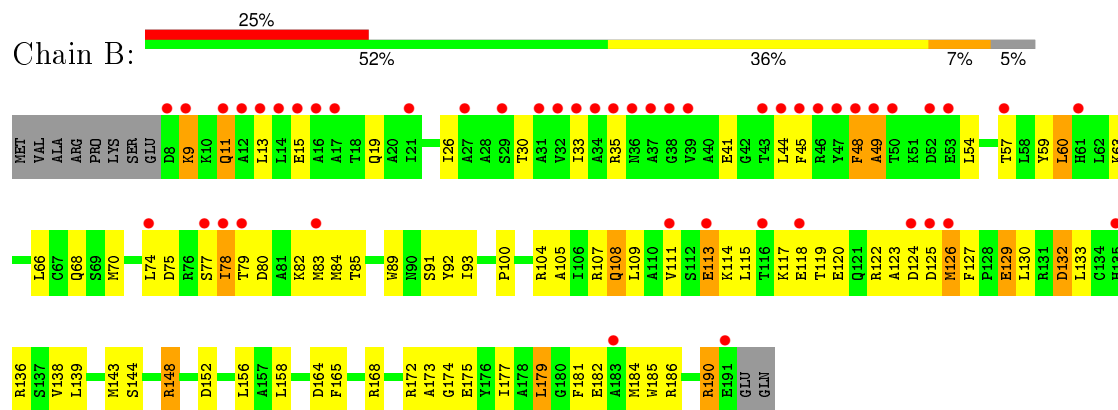
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ($\text{RSRZ} > 2$). 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.

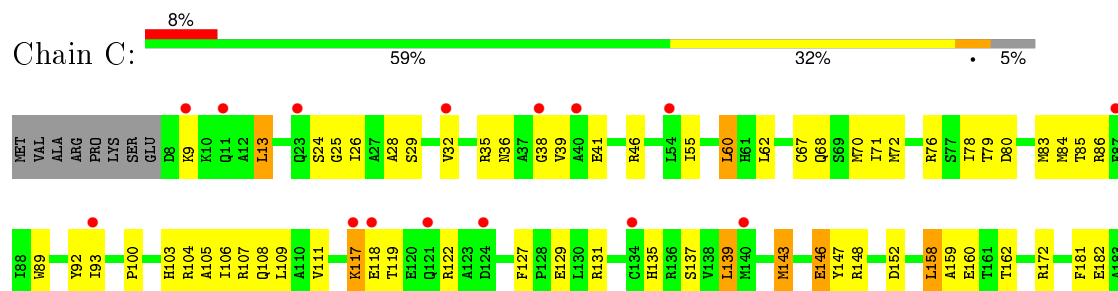
• Molecule 1: Putative regulatory protein

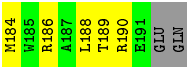


• Molecule 1: Putative regulatory protein

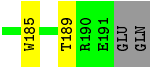
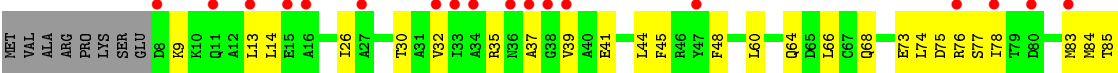


• Molecule 1: Putative regulatory protein





● Molecule 1: Putative regulatory protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	43.72Å 54.33Å 92.30Å 104.54° 97.32° 90.00°	Depositor
Resolution (Å)	44.28 – 2.51 40.88 – 2.51	Depositor EDS
% Data completeness (in resolution range)	97.6 (44.28-2.51) 90.0 (40.88-2.51)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.74 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.262 , 0.301 0.260 , 0.300	Depositor DCC
R_{free} test set	1399 reflections (5.41%)	DCC
Wilson B-factor (Å ²)	43.8	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.0	EDS
Estimated twinning fraction	0.026 for -h,k,-k-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 27288 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6038	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: RHQ, 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	0.95	2/1488 (0.1%)	0.87	0/2006
1	B	1.23	12/1488 (0.8%)	0.87	6/2006 (0.3%)
1	C	0.89	0/1488	0.85	1/2006 (0.0%)
1	D	0.88	0/1488	0.80	0/2006
All	All	1.00	14/5952 (0.2%)	0.85	7/8024 (0.1%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	113	GLU	CD-OE2	20.38	1.48	1.25
1	B	118	GLU	CD-OE2	9.42	1.36	1.25
1	B	35	ARG	CZ-NH2	-7.99	1.22	1.33
1	B	190	ARG	CZ-NH1	7.73	1.43	1.33
1	B	49	ALA	C-O	-7.07	1.09	1.23
1	B	35	ARG	CZ-NH1	7.05	1.42	1.33
1	A	178	ALA	CA-CB	6.57	1.66	1.52
1	B	41	GLU	CD-OE2	6.51	1.32	1.25
1	A	10	LYS	CD-CE	6.13	1.66	1.51
1	B	118	GLU	CG-CD	5.44	1.60	1.51
1	B	48	PHE	CG-CD1	5.42	1.46	1.38
1	B	129	GLU	CB-CG	5.16	1.61	1.52
1	B	68	GLN	CD-NE2	5.06	1.45	1.32
1	B	113	GLU	CD-OE1	5.04	1.31	1.25

