W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2021 – 08:03 PM EST

PDB ID	:	3M8N
Title	:	Crystal structure of a possible gutathione S-tranferase from Rhodopseu-domonas palustris
Authors	:	Damodharan, L.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2010-03-18
Resolution	:	2.04 Å(reported)

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

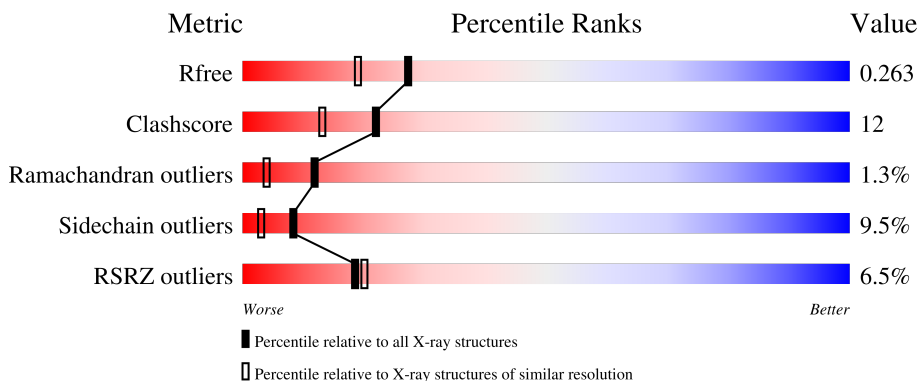|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

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 2.04 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	Percentile Ranks	Value
Rfree		0.263
Clashscore		12
Ramachandran outliers		1.3%
Sidechain outliers		9.5%
RSRZ outliers		6.5%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	225	% 67% 20% • 9%
1	B	225	2% 62% 16% • 19%
1	C	225	15% 61% 17% 7% 14%
1	D	225	4% 73% 21% • •

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 6636 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 Possible glutathione S-transferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	204	Total	C	N	O	S	Se	0	0	0
			1629	1046	275	301	2	5			
1	B	183	Total	C	N	O	S	Se	0	0	0
			1459	935	245	273	1	5			
1	C	193	Total	C	N	O	S	Se	0	0	0
			1525	983	257	278	2	5			
1	D	222	Total	C	N	O	S	Se	0	0	0
			1769	1132	305	325	2	5			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	expression tag	UNP Q6N1S2
A	0	SER	-	expression tag	UNP Q6N1S2
A	1	LEU	-	expression tag	UNP Q6N1S2
A	217	GLY	-	expression tag	UNP Q6N1S2
A	218	HIS	-	expression tag	UNP Q6N1S2
A	219	HIS	-	expression tag	UNP Q6N1S2
A	220	HIS	-	expression tag	UNP Q6N1S2
A	221	HIS	-	expression tag	UNP Q6N1S2
A	222	HIS	-	expression tag	UNP Q6N1S2
A	223	HIS	-	expression tag	UNP Q6N1S2
B	-1	MSE	-	expression tag	UNP Q6N1S2
B	0	SER	-	expression tag	UNP Q6N1S2
B	1	LEU	-	expression tag	UNP Q6N1S2
B	217	GLY	-	expression tag	UNP Q6N1S2
B	218	HIS	-	expression tag	UNP Q6N1S2
B	219	HIS	-	expression tag	UNP Q6N1S2
B	220	HIS	-	expression tag	UNP Q6N1S2
B	221	HIS	-	expression tag	UNP Q6N1S2
B	222	HIS	-	expression tag	UNP Q6N1S2
B	223	HIS	-	expression tag	UNP Q6N1S2
C	-1	MSE	-	expression tag	UNP Q6N1S2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	expression tag	UNP Q6N1S2
C	1	LEU	-	expression tag	UNP Q6N1S2
C	217	GLY	-	expression tag	UNP Q6N1S2
C	218	HIS	-	expression tag	UNP Q6N1S2
C	219	HIS	-	expression tag	UNP Q6N1S2
C	220	HIS	-	expression tag	UNP Q6N1S2
C	221	HIS	-	expression tag	UNP Q6N1S2
C	222	HIS	-	expression tag	UNP Q6N1S2
C	223	HIS	-	expression tag	UNP Q6N1S2
D	-1	MSE	-	expression tag	UNP Q6N1S2
D	0	SER	-	expression tag	UNP Q6N1S2
D	1	LEU	-	expression tag	UNP Q6N1S2
D	217	GLY	-	expression tag	UNP Q6N1S2
D	218	HIS	-	expression tag	UNP Q6N1S2
D	219	HIS	-	expression tag	UNP Q6N1S2
D	220	HIS	-	expression tag	UNP Q6N1S2
D	221	HIS	-	expression tag	UNP Q6N1S2
D	222	HIS	-	expression tag	UNP Q6N1S2
D	223	HIS	-	expression tag	UNP Q6N1S2

