



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:12 PM GMT

PDB ID : 3WG9  
Title : Crystal structure of RSP, a Rex-family repressor  
Authors : Zheng, Y.; Ko, T.-P.; Guo, R.-T.  
Deposited on : 2013-08-03  
Resolution : 1.97 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

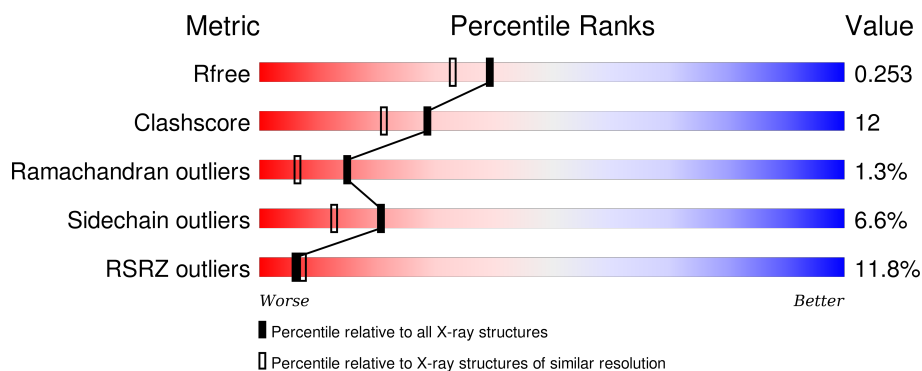
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.97 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	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)

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

Mol	Chain	Length	Quality of chain
1	A	224	<div> <div>15%</div> <div>75%</div> <div>16%</div> <div>7%</div> </div>
1	B	224	<div> <div>11%</div> <div>72%</div> <div>18%</div> <div>5%</div> </div>
1	C	224	<div> <div>12%</div> <div>74%</div> <div>16%</div> <div>8%</div> </div>
1	D	224	<div> <div>7%</div> <div>73%</div> <div>16%</div> <div>7%</div> </div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	902	-	-	X	-
2	SO4	D	301	-	-	X	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7554 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 Redox-sensing transcriptional repressor rex.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	0
			1682	1076	289	313	4			
1	B	212	Total	C	N	O	S	0	0	0
			1706	1091	293	318	4			
1	C	207	Total	C	N	O	S	0	0	0
			1666	1065	287	310	4			
1	D	209	Total	C	N	O	S	0	0	0
			1682	1075	289	314	4			

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



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

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

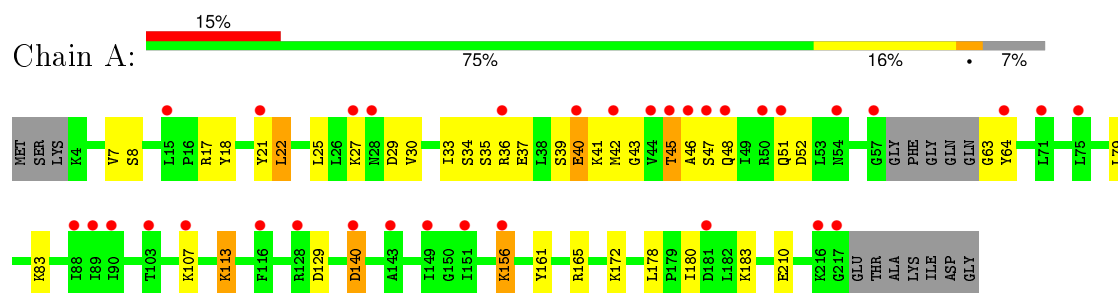
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	174	Total	O	0	0
			174	174		
3	B	223	Total	O	0	0
			223	223		
3	C	180	Total	O	0	0
			180	180		
3	D	216	Total	O	0	0
			216	216		

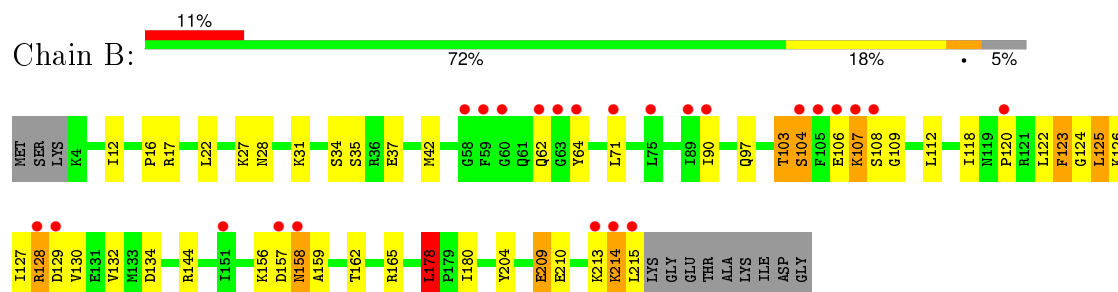
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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.