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	76	ARG	NE-CZ-NH2	10.57	125.59	120.30
1	B	35	ARG	NE-CZ-NH2	-8.51	116.05	120.30
1	B	190	ARG	NE-CZ-NH2	-8.07	116.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	107	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	B	75	ASP	CB-CG-OD1	-5.64	113.22	118.30
1	B	49	ALA	CA-C-O	5.50	131.65	120.10
1	B	49	ALA	O-C-N	-5.33	114.17	122.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1462	0	1450	43	1
1	B	1462	0	1450	64	0
1	C	1462	0	1450	67	1
1	D	1462	0	1450	47	0
2	A	33	0	31	0	0
2	B	33	0	31	4	0
2	C	33	0	31	6	0
2	D	33	0	31	5	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	1	0
4	A	13	0	0	3	0
4	B	8	0	0	1	0
4	C	8	0	0	0	0
4	D	9	0	0	0	0
All	All	6038	0	5924	214	1

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 18.

All (214) 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:25:GLY:HA2	1:C:108:GLN:OE1	1.59	1.01
1:C:158:LEU:HD11	1:D:158:LEU:HD21	1.52	0.92
1:B:122:ARG:O	1:B:126:MET:HB2	1.74	0.87
1:C:118:GLU:HB2	1:C:122:ARG:HH12	1.42	0.85
1:C:70:MET:HE3	1:C:92:TYR:HB2	1.57	0.84
1:D:13:LEU:HD11	1:D:39:VAL:HG21	1.63	0.80
1:C:158:LEU:CD1	1:D:158:LEU:HD21	2.14	0.78
1:C:32:VAL:HG12	1:C:36:ASN:HD21	1.47	0.77
1:A:84:MET:O	1:A:88:ILE:HG12	1.87	0.74
1:C:24:SER:HB2	1:C:28:ALA:HB2	1.70	0.73
1:C:70:MET:CE	1:C:92:TYR:HB2	2.21	0.71
1:B:130:LEU:HD12	1:B:133:LEU:HD23	1.72	0.70
1:B:74:LEU:HD21	1:B:129:GLU:OE1	1.92	0.70
1:D:152:ASP:HB3	2:D:301:RHQ:H212	1.75	0.69
1:B:138:VAL:HB	1:B:143:MET:HE1	1.73	0.69
1:C:9:LYS:HD2	1:C:39:VAL:HG11	1.74	0.69
1:B:138:VAL:HB	1:B:143:MET:CE	2.24	0.68
1:C:32:VAL:HG12	1:C:36:ASN:ND2	2.09	0.67
1:B:182:GLU:HG3	1:B:186:ARG:NH1	2.10	0.67
1:A:30:THR:HG22	4:A:403:HOH:O	1.94	0.67
1:A:17:ALA:O	1:A:21:ILE:HG12	1.95	0.66
1:C:84:MET:HE3	1:C:84:MET:HA	1.78	0.65
1:B:78:ILE:HD13	1:B:79:THR:H	1.61	0.64
1:C:35:ARG:O	1:C:38:GLY:N	2.30	0.64
1:B:11:GLN:HE21	1:B:11:GLN:N	1.95	0.64
1:D:60:LEU:HD21	1:D:119:THR:HG23	1.80	0.64
1:D:75:ASP:O	1:D:78:ILE:HB	1.98	0.64
1:C:107:ARG:HH11	1:C:107:ARG:HG3	1.63	0.64
1:D:152:ASP:OD1	2:D:301:RHQ:H31	1.98	0.63
1:C:117:LYS:N	1:C:117:LYS:HD3	2.13	0.63
1:B:48:PHE:CD1	1:B:57:THR:HG21	2.34	0.62
1:D:60:LEU:CD2	1:D:119:THR:HG23	2.29	0.62
1:C:118:GLU:HB2	1:C:122:ARG:NH1	2.14	0.62
1:D:13:LEU:HD12	1:D:37:ALA:HB1	1.81	0.61
1:A:62:LEU:HB3	1:A:106:ILE:HG12	1.82	0.61
1:B:85:THR:HG23	2:B:301:RHQ:HN11	1.65	0.61
1:A:30:THR:HG23	1:A:41:GLU:OE2	2.01	0.61
1:C:67:CYS:O	1:C:71:ILE:HG12	1.99	0.61
1:A:10:LYS:HG3	1:A:47:TYR:CD1	2.36	0.60
1:C:55:ILE:HG23	1:C:109:LEU:HD22	1.82	0.60
