



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 05:27 am BST

PDB ID : 2ORA
Title : RHODANESE (THIOSULFATE: CYANIDE SULFURTRANSFERASE)
Authors : Gliubich, F.; Gazerro, M.; Zanotti, G.; Delbono, S.; Berni, R.
Deposited on : 1996-02-22
Resolution : 1.99 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

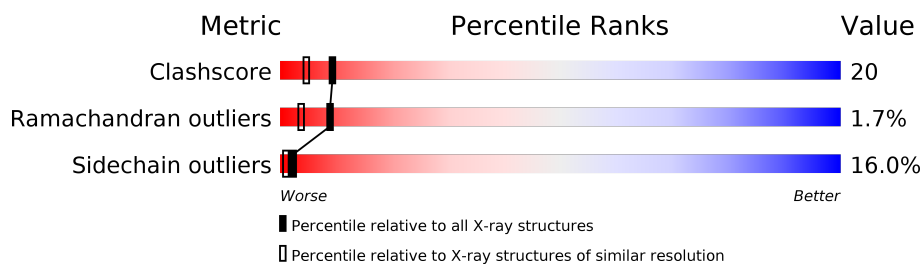
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	296	58% 25% 14% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2407 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 OXIDIZED RHODANESE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	293	2326	1486	405	426	9	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	247	CSO	CYS	CONFLICT	UNP P00586

- Molecule 2 is water.

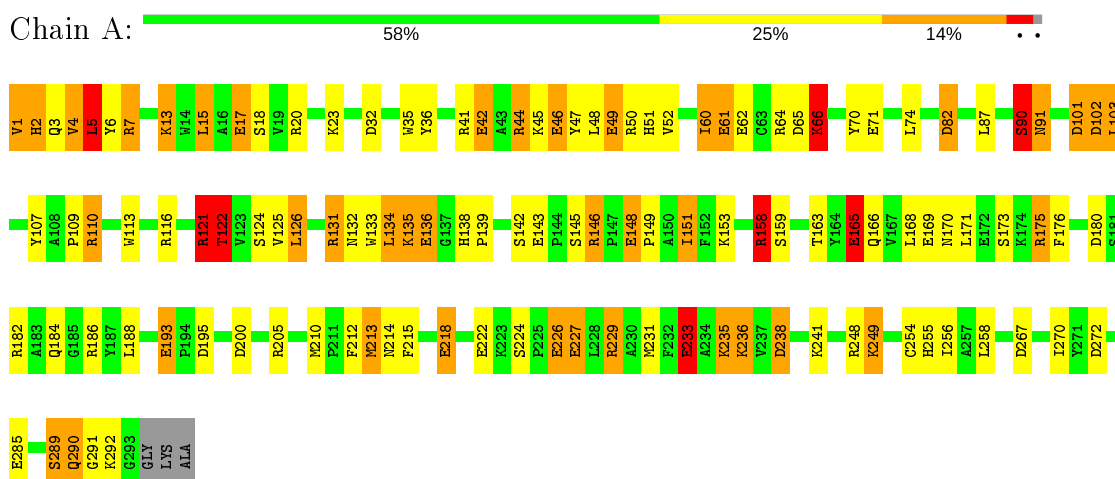
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	81	81	81	0	0

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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

- Molecule 1: OXIDIZED RHODANESE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	156.23Å 49.04Å 42.25Å 90.00° 98.60° 90.00°	Depositor
Resolution (Å)	9.00 – 1.99	Depositor
% Data completeness (in resolution range)	(Not available) (9.00-1.99)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2407	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