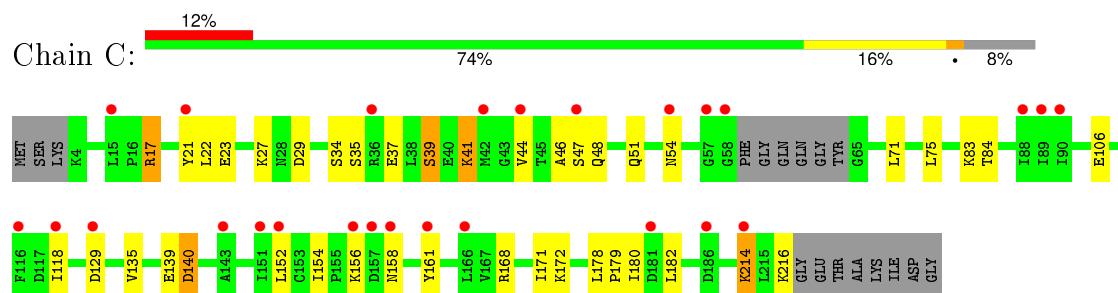
- Molecule 1: Redox-sensing transcriptional repressor rex



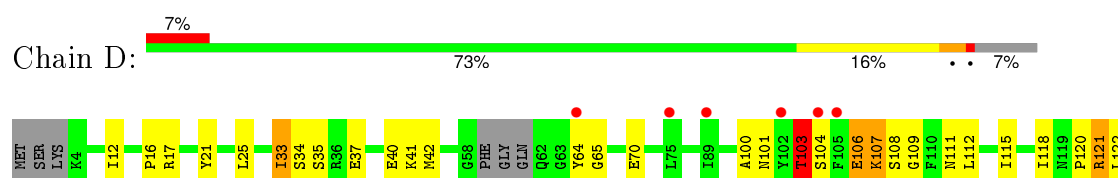
- Molecule 1: Redox-sensing transcriptional repressor rex

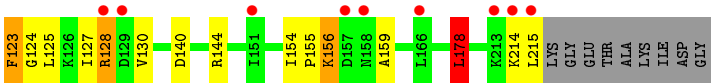


- Molecule 1: Redox-sensing transcriptional repressor rex



- Molecule 1: Redox-sensing transcriptional repressor rex





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.41 Å 90.10 Å 171.64 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 1.97 25.00 – 1.97	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.00-1.97) 96.1 (25.00-1.97)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.12 (at 1.98 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.198 , 0.252 0.201 , 0.253	Depositor DCC
$R_{free}$ test set	3945 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.7	Xtriage
Anisotropy	0.712	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 77797 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7554	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	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 41.80 % 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 2.2397e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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



## 5 Model quality

### 5.1 Standard geometry

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	0.76	0/1707	0.89	2/2300 (0.1%)
1	B	0.80	0/1733	0.92	3/2337 (0.1%)
1	C	0.73	0/1690	0.83	0/2277
1	D	0.78	0/1707	0.91	3/2301 (0.1%)
All	All	0.77	0/6837	0.89	8/9215 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	178	LEU	CA-CB-CG	7.41	132.35	115.30
1	A	22	LEU	CA-CB-CG	-6.71	99.86	115.30
1	B	165	ARG	NE-CZ-NH1	-6.19	117.20	120.30
1	D	178	LEU	CB-CG-CD2	6.01	121.22	111.00
1	B	134	ASP	CB-CG-OD1	5.94	123.64	118.30
1	D	17	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	B	178	LEU	CA-CB-CG	5.54	128.03	115.30
1	A	79	LEU	CB-CG-CD1	-5.05	102.41	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	103	THR	Peptide

## 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	1682	0	1722	41	1
1	B	1706	0	1738	40	0
1	C	1666	0	1710	29	1
1	D	1682	0	1717	46	0
2	A	10	0	0	2	0
2	C	10	0	0	1	0
2	D	5	0	0	5	0
3	A	174	0	0	8	0
3	B	223	0	0	10	1
3	C	180	0	0	1	1
3	D	216	0	0	4	0
All	All	7554	0	6887	157	2

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 12.