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	69	Total 69	O 69	0	0
3	B	73	Total 73	O 73	0	0
3	C	35	Total 35	O 35	0	0
3	D	62	Total 62	O 62	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Possible glutathione S-transferase
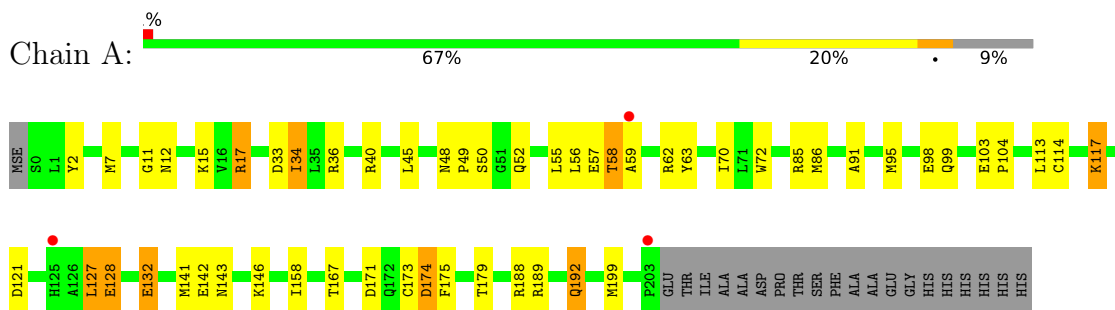
Chain A:

- Molecule 1: Possible glutathione S-transferase

Chain B:

- Molecule 1: Possible glutathione S-transferase

Chain C:

- Molecule 1: Possible glutathione S-transferase

Chain D:

MSE S0 L1 Y2 K3 L4 M7 Q8 R9 S10 G11 K15 V16 R17 R28 I34 R40 Q52 V53 P54 T58 A59 P60 A65 E66 I70 L71 W72 Y73 L74 A75 M86 D87 R88 L92 F96 F97 E98 Q99 H100 A101 L102 E103 L113 C114 L115 V116