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: CSO

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	0.92	19/2385 (0.8%)	1.65	53/3235 (1.6%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	218	GLU	CD-OE1	6.83	1.33	1.25
1	A	42	GLU	CD-OE2	6.16	1.32	1.25
1	A	148	GLU	CD-OE1	6.14	1.32	1.25
1	A	136	GLU	CD-OE1	6.01	1.32	1.25
1	A	143	GLU	CD-OE2	6.01	1.32	1.25
1	A	233	GLU	CD-OE2	6.00	1.32	1.25
1	A	71	GLU	CD-OE1	5.90	1.32	1.25
1	A	226	GLU	CD-OE1	5.88	1.32	1.25
1	A	227	GLU	CD-OE2	5.74	1.31	1.25
1	A	169	GLU	CD-OE1	5.72	1.31	1.25
1	A	222	GLU	CD-OE2	5.68	1.31	1.25
1	A	61	GLU	CD-OE2	5.55	1.31	1.25
1	A	165	GLU	CD-OE2	5.53	1.31	1.25
1	A	17	GLU	CD-OE2	5.52	1.31	1.25
1	A	193	GLU	CD-OE2	5.43	1.31	1.25
1	A	49	GLU	CD-OE1	5.40	1.31	1.25
1	A	46	GLU	CD-OE2	5.39	1.31	1.25
1	A	285	GLU	CD-OE2	5.19	1.31	1.25
1	A	62	GLU	CD-OE2	5.16	1.31	1.25

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	ARG	NE-CZ-NH1	16.27	128.43	120.30
1	A	5	LEU	O-C-N	-10.67	105.63	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	ARG	NE-CZ-NH1	10.13	125.36	120.30
1	A	102	ASP	CB-CG-OD2	-9.92	109.38	118.30
1	A	238	ASP	CB-CG-OD2	-9.32	109.91	118.30
1	A	66	LYS	N-CA-CB	8.79	126.42	110.60
1	A	5	LEU	C-N-CA	-8.59	100.22	121.70
1	A	65	ASP	CB-CG-OD1	-8.33	110.80	118.30
1	A	32	ASP	CB-CG-OD2	-7.69	111.38	118.30
1	A	238	ASP	CB-CG-OD1	7.62	125.16	118.30
1	A	158	ARG	NE-CZ-NH2	-7.55	116.52	120.30
1	A	32	ASP	CB-CG-OD1	7.38	124.94	118.30
1	A	5	LEU	CB-CG-CD1	7.34	123.48	111.00
1	A	131	ARG	NE-CZ-NH2	7.28	123.94	120.30
1	A	200	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	A	195	ASP	CB-CG-OD2	-6.96	112.04	118.30
1	A	4	VAL	O-C-N	6.91	133.76	122.70
1	A	205	ARG	NE-CZ-NH1	6.87	123.74	120.30
1	A	102	ASP	CB-CG-OD1	6.84	124.46	118.30
1	A	267	ASP	CB-CG-OD1	6.64	124.27	118.30
1	A	158	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	A	5	LEU	CA-C-N	6.37	131.21	117.20
1	A	5	LEU	CB-CA-C	-6.29	98.25	110.20
1	A	64	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	267	ASP	CB-CG-OD2	-6.25	112.68	118.30
1	A	180	ASP	CB-CG-OD1	6.24	123.91	118.30
1	A	195	ASP	CB-CG-OD1	6.20	123.88	118.30
1	A	125	VAL	N-CA-CB	-6.19	97.88	111.50
1	A	4	VAL	N-CA-C	-6.14	94.41	111.00
1	A	229	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	A	4	VAL	CG1-CB-CG2	-6.09	101.15	110.90
1	A	82	ASP	CB-CG-OD1	-5.97	112.93	118.30
1	A	110	ARG	CD-NE-CZ	5.88	131.83	123.60
1	A	65	ASP	CB-CG-OD2	5.87	123.58	118.30
1	A	229	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	60	ILE	CA-CB-CG2	5.73	122.36	110.90
1	A	4	VAL	CA-C-N	-5.71	104.64	117.20
1	A	169	GLU	CB-CA-C	-5.67	99.06	110.40
1	A	74	LEU	CB-CA-C	-5.66	99.45	110.20
1	A	20	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	A	90	SER	N-CA-CB	5.61	118.92	110.50
1	A	122	THR	N-CA-CB	5.53	120.81	110.30
1	A	200	ASP	CB-CG-OD1	5.45	123.21	118.30
1	A	272	ASP	CB-CG-OD1	5.43	123.19	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	ARG	NH1-CZ-NH2	-5.37	113.49	119.40
1	A	1	VAL	CB-CA-C	5.36	121.59	111.40
1	A	272	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	A	20	ARG	NE-CZ-NH2	5.27	122.94	120.30
1	A	101	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	121	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	110	ARG	CB-CG-CD	5.06	124.75	111.60
1	A	70	TYR	CA-CB-CG	-5.05	103.80	113.40
1	A	107	TYR	CB-CG-CD1	-5.04	117.98	121.00