All (157) 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:B:104:SER:HA	1:B:107:LYS:HB2	1.33	1.08
1:A:36:ARG:NH1	3:A:1169:HOH:O	1.87	1.07
2:A:902:SO4:O1	3:A:1032:HOH:O	1.73	1.03
1:B:144:ARG:HD3	3:B:420:HOH:O	1.63	0.98
1:B:34:SER:OG	1:B:37:GLU:HG3	1.66	0.95
1:B:17:ARG:NH1	3:B:459:HOH:O	1.95	0.93
1:D:156:LYS:H	1:D:156:LYS:HE3	1.37	0.88
1:A:25:LEU:HD13	1:A:33:ILE:HD13	1.58	0.85
1:A:39:SER:HB2	1:A:46:ALA:HA	1.62	0.80
1:D:101:ASN:OD1	3:D:581:HOH:O	2.01	0.78
1:D:127:ILE:O	1:D:130:VAL:HG23	1.82	0.78
1:B:104:SER:HA	1:B:107:LYS:CB	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:GLU:O	1:D:108:SER:O	2.04	0.74
1:A:45:THR:OG1	1:A:47:SER:HB3	1.89	0.73
1:A:156:LYS:HG3	1:A:178:LEU:HD11	1.72	0.71
1:B:158:ASN:N	3:B:442:HOH:O	2.17	0.71
1:B:97:GLN:HG2	1:B:127:ILE:HD13	1.73	0.71
1:B:125:LEU:HG	1:B:126:LYS:N	2.08	0.69
1:D:120:PRO:HA	1:D:123:PHE:CZ	2.29	0.68
1:A:17:ARG:HG2	1:A:42:MET:CE	2.25	0.66
1:A:48:GLN:O	1:A:52:ASP:N	2.20	0.66
1:D:120:PRO:HA	1:D:123:PHE:CE2	2.32	0.65
1:B:109:GLY:HA3	3:B:411:HOH:O	1.97	0.64
1:C:34:SER:OG	1:C:37:GLU:HG3	1.97	0.64
1:B:64:TYR:HB3	3:B:327:HOH:O	1.98	0.64
1:D:156:LYS:CE	1:D:156:LYS:H	2.09	0.64
1:D:156:LYS:HE3	1:D:156:LYS:N	2.12	0.63
1:D:101:ASN:ND2	1:D:128:ARG:HD3	2.13	0.63
1:A:17:ARG:NH1	3:A:1147:HOH:O	2.07	0.63
1:D:65:GLY:N	2:D:301:SO4:O1	2.32	0.63
1:A:64:TYR:HA	3:A:1100:HOH:O	1.98	0.63
1:B:107:LYS:O	1:B:109:GLY:N	2.32	0.62
1:A:39:SER:HB2	1:A:46:ALA:CA	2.28	0.62
1:D:104:SER:HA	1:D:107:LYS:HB2	1.82	0.62
1:C:22:LEU:HD12	1:C:75:LEU:HD12	1.81	0.62
1:D:34:SER:OG	1:D:37:GLU:HG3	1.98	0.62
1:B:104:SER:CA	1:B:107:LYS:HB2	2.18	0.62
1:D:104:SER:C	1:D:106:GLU:H	2.02	0.62
1:D:101:ASN:HD22	1:D:128:ARG:HD3	1.66	0.61
1:C:44:VAL:HG12	1:C:48:GLN:HB3	1.84	0.60
1:B:156:LYS:HD2	1:B:180:ILE:CD1	2.32	0.59
1:B:156:LYS:HD2	1:B:180:ILE:HD12	1.84	0.59
1:C:35:SER:O	1:C:39:SER:HB3	2.04	0.58
1:A:45:THR:C	1:A:47:SER:N	2.54	0.58
1:D:125:LEU:HD23	1:D:127:ILE:HD11	1.86	0.58
1:D:107:LYS:O	1:D:108:SER:C	2.40	0.58
1:C:22:LEU:HD12	1:C:75:LEU:CD1	2.32	0.58
1:C:17:ARG:HG2	1:C:17:ARG:HH21	1.69	0.58
1:D:109:GLY:HA3	3:D:571:HOH:O	2.05	0.57
1:C:154:ILE:O	1:C:178:LEU:HD21	2.03	0.57
1:A:17:ARG:HG2	1:A:42:MET:HE2	1.85	0.57
1:B:107:LYS:HE2	1:B:112:LEU:H	1.69	0.56