1:C:111:VAL:HG12	1:C:111:VAL:O	2.01	0.60
1:C:107:ARG:NE	1:C:160:GLU:OE1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:MET:HE2	1:D:133:LEU:HD13	1.83	0.59
1:B:59:TYR:O	1:B:63:LYS:HB2	2.03	0.59
1:B:148:ARG:HH11	1:B:148:ARG:HG3	1.68	0.58
1:A:113:GLU:OE1	1:B:168:ARG:HD3	2.04	0.58
1:C:146:GLU:HG2	1:C:147:TYR:CD2	2.39	0.57
1:A:121:GLN:HG3	1:A:122:ARG:N	2.19	0.57
1:B:30:THR:HA	1:B:33:ILE:HD12	1.85	0.57
1:C:92:TYR:OH	1:C:103:HIS:NE2	2.27	0.56
1:C:9:LYS:HD2	1:C:39:VAL:CG1	2.35	0.56
1:B:45:PHE:HA	1:B:48:PHE:O	2.05	0.56
1:D:107:ARG:HD2	1:D:160:GLU:OE2	2.05	0.56
1:A:66:LEU:HD11	1:A:92:TYR:HD1	1.70	0.56
1:C:80:ASP:HB3	1:C:83:MET:HB3	1.87	0.56
1:A:63:LYS:NZ	1:A:67:CYS:SG	2.79	0.56
1:D:66:LEU:HD11	1:D:92:TYR:HD1	1.71	0.56
1:B:148:ARG:NH1	1:B:148:ARG:HG3	2.21	0.56
1:C:89:TRP:CZ2	1:C:93:ILE:HD11	2.41	0.56
1:D:138:VAL:HB	1:D:143:MET:HE1	1.89	0.55
1:B:125:ASP:C	1:B:127:PHE:H	2.08	0.55
1:A:111:VAL:HG23	1:B:165:PHE:HZ	1.70	0.55
1:B:59:TYR:CD1	1:B:109:LEU:HB3	2.42	0.55
1:D:127:PHE:CE2	1:D:129:GLU:HB2	2.42	0.55
1:C:139:LEU:CD1	1:C:190:ARG:HA	2.36	0.55
1:B:30:THR:N	4:B:407:HOH:O	2.29	0.55
1:A:118:GLU:OE1	1:A:118:GLU:N	2.39	0.55
1:A:128:PRO:HB2	4:A:408:HOH:O	2.06	0.54
1:A:65:ASP:OD2	1:A:102:ARG:NH1	2.40	0.54
1:C:78:ILE:CG2	1:C:83:MET:HG2	2.37	0.54
1:A:76:ARG:NH2	1:A:129:GLU:OE1	2.41	0.54
1:B:70:MET:HG2	1:B:91:SER:HB2	1.91	0.53
1:B:63:LYS:HE3	1:B:123:ALA:HB1	1.90	0.53
1:D:45:PHE:HA	1:D:48:PHE:O	2.09	0.53
1:B:173:ALA:O	1:B:177:ILE:HG13	2.09	0.52
1:D:76:ARG:C	1:D:78:ILE:H	2.12	0.52
1:B:144:SER:O	1:B:148:ARG:HB2	2.09	0.52
1:C:29:SER:HB3	1:C:32:VAL:HG23	1.92	0.52
1:B:125:ASP:O	1:B:127:PHE:N	2.43	0.52
1:C:62:LEU:HB3	1:C:106:ILE:HD12	1.92	0.52
1:A:68:GLN:O	1:A:72:MET:HG3	2.09	0.52
1:B:66:LEU:HD11	1:B:92:TYR:HD1	1.74	0.52
1:A:74:LEU:HD12	1:A:84:MET:HE1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:LEU:HD13	1:C:189:THR:O	2.10	0.51
1:A:132:ASP:HB3	1:A:136:ARG:HH12	1.76	0.51
1:B:113:GLU:C	1:B:115:LEU:H	2.14	0.51
1:A:93:ILE:HG21	1:A:177:ILE:HG12	1.93	0.51
1:C:60:LEU:HD13	1:C:119:THR:HG23	1.93	0.51
1:D:78:ILE:HD11	1:D:84:MET:HA	1.93	0.50
1:B:111:VAL:HG23	1:B:111:VAL:O	2.11	0.50
1:D:151:GLY:O	2:D:301:RHQ:H161	2.12	0.50
1:A:100:PRO:O	1:A:104:ARG:HD3	2.11	0.50
1:C:9:LYS:O	1:C:13:LEU:HD22	2.11	0.50
1:B:13:LEU:HD22	1:B:44:LEU:HD12	1.93	0.50
1:D:78:ILE:HG23	1:D:78:ILE:O	2.12	0.50
1:B:45:PHE:HD1	1:B:49:ALA:O	1.95	0.50
1:A:160:GLU:HA	1:A:163:MET:HE1	1.93	0.50
1:A:58:LEU:HD23	1:A:109:LEU:HD21	1.94	0.50
1:A:26:ILE:HD12	1:A:114:LYS:HE2	1.94	0.49