K117 G118 D121 H125 A126 L127 E128 E132 A153 I158 D171 Q172 C173 D174 L177 S178 T179 N184 R188 M199 D200 W201 T202 P203 GLU THR I206 T211 S212 H221 H222 H223
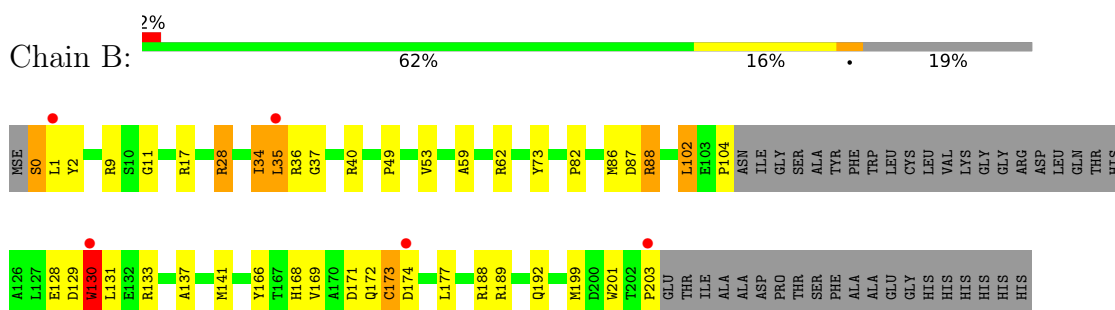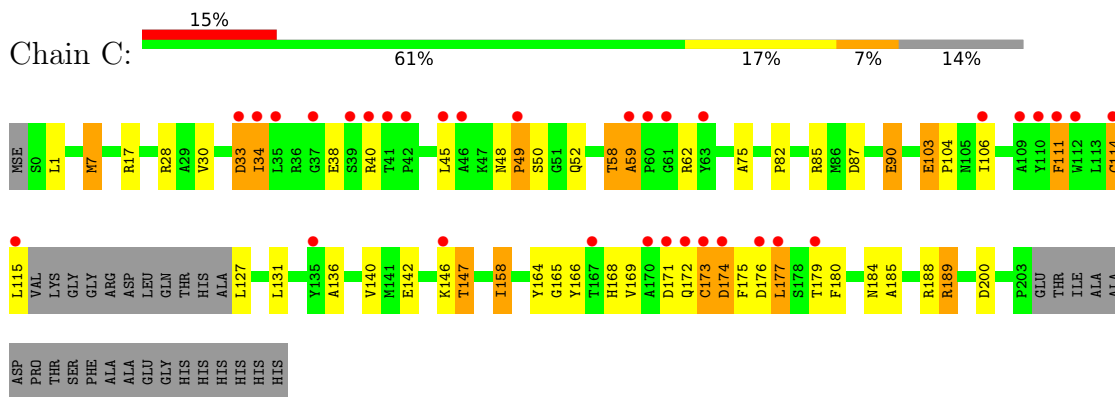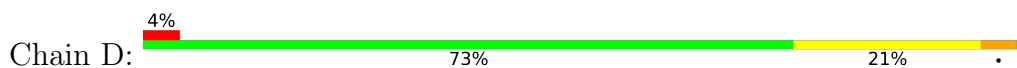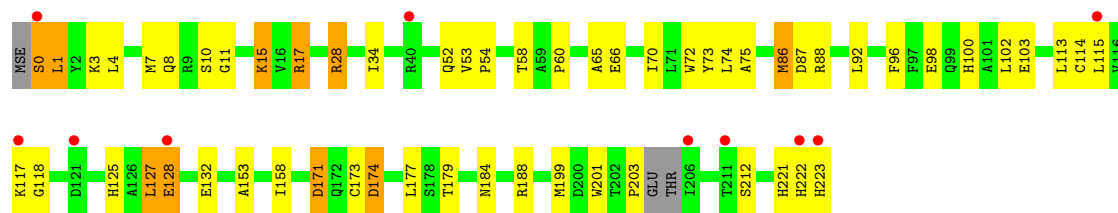
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	56.97Å　　105.09Å　　152.13Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	45.67　–　2.04 45.67　–　2.04	Depositor EDS
% Data completeness (in resolution range)	91.3 (45.67-2.04) 91.3 (45.67-2.04)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.73 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.199　,　0.259 0.205　,　0.263	Depositor DCC
R_{free} test set	1718 reflections (3.20%)	wwPDB-VP
Wilson B-factor (Å^2)	35.5	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 54.2	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6636	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	1.07	0/1668	1.00	5/2266 (0.2%)
1	B	1.14	1/1492 (0.1%)	1.07	4/2026 (0.2%)
1	C	0.95	1/1561 (0.1%)	0.93	1/2122 (0.0%)
1	D	1.01	0/1815	0.98	4/2466 (0.2%)
All	All	1.04	2/6536 (0.0%)	0.99	14/8880 (0.2%)