1:B:103:THR:HA	1:B:106:GLU:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:GLU:OE1	3:B:486:HOH:O	2.18	0.56
1:D:25:LEU:HD11	1:D:33:ILE:HD13	1.88	0.56
1:C:17:ARG:NH2	2:C:301:SO4:O2	2.40	0.54
1:D:107:LYS:O	1:D:109:GLY:N	2.40	0.54
1:B:127:ILE:O	1:B:128:ARG:HB3	2.08	0.54
1:D:100:ALA:O	1:D:103:THR:HB	2.07	0.53
1:D:123:PHE:N	1:D:123:PHE:CD1	2.74	0.53
1:A:33:ILE:HG22	1:A:34:SER:O	2.09	0.53
1:D:154:ILE:O	1:D:178:LEU:HD22	2.09	0.52
1:D:140:ASP:OD1	1:D:144:ARG:NH1	2.42	0.52
1:A:36:ARG:NH2	1:A:46:ALA:HB2	2.24	0.52
1:D:159:ALA:HB2	1:D:178:LEU:HD11	1.91	0.52
1:B:159:ALA:HB2	1:B:178:LEU:HD11	1.90	0.52
1:A:172:LYS:HB3	3:A:1068:HOH:O	2.08	0.52
1:B:22:LEU:CD1	1:B:71:LEU:HG	2.40	0.51
1:B:123:PHE:CD1	1:B:123:PHE:N	2.76	0.51
1:C:22:LEU:CD1	1:C:75:LEU:HD12	2.41	0.51
1:C:118:ILE:HG22	1:C:135:VAL:HG11	1.93	0.51
1:A:17:ARG:NE	2:A:902:SO4:O2	2.41	0.51
1:B:204:TYR:CD2	1:B:204:TYR:C	2.85	0.50
1:D:106:GLU:OE1	1:D:106:GLU:HA	2.11	0.50
1:B:214:LYS:O	1:B:215:LEU:C	2.50	0.50
1:C:23:GLU:HG2	1:C:27:LYS:HE2	1.93	0.49
1:D:107:LYS:HE3	1:D:111:ASN:HA	1.93	0.49
1:D:104:SER:HA	1:D:107:LYS:CB	2.42	0.49
1:A:156:LYS:HE3	1:A:156:LYS:H	1.78	0.49
1:B:17:ARG:CZ	1:B:42:MET:HE3	2.43	0.48
1:A:33:ILE:HG23	1:A:37:GLU:HB2	1.95	0.48
1:B:64:TYR:HE1	3:B:521:HOH:O	1.97	0.48
1:B:122:LEU:O	1:B:124:GLY:N	2.47	0.48
1:B:34:SER:HG	1:B:37:GLU:HG3	1.74	0.48
1:D:121:ARG:HD2	3:D:452:HOH:O	2.12	0.48
1:B:27:LYS:HB2	1:B:27:LYS:HE3	1.62	0.48
1:B:209:GLU:HG2	3:B:423:HOH:O	2.13	0.48
1:A:161:TYR:CE2	1:A:165:ARG:HD2	2.49	0.48
1:C:17:ARG:CG	1:C:17:ARG:HH21	2.26	0.48
1:D:21:TYR:CZ	1:D:41:LYS:HG2	2.50	0.47
1:D:127:ILE:O	1:D:130:VAL:CG2	2.58	0.47
1:C:140:ASP:N	1:C:140:ASP:OD1	2.44	0.47
1:A:48:GLN:HG2	3:A:1057:HOH:O	2.12	0.47
1:A:18:TYR:OH	1:A:52:ASP:OD2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ARG:HG2	3:B:407:HOH:O	2.14	0.47
1:D:115:ILE:HD12	1:D:127:ILE:HD12	1.97	0.47
1:B:22:LEU:HD13	1:B:71:LEU:HG	1.97	0.47
1:C:152:LEU:HD12	1:C:182:LEU:HD11	1.97	0.47
1:C:21:TYR:CE2	1:C:41:LYS:HG3	2.50	0.47
1:D:21:TYR:CE1	1:D:41:LYS:HG2	2.50	0.47
1:A:18:TYR:CE1	1:A:42:MET:HG3	2.50	0.46
1:A:25:LEU:HD13	1:A:33:ILE:CD1	2.35	0.46
1:A:156:LYS:CE	1:A:156:LYS:H	2.29	0.46
1:D:35:SER:HB3	2:D:301:SO4:S	2.55	0.46