1:D:138:VAL:HB	1:D:143:MET:CE	2.42	0.49
1:D:89:TRP:CD1	1:D:181:PHE:HB2	2.47	0.49
1:C:139:LEU:HD12	1:C:190:ARG:HA	1.95	0.49
1:A:75:ASP:HB3	1:A:78:ILE:HG13	1.93	0.49
1:D:26:ILE:CD1	1:D:109:LEU:HD12	2.42	0.49
1:D:106:ILE:HG22	1:D:107:ARG:N	2.28	0.49
1:A:111:VAL:HG23	1:B:165:PHE:CZ	2.46	0.49
1:B:11:GLN:O	1:B:15:GLU:HB2	2.13	0.48
1:C:143:MET:CE	2:C:301:RHQ:H181	2.44	0.48
1:B:85:THR:OG1	1:B:133:LEU:HD21	2.12	0.48
1:C:146:GLU:HG3	1:C:147:TYR:CE2	2.49	0.48
1:A:121:GLN:NE2	1:A:125:ASP:OD2	2.46	0.48
1:B:26:ILE:HG12	1:B:108:GLN:HB3	1.94	0.48
1:C:89:TRP:CE2	1:C:93:ILE:HD11	2.48	0.48
1:D:64:GLN:HE21	1:D:68:GLN:CD	2.17	0.48
1:A:182:GLU:HB3	1:A:186:ARG:HH12	1.79	0.48
2:C:301:RHQ:O27	2:C:301:RHQ:C9	2.62	0.48
1:A:26:ILE:CD1	1:A:114:LYS:HE2	2.44	0.47
1:D:85:THR:HG23	2:D:301:RHQ:HN11	1.80	0.47
1:A:127:PHE:HD1	1:A:130:LEU:H	1.60	0.47
1:C:68:GLN:O	1:C:72:MET:HG3	2.14	0.47
1:C:137:SER:O	1:C:190:ARG:HG2	2.14	0.47
1:C:26:ILE:HD11	1:C:108:GLN:C	2.35	0.47
1:C:146:GLU:CG	1:C:147:TYR:CE2	2.98	0.47
1:D:73:GLU:OE1	1:D:91:SER:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:ARG:HH11	1:C:46:ARG:HG2	1.80	0.47
1:D:75:ASP:N	1:D:87:PHE:HE2	2.11	0.47
1:B:120:GLU:O	1:B:124:ASP:N	2.48	0.47
1:B:80:ASP:HB3	1:B:83:MET:HB2	1.97	0.47
1:B:84:MET:HE2	1:B:133:LEU:HD22	1.97	0.46
1:D:107:ARG:HG3	1:D:156:LEU:HB3	1.97	0.46
1:B:152:ASP:OD1	2:B:301:RHQ:H31	2.16	0.46
1:C:84:MET:CE	1:C:84:MET:HA	2.45	0.46
1:C:70:MET:HE3	1:C:92:TYR:CB	2.38	0.46
1:C:107:ARG:CG	1:C:107:ARG:HH11	2.29	0.46
1:C:93:ILE:CD1	1:C:162:THR:HG21	2.46	0.46
1:B:132:ASP:O	1:B:136:ARG:HG3	2.16	0.46
1:D:32:VAL:HG22	1:D:35:ARG:HH22	1.80	0.46
1:A:126:MET:C	1:A:128:PRO:HD3	2.36	0.45
1:B:117:LYS:HA	1:B:120:GLU:HG2	1.97	0.45
1:B:100:PRO:HB2	1:B:104:ARG:HH21	1.82	0.45
1:C:117:LYS:HD3	1:C:117:LYS:H	1.81	0.45
1:A:111:VAL:O	1:A:111:VAL:HG22	2.16	0.45
1:D:9:LYS:O	1:D:13:LEU:HD13	2.16	0.45
1:C:117:LYS:NZ	1:C:117:LYS:H	2.14	0.45
1:B:138:VAL:HB	1:B:143:MET:HE2	1.99	0.45
1:B:175:GLU:O	1:B:179:LEU:HB2	2.16	0.45
1:D:74:LEU:HD11	1:D:78:ILE:HG12	1.98	0.44
1:A:129:GLU:HG3	4:A:408:HOH:O	2.17	0.44
1:B:105:ALA:O	1:B:109:LEU:HD13	2.17	0.44
1:D:13:LEU:HD11	1:D:39:VAL:CG2	2.40	0.44
1:B:108:GLN:OE1	1:B:108:GLN:N	2.50	0.44
1:C:172:ARG:HH11	1:C:172:ARG:HG3	1.82	0.44
1:A:76:ARG:C	1:A:78:ILE:N	2.71	0.44
1:D:64:GLN:NE2	1:D:68:GLN:HG3	2.32	0.44
1:D:185:TRP:CE3	1:D:189:THR:HG21	2.53	0.44
1:B:125:ASP:C	1:B:127:PHE:N	2.71	0.44
1:C:62:LEU:CB	1:C:106:ILE:HD12	2.46	0.44
1:D:13:LEU:CD2	1:D:44:LEU:HA	2.47	0.44
1:D:13:LEU:HD21	1:D:44:LEU:HA	2.00	0.44