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
1	D	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	130	TRP	CB-CG	5.71	1.60	1.50
1	C	90	GLU	CG-CD	5.71	1.60	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	ARG	NE-CZ-NH2	-12.72	113.94	120.30
1	A	17	ARG	NE-CZ-NH1	9.00	124.80	120.30
1	B	189	ARG	NE-CZ-NH2	-9.00	115.80	120.30
1	D	17	ARG	NE-CZ-NH2	-7.85	116.37	120.30
1	B	88	ARG	NE-CZ-NH1	-7.57	116.51	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	17	ARG	NE-CZ-NH2	-7.25	116.67	120.30
1	B	87	ASP	CB-CG-OD1	6.41	124.06	118.30
1	A	189	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	D	17	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	17	ARG	CD-NE-CZ	5.51	131.31	123.60
1	D	1	LEU	CB-CA-C	5.29	120.25	110.20
1	D	88	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	98	GLU	OE1-CD-OE2	-5.08	117.20	123.30
1	B	189	ARG	CG-CD-NE	-5.05	101.19	111.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	0	SER	Peptide
1	D	0	SER	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1629	0	1582	36	0
1	B	1459	0	1409	37	0
1	C	1525	0	1470	46	0
1	D	1769	0	1695	39	0
2	B	10	0	0	0	0
2	D	5	0	0	0	0
3	A	69	0	0	3	0
3	B	73	0	0	4	0
3	C	35	0	0	0	0
3	D	62	0	0	8	0
All	All	6636	0	6156	148	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (148) 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:102:LEU:O	1:B:130:TRP:HZ3	1.35	1.08
1:D:28:ARG:HH11	1:D:28:ARG:HG3	1.21	1.02
1:A:58:THR:HG21	1:B:86:MSE:SE	2.10	1.02
1:D:28:ARG:HH11	1:D:28:ARG:CG	1.78	0.95
1:B:102:LEU:O	1:B:130:TRP:CZ3	2.24	0.91
1:B:28:ARG:HH11	1:B:28:ARG:HG2	1.37	0.90
1:B:59:ALA:HB3	1:B:62:ARG:HB3	1.62	0.81
1:B:36:ARG:HG2	1:B:37:GLY:H	1.46	0.81
1:D:28:ARG:NH1	1:D:28:ARG:HG3	1.92	0.81
1:A:57:GLU:HG2	1:A:63:TYR:CE1	2.16	0.80
1:D:34:ILE:HD11	1:D:53:VAL:HG22	1.65	0.78
1:A:58:THR:HG22	1:A:59:ALA:N	1.96	0.78
1:D:113:LEU:HD11	1:D:127:LEU:HD21	1.69	0.75
1:B:36:ARG:HG2	1:B:37:GLY:N	2.03	0.74
1:A:188:ARG:O	1:A:192:GLN:HG2	1.87	0.73
1:B:129:ASP:O	1:B:133:ARG:HB2	1.89	0.72
1:B:36:ARG:CG	1:B:37:GLY:H	2.05	0.70
1:C:127:LEU:O	1:C:131:LEU:HD12	1.91	0.69
1:C:172:GLN:C	1:C:174:ASP:H	1.95	0.69
1:A:173:CYS:O	1:A:174:ASP:HB2	1.91	0.69
1:D:28:ARG:NH1	1:D:28:ARG:CG	2.48	0.69
1:A:57:GLU:CG	1:A:63:TYR:CE1	2.78	0.67
1:C:7:MSE:CG	1:C:34:ILE:HD13	2.26	0.66
1:D:113:LEU:HD21	1:D:127:LEU:HD11	1.78	0.65
1:D:171:ASP:HB2	3:D:276:HOH:O	1.96	0.64
1:D:128:GLU:O	1:D:132:GLU:HG3	1.97	0.64
1:C:111:PHE:C	1:C:111:PHE:HD1	2.03	0.62
1:C:7:MSE:HB2	1:C:34:ILE:HD13	1.83	0.61
1:C:28:ARG:NH1	1:C:30:VAL:HG22	2.15	0.61
1:C:111:PHE:C	1:C:111:PHE:CD1	2.73	0.61
1:A:12:ASN:HA	1:A:15:LYS:HD3	1.83	0.60