1:A:36:ARG:NE	1:A:36:ARG:HA	2.31	0.46
1:C:158:ASN:OD1	1:C:161:TYR:HB3	2.16	0.46
1:A:40:GLU:OE1	1:A:41:LYS:HD2	2.15	0.46
1:C:154:ILE:O	1:C:178:LEU:HD11	2.17	0.45
1:C:214:LYS:HB2	1:C:214:LYS:NZ	2.32	0.45
1:C:51:GLN:O	1:C:54:ASN:HB2	2.16	0.45
1:A:47:SER:O	1:A:51:GLN:N	2.44	0.45
1:B:12:ILE:O	1:B:16:PRO:HD3	2.17	0.45
1:D:107:LYS:HZ1	1:D:112:LEU:H	1.65	0.45
1:A:36:ARG:NH2	3:A:1033:HOH:O	2.48	0.45
1:D:64:TYR:HA	2:D:301:SO4:O2	2.17	0.44
1:B:28:ASN:ND2	3:B:519:HOH:O	2.30	0.44
1:A:45:THR:O	1:A:46:ALA:C	2.56	0.44
1:B:209:GLU:HG3	1:B:210:GLU:H	1.82	0.44
1:A:7:VAL:HG12	1:A:8:SER:N	2.32	0.44
1:A:45:THR:C	1:A:47:SER:H	2.19	0.44
1:A:156:LYS:HG2	1:A:180:ILE:HG21	1.99	0.44
1:C:34:SER:HG	1:C:37:GLU:HG3	1.83	0.44
1:C:37:GLU:O	1:C:41:LYS:HG2	2.17	0.44
1:D:215:LEU:HD23	1:D:215:LEU:HA	1.63	0.44
1:B:120:PRO:HA	1:B:123:PHE:CE2	2.53	0.44
1:D:104:SER:O	1:D:107:LYS:HB2	2.18	0.44
1:D:65:GLY:HA2	2:D:301:SO4:O1	2.18	0.43
1:D:122:LEU:O	1:D:124:GLY:N	2.51	0.43
1:A:113:LYS:HA	1:A:113:LYS:HD2	1.76	0.43
1:C:35:SER:HB2	1:C:46:ALA:HB1	1.99	0.43
1:C:106:GLU:HG2	3:C:535:HOH:O	2.18	0.43
1:A:30:VAL:HG11	1:A:33:ILE:HD11	2.01	0.43
1:D:107:LYS:NZ	1:D:112:LEU:H	2.16	0.43
1:A:63:GLY:N	3:A:1149:HOH:O	2.52	0.43
1:D:42:MET:HB3	1:D:42:MET:HE2	1.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:TYR:HE1	1:A:42:MET:HG3	1.83	0.43
1:C:34:SER:OG	1:C:37:GLU:CG	2.66	0.42
1:C:139:GLU:OE2	1:C:168:ARG:NH1	2.52	0.42
1:A:156:LYS:N	1:A:156:LYS:HE3	2.34	0.42
1:C:41:LYS:HB3	1:C:41:LYS:HE2	1.80	0.42
1:D:65:GLY:CA	2:D:301:SO4:O1	2.67	0.42
1:C:22:LEU:HD11	1:C:71:LEU:HD23	2.00	0.42
1:A:45:THR:O	1:A:47:SER:N	2.53	0.42
1:D:12:ILE:O	1:D:16:PRO:HD3	2.20	0.42
1:B:106:GLU:HA	1:B:106:GLU:OE1	2.20	0.41
1:A:156:LYS:HA	1:A:178:LEU:HD21	2.02	0.41
1:D:154:ILE:HB	1:D:155:PRO:CD	2.50	0.41
1:B:127:ILE:O	1:B:130:VAL:HB	2.20	0.41
1:C:22:LEU:HD11	1:C:71:LEU:CD2	2.50	0.41
1:A:21:TYR:OH	1:A:41:LYS:HD3	2.21	0.41
1:D:115:ILE:HG21	1:D:115:ILE:HD13	1.87	0.41
1:B:90:ILE:HG21	1:B:162:THR:HG21	2.03	0.41
1:B:125:LEU:HD23	1:B:132:VAL:HG21	2.03	0.41
1:C:178:LEU:HA	1:C:179:PRO:HD3	1.79	0.41
1:D:156:LYS:CD	3:D:592:HOH:O	2.70	0.40
1:A:140:ASP:OD1	1:A:140:ASP:N	2.33	0.40
1:B:42:MET:HB3	1:B:42:MET:HE2	1.58	0.40