1:A:26:ILE:HD12	1:A:114:LYS:CE	2.47	0.44
1:B:11:GLN:H	1:B:11:GLN:HE21	1.66	0.43
1:C:84:MET:O	1:C:84:MET:HE2	2.19	0.43
1:C:92:TYR:HH	1:C:103:HIS:CD2	2.30	0.43
1:C:152:ASP:OD1	2:C:301:RHQ:H31	2.19	0.43
1:C:100:PRO:CB	1:C:104:ARG:HH12	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:ARG:HG3	1:C:135:HIS:CE1	2.53	0.43
1:D:92:TYR:HE2	1:D:159:ALA:HB1	1.84	0.43
1:A:154:LEU:HD22	1:B:158:LEU:HD22	2.01	0.43
1:D:101:ALA:HB3	3:D:302:SO4:O1	2.19	0.43
1:D:84:MET:CE	1:D:133:LEU:HD13	2.49	0.43
1:C:139:LEU:HD13	1:C:189:THR:C	2.37	0.43
1:C:172:ARG:NH1	1:C:172:ARG:HG3	2.32	0.43
1:B:89:TRP:O	1:B:93:ILE:HG12	2.19	0.43
1:B:82:LYS:HD2	1:B:185:TRP:NE1	2.33	0.42
1:B:15:GLU:O	1:B:19:GLN:HG2	2.19	0.42
1:D:92:TYR:OH	1:D:103:HIS:CD2	2.72	0.42
1:B:89:TRP:CD1	1:B:181:PHE:HB2	2.54	0.42
1:C:86:ARG:HB2	1:C:181:PHE:CE2	2.53	0.42
1:B:59:TYR:HD1	1:B:109:LEU:HB3	1.84	0.42
1:D:172:ARG:O	1:D:173:ALA:C	2.58	0.42
1:B:63:LYS:HE2	2:B:301:RHQ:H253	2.01	0.42
1:C:172:ARG:CZ	1:D:146:GLU:OE2	2.68	0.42
1:D:44:LEU:HD23	1:D:44:LEU:C	2.39	0.42
1:D:173:ALA:O	1:D:177:ILE:HG13	2.20	0.42
1:C:131:ARG:HG3	1:C:135:HIS:HE1	1.84	0.42
1:A:80:ASP:HB3	1:A:83:MET:HB3	2.01	0.42
1:B:44:LEU:HD21	1:B:54:LEU:HD22	2.02	0.42
1:C:147:TYR:CE1	1:D:172:ARG:HD3	2.54	0.42
1:A:76:ARG:C	1:A:78:ILE:H	2.22	0.42
1:B:172:ARG:O	1:B:174:GLY:N	2.53	0.42
1:B:60:LEU:HD11	1:B:119:THR:HG23	2.01	0.42
1:A:66:LEU:HD13	1:A:95:TRP:CE3	2.55	0.41
1:B:85:THR:HG23	2:B:301:RHQ:N1	2.32	0.41
1:C:92:TYR:HE2	1:C:159:ALA:HB1	1.85	0.41
1:B:63:LYS:HB3	1:B:126:MET:HE1	2.02	0.41
1:D:151:GLY:C	2:D:301:RHQ:H161	2.41	0.41
2:C:301:RHQ:H221	2:C:301:RHQ:H101	1.80	0.41
1:A:158:LEU:CD1	1:B:158:LEU:HD21	2.51	0.41
1:B:82:LYS:HD2	1:B:185:TRP:CE2	2.56	0.41
1:A:179:LEU:HA	1:A:179:LEU:HD12	1.95	0.41
1:C:105:ALA:O	1:C:109:LEU:HG	2.21	0.41
1:A:89:TRP:O	1:A:93:ILE:HG12	2.20	0.41
1:C:117:LYS:HZ2	1:C:117:LYS:H	1.67	0.41
1:C:148:ARG:NH2	2:C:301:RHQ:H292	2.36	0.41
1:C:86:ARG:HA	1:C:181:PHE:CE1	2.56	0.41
1:C:143:MET:HE1	2:C:301:RHQ:H181	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:LEU:HD22	1:A:188:LEU:C	2.41	0.40
1:C:182:GLU:HB3	1:C:186:ARG:NH1	2.36	0.40
1:B:48:PHE:HD1	1:B:57:THR:HG21	1.82	0.40
1:A:66:LEU:O	1:A:70:MET:HG3	2.21	0.40
1:B:172:ARG:O	1:B:175:GLU:N	2.53	0.40
1:B:54:LEU:HA	1:B:57:THR:HG22	2.03	0.40
1:C:85:THR:O	1:C:86:ARG:C	2.59	0.40
1:D:30:THR:HG23	1:D:41:GLU:OE2	2.21	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	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ASP:OD2	1:C:79:THR:CG2[1_454]	2.00	0.20