3:A:256:HOH:O	1:D:60:PRO:HD3	2.02	0.59
1:A:128:GLU:O	1:A:132:GLU:HB3	2.02	0.59
1:A:11:GLY:HA2	1:A:199:MSE:CE	2.33	0.59
1:D:173:CYS:O	1:D:174:ASP:HB2	2.02	0.58
1:C:185:ALA:C	1:C:189:ARG:HH21	2.06	0.58
1:A:117:LYS:HZ2	1:C:147:THR:HG22	1.67	0.58
1:C:166:TYR:O	1:C:169:VAL:HG22	2.03	0.58
1:A:113:LEU:HD21	1:A:127:LEU:HD11	1.87	0.57
1:A:117:LYS:NZ	1:C:147:THR:HG22	2.20	0.57
1:C:114:CYS:O	1:C:115:LEU:HG	2.05	0.57
1:D:201:TRP:CH2	1:D:203:PRO:HA	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:THR:CG2	1:A:59:ALA:H	2.19	0.56
1:D:34:ILE:HD11	1:D:53:VAL:CG2	2.36	0.55
1:A:95:MSE:SE	1:A:158:ILE:HD12	2.57	0.55
1:C:172:GLN:O	1:C:174:ASP:N	2.38	0.55
1:C:7:MSE:CB	1:C:34:ILE:HD13	2.37	0.54
1:C:33:ASP:HB2	1:C:38:GLU:OE1	2.09	0.53
1:B:173:CYS:O	1:B:173:CYS:SG	2.67	0.53
1:B:34:ILE:C	1:B:36:ARG:H	2.11	0.53
1:C:172:GLN:OE1	1:C:172:GLN:N	2.42	0.53
1:B:34:ILE:HD11	1:B:53:VAL:HG12	1.90	0.53
1:D:127:LEU:O	1:D:128:GLU:C	2.48	0.52
1:B:36:ARG:CG	1:B:37:GLY:N	2.69	0.52
1:A:40:ARG:NH1	3:A:252:HOH:O	2.43	0.52
1:D:8:GLN:O	1:D:17:ARG:NH2	2.42	0.52
1:A:58:THR:HG23	3:A:283:HOH:O	2.09	0.52
1:A:91:ALA:O	1:A:95:MSE:HG3	2.10	0.51
1:B:28:ARG:NH1	1:B:28:ARG:HG2	2.16	0.51
1:C:172:GLN:C	1:C:174:ASP:N	2.63	0.51
1:C:28:ARG:HH12	1:C:30:VAL:HG22	1.75	0.51
1:B:166:TYR:O	1:B:169:VAL:HG22	2.11	0.51
1:B:82:PRO:O	1:B:88:ARG:HD2	2.11	0.51
1:C:111:PHE:HD1	1:C:111:PHE:O	1.94	0.51
1:B:133:ARG:HB3	3:B:286:HOH:O	2.10	0.51
1:D:15:LYS:NZ	1:D:98:GLU:OE2	2.42	0.51
1:D:11:GLY:HA2	1:D:199:MSE:CE	2.41	0.50
1:C:90:GLU:HG3	3:D:235:HOH:O	2.12	0.50
1:C:85:ARG:NH1	1:D:73:TYR:O	2.45	0.50
1:D:52:GLN:HB2	3:D:262:HOH:O	2.10	0.50
1:C:34:ILE:HD12	1:C:34:ILE:N	2.25	0.50
1:B:192:GLN:NE2	3:B:266:HOH:O	2.45	0.49
1:A:171:ASP:HA	1:A:175:PHE:O	2.11	0.49
1:A:103:GLU:HB3	1:A:104:PRO:HD3	1.94	0.49
1:C:7:MSE:HG3	1:C:34:ILE:HD13	1.93	0.49
1:C:142:GLU:O	1:C:146:LYS:HG3	2.12	0.49
1:B:129:ASP:HB2	1:D:222:HIS:CE1	2.48	0.49
1:A:55:LEU:HG	1:A:63:TYR:HB3	1.95	0.48
1:B:17:ARG:NH1	3:B:243:HOH:O	2.43	0.48
1:C:7:MSE:SE	1:C:34:ILE:HB	2.63	0.48
1:A:114:CYS:SG	1:A:173:CYS:HB3	2.53	0.48
1:D:75:ALA:HB2	1:D:158:ILE:HG21	1.96	0.48
1:B:34:ILE:HB	1:B:35:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:ASP:HB3	1:D:153:ALA:HB2	1.96	0.48
1:B:34:ILE:HD11	1:B:53:VAL:CG1	2.45	0.47
1:B:86:MSE:HE2	3:B:253:HOH:O	2.14	0.47
1:A:48:ASN:HA	1:A:49:PRO:HD3	1.81	0.47
1:A:50:SER:HB2	1:A:52:GLN:HG3	1.96	0.47
1:A:7:MSE:SE	1:A:34:ILE:HB	2.65	0.47
1:D:114:CYS:SG	1:D:173:CYS:HB3	2.54	0.47
1:A:7:MSE:O	1:A:17:ARG:NH2	2.48	0.46
1:D:7:MSE:SE	1:D:34:ILE:HG12	2.66	0.46
1:A:33:ASP:OD2	1:A:36:ARG:HD2	2.15	0.46
1:B:11:GLY:HA2	1:B:199:MSE:CE	2.45	0.46