All (2) 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)
3:B:466:HOH:O	3:C:401:HOH:O[4_456]	2.11	0.09
1:A:210:GLU:OE2	1:C:51:GLN:NE2[4_556]	2.13	0.07

## 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	205/224 (92%)	196 (96%)	7 (3%)	2 (1%)	19	10
1	B	210/224 (94%)	200 (95%)	5 (2%)	5 (2%)	7	2
1	C	203/224 (91%)	199 (98%)	4 (2%)	0	100	100
1	D	205/224 (92%)	196 (96%)	5 (2%)	4 (2%)	9	3
All	All	823/896 (92%)	791 (96%)	21 (3%)	11 (1%)	15	6

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	ASP
1	B	123	PHE
1	B	157	ASP
1	B	214	LYS
1	D	103	THR
1	D	106	GLU
1	D	123	PHE
1	B	108	SER
1	B	125	LEU
1	D	214	LYS
1	A	43	GLY

### 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	185/196 (94%)	173 (94%)	12 (6%)	21	13
1	B	187/196 (95%)	175 (94%)	12 (6%)	22	14
1	C	184/196 (94%)	169 (92%)	15 (8%)	14	8
1	D	185/196 (94%)	175 (95%)	10 (5%)	27	19
All	All	741/784 (94%)	692 (93%)	49 (7%)	21	13

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LEU
1	A	27	LYS
1	A	35	SER
1	A	40	GLU
1	A	45	THR
1	A	83	LYS
1	A	107	LYS
1	A	113	LYS
1	A	129	ASP
1	A	140	ASP
1	A	156	LYS
1	A	183	LYS
1	B	31	LYS
1	B	35	SER
1	B	62	GLN
1	B	104	SER
1	B	107	LYS
1	B	118	ILE
1	B	128	ARG
1	B	129	ASP
1	B	158	ASN
1	B	178	LEU
1	B	209	GLU
1	B	213	LYS
1	C	17	ARG
1	C	29	ASP
1	C	39	SER
1	C	41	LYS
1	C	47	SER
1	C	83	LYS
1	C	84	THR
1	C	129	ASP
1	C	140	ASP
1	C	156	LYS
1	C	171	ILE
1	C	172	LYS
1	C	180	ILE
1	C	214	LYS
1	C	216	LYS
1	D	33	ILE
1	D	40	GLU
1	D	70	GLU
1	D	103	THR

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Mol	Chain	Res	Type
1	D	107	LYS
1	D	118	ILE
1	D	121	ARG
1	D	128	ARG
1	D	156	LYS
1	D	178	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	B	62	GLN
1	B	101	ASN
1	B	111	ASN
1	B	158	ASN
1	C	101	ASN
1	D	62	GLN
1	D	101	ASN
1	D	111	ASN
1	D	194	HIS

### 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](#)

5 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	901	-	4,4,4	0.27	0	6,6,6	0.52	0
2	SO4	A	902	-	4,4,4	0.12	0	6,6,6	0.41	0
2	SO4	C	301	-	4,4,4	0.25	0	6,6,6	0.53	0
2	SO4	C	302	-	4,4,4	0.14	0	6,6,6	0.37	0
2	SO4	D	301	-	4,4,4	0.13	0	6,6,6	0.37	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	901	-	-	0/0/0/0	0/0/0/0
2	SO4	A	902	-	-	0/0/0/0	0/0/0/0
2	SO4	C	301	-	-	0/0/0/0	0/0/0/0
2	SO4	C	302	-	-	0/0/0/0	0/0/0/0
2	SO4	D	301	-	-	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.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	902	SO4	2	0
2	C	301	SO4	1	0
2	D	301	SO4	5	0