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	182/194 (94%)	177 (97%)	5 (3%)	0	100	100
1	B	182/194 (94%)	166 (91%)	12 (7%)	4 (2%)	8	13
1	C	182/194 (94%)	177 (97%)	4 (2%)	1 (0%)	34	55
1	D	182/194 (94%)	171 (94%)	10 (6%)	1 (0%)	34	55
All	All	728/776 (94%)	691 (95%)	31 (4%)	6 (1%)	24	41

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	9	LYS
1	B	77	SER

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Mol	Chain	Res	Type
1	B	126	MET
1	D	77	SER
1	B	114	LYS
1	C	41	GLU

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	149/158 (94%)	136 (91%)	13 (9%)	13	24
1	B	149/158 (94%)	136 (91%)	13 (9%)	13	24
1	C	149/158 (94%)	138 (93%)	11 (7%)	17	31
1	D	149/158 (94%)	142 (95%)	7 (5%)	32	56
All	All	596/632 (94%)	552 (93%)	44 (7%)	17	31

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	60	LEU
1	A	97	LEU
1	A	104	ARG
1	A	106	ILE
1	A	109	LEU
1	A	121	GLN
1	A	127	PHE
1	A	139	LEU
1	A	158	LEU
1	A	160	GLU
1	A	175	GLU
1	A	179	LEU
1	B	9	LYS
1	B	11	GLN
1	B	60	LEU
1	B	78	ILE

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Mol	Chain	Res	Type
1	B	108	GLN
1	B	132	ASP
1	B	139	LEU
1	B	148	ARG
1	B	156	LEU
1	B	164	ASP
1	B	179	LEU
1	B	184	MET
1	B	190	ARG
1	C	13	LEU
1	C	60	LEU
1	C	117	LYS
1	C	127	PHE
1	C	129	GLU
1	C	139	LEU
1	C	143	MET
1	C	146	GLU
1	C	158	LEU
1	C	184	MET
1	C	188	LEU
1	D	14	LEU
1	D	83	MET
1	D	106	ILE
1	D	139	LEU
1	D	154	LEU
1	D	156	LEU
1	D	179	LEU

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

Mol	Chain	Res	Type
1	A	90	ASN
1	A	98	ASN
1	A	121	GLN
1	B	11	GLN
1	B	36	ASN
1	B	64	GLN
1	B	103	HIS
1	B	121	GLN
1	C	36	ASN
1	C	64	GLN
1	D	64	GLN