1:D:70:ILE:O	1:D:74:LEU:HG	2.16	0.46
1:A:142:GLU:HG3	1:A:146:LYS:HE2	1.96	0.46
1:B:172:GLN:OE1	1:B:172:GLN:HA	2.16	0.46
1:B:11:GLY:HA2	1:B:199:MSE:HE1	1.97	0.45
1:C:7:MSE:HB2	1:C:34:ILE:CD1	2.45	0.45
1:A:57:GLU:HG2	1:A:63:TYR:CD1	2.50	0.45
1:C:48:ASN:HA	1:C:49:PRO:HD2	1.67	0.45
1:D:102:LEU:HD23	3:D:229:HOH:O	2.17	0.45
1:D:177:LEU:HD23	1:D:184:ASN:HD21	1.82	0.45
1:C:90:GLU:CG	3:D:235:HOH:O	2.64	0.45
1:A:85:ARG:NH2	1:B:73:TYR:O	2.47	0.45
1:A:34:ILE:HD13	1:A:34:ILE:N	2.31	0.45
1:C:158:ILE:HG13	1:C:158:ILE:H	1.54	0.45
1:C:136:ALA:O	1:C:140:VAL:HG23	2.18	0.44
1:C:103:GLU:N	1:C:104:PRO:CD	2.81	0.44
1:D:117:LYS:HD2	3:D:270:HOH:O	2.17	0.44
1:D:1:LEU:HD23	1:D:1:LEU:HA	1.85	0.44
1:D:212:SER:OG	1:D:221:HIS:HE1	2.00	0.44
1:D:96:PHE:O	1:D:100:HIS:CD2	2.70	0.44
1:C:82:PRO:HB2	1:C:87:ASP:HB3	2.00	0.44
1:C:40:ARG:HG2	1:C:45:LEU:HD21	2.00	0.43
1:C:75:ALA:CB	1:C:158:ILE:HG12	2.48	0.43
1:A:86:MSE:HE2	1:B:62:ARG:HG3	2.00	0.43
1:C:90:GLU:HB2	3:D:235:HOH:O	2.17	0.43
1:C:82:PRO:CB	1:C:87:ASP:HB3	2.49	0.43
1:D:4:LEU:HD11	1:D:54:PRO:HB2	2.00	0.43
1:A:62:ARG:NH1	1:B:86:MSE:HE3	2.33	0.43
1:B:201:TRP:CZ2	1:B:203:PRO:HA	2.54	0.43
1:C:177:LEU:HB3	1:C:184:ASN:HD21	1.83	0.42
1:D:113:LEU:HD12	1:D:173:CYS:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:ALA:O	1:D:66:GLU:HB2	2.19	0.42
1:C:59:ALA:HB3	1:C:62:ARG:CB	2.50	0.42
1:C:82:PRO:HB2	1:C:87:ASP:CB	2.50	0.42
1:C:48:ASN:OD1	1:C:52:GLN:HG3	2.19	0.42
1:B:133:ARG:HG3	1:D:221:HIS:CD2	2.55	0.42
1:A:45:LEU:HA	1:A:45:LEU:HD23	1.88	0.41
1:B:137:ALA:O	1:B:141:MSE:HG3	2.20	0.41
1:C:106:ILE:O	1:C:106:ILE:HG22	2.20	0.41
1:C:177:LEU:HD12	1:C:180:PHE:HB2	2.01	0.41
1:C:58:THR:HG23	1:D:86:MSE:SE	2.71	0.41
1:B:34:ILE:HG22	1:B:35:LEU:H	1.85	0.41
1:C:59:ALA:HB3	1:C:62:ARG:HB3	2.01	0.41
1:D:72:TRP:CZ3	1:D:92:LEU:HG	2.55	0.41
1:B:34:ILE:C	1:B:36:ARG:N	2.74	0.41
1:B:59:ALA:HB3	1:B:62:ARG:CB	2.42	0.41
1:C:34:ILE:N	1:C:34:ILE:CD1	2.83	0.41
1:B:168:HIS:O	1:B:171:ASP:HB3	2.21	0.41
1:A:141:MSE:HE1	1:A:167:THR:OG1	2.21	0.41
1:C:164:TYR:O	1:C:165:GLY:C	2.59	0.41
1:A:56:LEU:HD22	1:A:70:ILE:HG23	2.03	0.40
1:D:118:GLY:HA2	3:D:230:HOH:O	2.20	0.40
1:D:212:SER:OG	1:D:221:HIS:CE1	2.74	0.40
1:A:72:TRP:HA	1:A:158:ILE:HD13	2.03	0.40
1:B:104:PRO:HA	1:B:130:TRP:CE3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	202/225 (90%)	196 (97%)	4 (2%)	2 (1%)	15	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	179/225 (80%)	171 (96%)	7 (4%)	1 (1%)	25	15
1	C	189/225 (84%)	173 (92%)	10 (5%)	6 (3%)	4	0
1	D	218/225 (97%)	207 (95%)	10 (5%)	1 (0%)	29	18
All	All	788/900 (88%)	747 (95%)	31 (4%)	10 (1%)	12	4