## 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	209/224 (93%)	0.80	34 (16%) <b>2</b> <b>3</b>	26, 48, 76, 95	0
1	B	212/224 (94%)	0.53	24 (11%) <b>7</b> <b>8</b>	24, 42, 75, 89	0
1	C	207/224 (92%)	0.71	26 (12%) <b>5</b> <b>6</b>	28, 51, 70, 84	0
1	D	209/224 (93%)	0.56	15 (7%) <b>18</b> <b>22</b>	28, 44, 75, 93	0
All	All	837/896 (93%)	0.65	99 (11%) <b>6</b> <b>7</b>	24, 47, 75, 95	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	105	PHE	9.4
1	B	105	PHE	6.3
1	D	129	ASP	5.6
1	A	21	TYR	5.1
1	A	64	TYR	4.9
1	A	44	VAL	4.7
1	A	36	ARG	4.4
1	C	90	ILE	4.2
1	B	213	LYS	4.2
1	B	60	GLY	4.1
1	C	58	GLY	4.1
1	D	214	LYS	4.0
1	C	161	TYR	3.8
1	A	28	ASN	3.8
1	D	158	ASN	3.8
1	A	90	ILE	3.8
1	C	157	ASP	3.7
1	D	157	ASP	3.7
1	A	45	THR	3.6
1	D	104	SER	3.6
1	B	71	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	57	GLY	3.5
1	B	214	LYS	3.5
1	A	57	GLY	3.5
1	C	36	ARG	3.5
1	B	75	LEU	3.5
1	C	158	ASN	3.5
1	B	104	SER	3.5
1	D	213	LYS	3.4
1	D	215	LEU	3.4
1	C	214	LYS	3.3
1	A	107	LYS	3.3
1	D	151	ILE	3.3
1	A	103	THR	3.2
1	B	107	LYS	3.2
1	C	44	VAL	3.1
1	B	58	GLY	3.1
1	A	143	ALA	3.1
1	A	47	SER	3.1
1	C	89	ILE	3.0
1	C	151	ILE	3.0
1	D	64	TYR	3.0
1	B	157	ASP	2.9
1	B	62	GLN	2.9
1	A	181	ASP	2.8
1	A	88	ILE	2.8
1	B	64	TYR	2.8
1	C	54	ASN	2.8
1	B	63	GLY	2.8
1	A	46	ALA	2.8
1	A	48	GLN	2.8
1	A	51	GLN	2.7
1	A	151	ILE	2.6
1	A	15	LEU	2.6
1	A	54	ASN	2.6
1	C	156	LYS	2.6
1	C	21	TYR	2.6
1	C	42	MET	2.6
1	D	128	ARG	2.6
1	A	40	GLU	2.5
1	B	128	ARG	2.5
1	B	215	LEU	2.5
1	C	129	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	89	ILE	2.4
1	C	181	ASP	2.4
1	A	27	LYS	2.4
1	A	42	MET	2.4
1	B	89	ILE	2.4
1	B	151	ILE	2.4
1	B	129	ASP	2.4
1	A	128	ARG	2.4
1	A	50	ARG	2.4
1	A	89	ILE	2.3
1	C	143	ALA	2.3
1	A	217	GLY	2.3
1	A	116	PHE	2.3
1	A	156	LYS	2.3
1	D	102	TYR	2.3
1	C	166	LEU	2.3
1	D	75	LEU	2.3
1	C	118	ILE	2.3
1	C	186	ASP	2.2
1	B	106	GLU	2.2
1	D	166	LEU	2.2
1	A	149	ILE	2.2
1	B	158	ASN	2.2
1	B	90	ILE	2.2
1	B	120	PRO	2.1
1	C	116	PHE	2.1
1	A	71	LEU	2.1
1	C	15	LEU	2.1
1	C	47	SER	2.1
1	A	140	ASP	2.1
1	A	75	LEU	2.1
1	C	152	LEU	2.1
1	A	216	LYS	2.1
1	B	59	PHE	2.0
1	C	88	ILE	2.0
1	B	108	SER	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	D	301	5/5	0.96	0.31	3.99	73,74,75,77	0
2	SO4	A	901	5/5	0.98	0.15	0.62	39,44,46,47	0
2	SO4	C	302	5/5	0.97	0.11	0.13	50,51,55,55	0
2	SO4	C	301	5/5	0.95	0.12	0.05	64,65,67,67	0
2	SO4	A	902	5/5	0.95	0.09	-1.01	69,71,72,73	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.