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Mol	Chain	Res	Type
1	D	90	ASN
1	D	103	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 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	RHQ	A	301	-	33,36,36	1.82	4 (12%)	40,51,51	1.80	10 (25%)
3	SO4	A	302	-	4,4,4	0.68	0	6,6,6	2.22	3 (50%)
2	RHQ	B	301	-	33,36,36	1.64	4 (12%)	40,51,51	1.66	10 (25%)
3	SO4	B	302	-	4,4,4	0.37	0	6,6,6	0.40	0
2	RHQ	C	301	-	33,36,36	1.79	5 (15%)	40,51,51	1.76	6 (15%)
3	SO4	C	302	-	4,4,4	0.36	0	6,6,6	0.34	0
2	RHQ	D	301	-	33,36,36	1.62	2 (6%)	40,51,51	1.65	10 (25%)
3	SO4	D	302	-	4,4,4	0.47	0	6,6,6	0.83	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	RHQ	A	301	-	-	0/15/21/21	0/4/4/4
3	SO4	A	302	-	-	0/0/0/0	0/0/0/0
2	RHQ	B	301	-	-	0/15/21/21	0/4/4/4
3	SO4	B	302	-	-	0/0/0/0	0/0/0/0
2	RHQ	C	301	-	-	0/15/21/21	0/4/4/4
3	SO4	C	302	-	-	0/0/0/0	0/0/0/0
2	RHQ	D	301	-	-	0/15/21/21	0/4/4/4
3	SO4	D	302	-	-	0/0/0/0	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	RHQ	C2-C1	-5.90	1.38	1.48
2	C	301	RHQ	C2-C1	-5.65	1.39	1.48
2	B	301	RHQ	C2-C1	-4.72	1.40	1.48
2	D	301	RHQ	C2-C1	-4.56	1.41	1.48
2	B	301	RHQ	C3-C4	2.14	1.41	1.37
2	C	301	RHQ	C3-C4	2.48	1.41	1.37
2	B	301	RHQ	C2-C9	2.56	1.42	1.38
2	A	301	RHQ	C24-N2	2.66	1.55	1.48
2	A	301	RHQ	O1-C1	2.73	1.38	1.35
2	C	301	RHQ	C6-C1	3.14	1.43	1.36
2	C	301	RHQ	C24-N2	3.29	1.57	1.48
2	C	301	RHQ	O2-C26	5.35	1.46	1.33
2	B	301	RHQ	O2-C26	5.75	1.47	1.33
2	D	301	RHQ	O2-C26	5.98	1.47	1.33
2	A	301	RHQ	O2-C26	6.44	1.48	1.33

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	RHQ	C24-N2-C5	-6.92	107.97	120.84
2	A	301	RHQ	C24-N2-C5	-5.35	110.89	120.84
2	A	301	RHQ	C3-C2-C9	-3.40	120.36	124.27
2	D	301	RHQ	C24-N2-C5	-3.39	114.53	120.84
2	D	301	RHQ	O2-C26-O27	-3.15	117.88	123.66
2	B	301	RHQ	C25-C24-N2	-3.12	102.26	110.31
2	B	301	RHQ	C10-C11-N1	-3.11	116.19	121.95
2	B	301	RHQ	O2-C26-O27	-2.93	118.28	123.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	RHQ	C3-C2-C9	-2.81	121.03	124.27
2	B	301	RHQ	C24-N2-C5	-2.80	115.63	120.84
2	A	301	RHQ	O2-C26-O27	-2.78	118.54	123.66
2	A	301	RHQ	C22-N1-C11	-2.71	118.58	123.44
2	C	301	RHQ	O2-C26-O27	-2.64	118.80	123.66
3	A	302	SO4	O4-S-O3	-2.55	98.60	108.98
2	D	301	RHQ	C10-C11-N1	-2.31	117.66	121.95
2	B	301	RHQ	C22-N1-C11	-2.30	119.31	123.44
2	D	301	RHQ	C18-C19-C26	-2.14	114.28	118.68
2	B	301	RHQ	C3-C2-C9	-2.13	121.82	124.27
3	A	302	SO4	O4-S-O2	-2.10	90.64	110.19
2	A	301	RHQ	C18-C19-C26	-2.04	114.48	118.68
2	D	301	RHQ	C6-C1-C2	2.05	121.49	118.52
2	D	301	RHQ	C13-C8-C7	2.06	118.89	116.42
2	C	301	RHQ	O1-C7-C10	2.18	118.95	116.18
2	C	301	RHQ	C13-C12-C11	2.20	120.27	118.25
2	D	301	RHQ	C14-C19-C26	2.33	126.65	122.86
2	A	301	RHQ	O1-C7-C10	2.33	119.15	116.18
2	A	301	RHQ	C28-O2-C26	2.43	122.07	116.46
2	D	301	RHQ	C12-C11-N1	2.45	122.52	119.52
2	C	301	RHQ	C6-C1-C2	2.60	122.27	118.52
2	B	301	RHQ	C6-C1-C2	2.62	122.31	118.52
2	A	301	RHQ	C13-C12-C11	2.64	120.68	118.25
2	B	301	RHQ	C13-C8-C7	2.67	119.61	116.42
2	B	301	RHQ	C12-C11-N1	2.94	123.13	119.52
2	A	301	RHQ	C23-C22-N1	3.05	118.88	111.61
2	A	301	RHQ	O2-C26-C19	3.78	119.03	112.16
2	B	301	RHQ	O2-C26-C19	3.86	119.19	112.16
3	A	302	SO4	O2-S-O1	4.01	122.21	109.50
2	C	301	RHQ	O2-C26-C19	4.09	119.61	112.16
2	D	301	RHQ	O2-C26-C19	4.78	120.85	112.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	RHQ	4	0
2	C	301	RHQ	6	0
2	D	301	RHQ	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	302	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	184/194 (94%)	0.65	11 (5%)	25 28	25, 41, 63, 72	12 (6%)
1	B	184/194 (94%)	1.52	48 (26%)	1 1	23, 62, 106, 109	4 (2%)
1	C	184/194 (94%)	0.80	15 (8%)	14 15	27, 49, 67, 74	5 (2%)
1	D	184/194 (94%)	1.06	26 (14%)	4 3	32, 52, 79, 92	4 (2%)
All	All	736/776 (94%)	1.01	100 (13%)	4 4	23, 49, 95, 109	25 (3%)