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	49	PRO
1	C	173	CYS
1	C	175	PHE
1	B	2	TYR
1	A	58	THR
1	A	174	ASP
1	C	174	ASP
1	C	176	ASP
1	D	174	ASP
1	C	59	ALA

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	168/178 (94%)	157 (94%)	11 (6%)	17	9
1	B	150/178 (84%)	134 (89%)	16 (11%)	6	2
1	C	154/178 (86%)	135 (88%)	19 (12%)	4	1
1	D	181/178 (102%)	165 (91%)	16 (9%)	10	4
All	All	653/712 (92%)	591 (90%)	62 (10%)	8	3

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	TYR

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Mol	Chain	Res	Type
1	A	34	ILE
1	A	99	GLN
1	A	117	LYS
1	A	121	ASP
1	A	127	LEU
1	A	128	GLU
1	A	132	GLU
1	A	143	ASN
1	A	179	THR
1	A	192	GLN
1	B	0	SER
1	B	1	LEU
1	B	9	ARG
1	B	28	ARG
1	B	34	ILE
1	B	35	LEU
1	B	40	ARG
1	B	49	PRO
1	B	102	LEU
1	B	128	GLU
1	B	130	TRP
1	B	131	LEU
1	B	173	CYS
1	B	174	ASP
1	B	177	LEU
1	B	188	ARG
1	C	1	LEU
1	C	7	MSE
1	C	33	ASP
1	C	34	ILE
1	C	50	SER
1	C	58	THR
1	C	103	GLU
1	C	111	PHE
1	C	114	CYS
1	C	147	THR
1	C	158	ILE
1	C	168	HIS
1	C	171	ASP
1	C	173	CYS
1	C	177	LEU
1	C	179	THR