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	39	VAL	8.0
1	B	47	TYR	8.0
1	B	48	PHE	6.9
1	B	33	ILE	6.6
1	B	9	LYS	6.2
1	B	44	LEU	5.8
1	B	49	ALA	5.8
1	B	16	ALA	5.7
1	B	13	LEU	5.4
1	D	78	ILE	4.7
1	B	46	ARG	4.6
1	B	43	THR	4.4
1	B	36	ASN	4.2
1	B	52	ASP	4.2
1	B	34	ALA	4.0
1	B	37	ALA	4.0
1	B	57	THR	3.9
1	D	34	ALA	3.9
1	B	35	ARG	3.6
1	D	38	GLY	3.6
1	B	125	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	83	MET	3.5
1	B	50	THR	3.5
1	B	21	ILE	3.5
1	B	38	GLY	3.5
1	B	113	GLU	3.4
1	A	79	THR	3.4
1	B	32	VAL	3.4
1	D	133	LEU	3.2
1	D	83	MET	3.2
1	B	15	GLU	3.2
1	B	12	ALA	3.1
1	B	78	ILE	3.1
1	D	27	ALA	3.0
1	D	39	VAL	3.0
1	A	87	PHE	3.0
1	B	27	ALA	2.9
1	B	29	SER	2.9
1	D	140	MET	2.9
1	D	76	ARG	2.9
1	C	38	GLY	2.9
1	D	33	ILE	2.8
1	B	14	LEU	2.8
1	B	191	GLU	2.8
1	A	91	SER	2.7
1	D	47	TYR	2.7
1	D	36	ASN	2.7
1	B	61	HIS	2.7
1	B	135	HIS	2.6
1	B	79	THR	2.6
1	B	77	SER	2.6
1	D	94	SER	2.6
1	B	45	PHE	2.6
1	D	32	VAL	2.5
1	B	31	ALA	2.5
1	D	145	ASP	2.5
1	D	8	ASP	2.5
1	D	126	MET	2.5
1	C	140	MET	2.5
1	B	11	GLN	2.5
1	C	121	GLN	2.5
1	C	32	VAL	2.4
1	D	16	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	69	SER	2.4
1	A	123	ALA	2.4
1	D	11	GLN	2.4
1	B	53	GLU	2.4
1	D	37	ALA	2.4
1	A	181	PHE	2.4
1	C	11	GLN	2.4
1	B	111	VAL	2.3
1	D	159	ALA	2.3
1	A	127	PHE	2.3
1	C	134	CYS	2.3
1	B	183	ALA	2.3
1	C	9	LYS	2.3
1	B	8	ASP	2.3
1	A	106	ILE	2.2
1	D	80	ASP	2.2
1	D	136	ARG	2.2
1	C	117	LYS	2.2
1	C	23	GLN	2.2
1	A	134	CYS	2.2
1	C	87	PHE	2.2
1	D	124	ASP	2.2
1	B	126	MET	2.1
1	C	118	GLU	2.1
1	B	124	ASP	2.1
1	C	124	ASP	2.1
1	C	54	LEU	2.1
1	D	15	GLU	2.1
1	A	60	LEU	2.1
1	D	13	LEU	2.1
1	C	93	ILE	2.0
1	B	17	ALA	2.0
1	B	74	LEU	2.0
1	A	137	SER	2.0
1	C	40	ALA	2.0
1	B	118	GLU	2.0
1	B	116	THR	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 [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	RHQ	B	301	33/33	0.80	0.29	1.62	62,69,76,76	0
2	RHQ	D	301	33/33	0.87	0.24	1.17	64,67,72,74	0
2	RHQ	A	301	33/33	0.85	0.25	0.84	53,57,62,64	0
2	RHQ	C	301	33/33	0.86	0.24	0.77	51,56,61,62	0
3	SO4	A	302	5/5	0.97	0.13	-0.93	45,47,50,51	0
3	SO4	C	302	5/5	0.95	0.12	-0.96	53,54,59,59	0
3	SO4	B	302	5/5	0.92	0.12	-1.24	80,81,81,82	0
3	SO4	D	302	5/5	0.98	0.11	-1.39	60,61,64,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.