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Mol	Chain	Res	Type
1	C	188	ARG
1	C	189	ARG
1	C	200	ASP
1	D	0	SER
1	D	3	LYS
1	D	10	SER
1	D	15	LYS
1	D	28	ARG
1	D	58	THR
1	D	86	MSE
1	D	103	GLU
1	D	115	LEU
1	D	125	HIS
1	D	127	LEU
1	D	128	GLU
1	D	171	ASP
1	D	179	THR
1	D	188	ARG
1	D	223	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	B	144	HIS
1	B	184	ASN
1	B	192	GLN
1	C	52	GLN
1	C	105	ASN
1	D	48	ASN
1	D	105	ASN
1	D	144	HIS
1	D	172	GLN
1	D	184	ASN
1	D	221	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 monosaccharides in this entry.

5.6   Ligand geometry ⓘ

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	SO4	B	230	-	4,4,4	0.21	0	6,6,6	0.99	0
2	SO4	D	231	-	4,4,4	0.14	0	6,6,6	0.96	0
2	SO4	B	232	-	4,4,4	0.13	0	6,6,6	0.36	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7   Other polymers ⓘ

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	199/225 (88%)	-0.10	3 (1%)	73	76	18, 31, 50, 55	0
1	B	178/225 (79%)	0.15	5 (2%)	53	58	18, 28, 59, 66	0
1	C	188/225 (83%)	0.74	33 (17%)	1	1	24, 46, 81, 88	0
1	D	217/225 (96%)	0.23	10 (4%)	32	35	23, 37, 59, 69	0
All	All	782/900 (86%)	0.25	51 (6%)	18	20	18, 35, 63, 88	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	35	LEU	5.8
1	C	40	ARG	5.2
1	C	114	CYS	4.9
1	C	110	TYR	4.4
1	D	206	ILE	4.4
1	C	33	ASP	3.9
1	B	35	LEU	3.8
1	D	0	SER	3.8
1	C	112	TRP	3.8
1	C	45	LEU	3.7
1	A	59	ALA	3.7
1	B	1	LEU	3.6
1	B	174	ASP	3.6
1	C	177	LEU	3.6
1	C	34	ILE	3.6
1	C	174	ASP	3.6
1	C	170	ALA	3.5
1	C	109	ALA	3.4
1	B	130	TRP	3.3
1	D	222	HIS	3.2
1	D	115	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	41	THR	3.2
1	D	117	LYS	3.1
1	C	49	PRO	3.1
1	C	42	PRO	3.1
1	C	46	ALA	2.8
1	C	173	CYS	2.8
1	A	125	HIS	2.7
1	C	39	SER	2.7
1	C	111	PHE	2.7
1	D	121	ASP	2.6
1	C	176	ASP	2.6
1	D	211	THR	2.6
1	C	37	GLY	2.5
1	C	61	GLY	2.4
1	C	115	LEU	2.4
1	C	172	GLN	2.4
1	C	106	ILE	2.4
1	C	60	PRO	2.3
1	C	59	ALA	2.3
1	D	40	ARG	2.3
1	C	135	TYR	2.3
1	A	203	PRO	2.3
1	C	179	THR	2.2
1	C	171	ASP	2.2
1	D	128	GLU	2.2
1	B	203	PRO	2.2
1	C	63	TYR	2.2
1	C	167	THR	2.1
1	D	223	HIS	2.1
1	C	146	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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
2	SO4	D	231	5/5	0.94	0.10	59,62,64,64	0
2	SO4	B	230	5/5	0.95	0.10	55,58,58,62	0
2	SO4	B	232	5/5	0.96	0.12	83,84,85,86	0

6.5 Other polymers ⓘ

There are no such residues in this entry.