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	2326	0	2262	91	0
2	A	81	0	0	7	0
All	All	2407	0	2262	91	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 20.

All (91) 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:A:158:ARG:HH22	1:A:163:THR:HG23	1.31	0.95
1:A:44:ARG:HE	1:A:48:LEU:HD11	1.39	0.84
1:A:35:TRP:CD1	1:A:60:ILE:HD11	2.16	0.81
1:A:5:LEU:HA	2:A:326:HOH:O	1.82	0.80
1:A:44:ARG:HD2	1:A:44:ARG:O	1.82	0.80
1:A:122:THR:N	2:A:329:HOH:O	2.17	0.78
1:A:290:GLN:HA	1:A:290:GLN:NE2	1.99	0.77
1:A:138:HIS:HB3	1:A:139:PRO:HD2	1.66	0.76
1:A:224:SER:OG	1:A:227:GLU:HG3	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ASN:HD21	1:A:176:PHE:H	1.35	0.74
1:A:121:ARG:O	1:A:122:THR:HG23	1.88	0.74
1:A:91:ASN:H	1:A:91:ASN:ND2	1.86	0.74
1:A:4:VAL:HG12	1:A:5:LEU:HD12	1.70	0.72
1:A:163:THR:H	1:A:166:GLN:HE21	1.37	0.71
1:A:215:PHE:CE2	1:A:256:ILE:HD13	2.28	0.68
1:A:254:CYS:SG	1:A:270:ILE:HD13	2.34	0.68
1:A:109:PRO:HG2	1:A:255:HIS:CE1	2.29	0.68
1:A:290:GLN:HE21	1:A:290:GLN:HA	1.57	0.68
1:A:158:ARG:HH22	1:A:163:THR:CG2	2.06	0.67
1:A:4:VAL:HG12	1:A:5:LEU:CD1	2.25	0.67
1:A:102:ASP:O	1:A:131:ARG:NH1	2.29	0.65
1:A:113:TRP:CD1	1:A:270:ILE:HD12	2.32	0.65
1:A:101:ASP:OD2	1:A:103:LEU:HB2	1.97	0.64
1:A:3:GLN:HE22	1:A:116:ARG:HH21	1.45	0.64
1:A:214:ASN:HB3	1:A:231:MET:HE3	1.80	0.63
1:A:170:ASN:ND2	1:A:176:PHE:H	1.98	0.61
1:A:4:VAL:HA	2:A:325:HOH:O	2.00	0.60
1:A:233:GLU:O	1:A:236:LYS:HE3	2.01	0.60
1:A:44:ARG:C	1:A:44:ARG:HD2	2.22	0.60
1:A:52:VAL:HG22	1:A:133:TRP:CE2	2.37	0.59
1:A:168:LEU:O	1:A:171:LEU:HB2	2.02	0.59
1:A:173:SER:HB2	1:A:175:ARG:HG2	1.86	0.58
1:A:136:GLU:OE1	1:A:138:HIS:HE1	1.86	0.57
1:A:238:ASP:OD2	1:A:241:LYS:HD2	2.05	0.57
1:A:49:GLU:O	1:A:142:SER:HB3	2.05	0.56
1:A:4:VAL:HG13	1:A:5:LEU:HG	1.86	0.56
1:A:165:GLU:CD	1:A:165:GLU:H	2.07	0.56
1:A:44:ARG:NH1	1:A:44:ARG:HG3	2.20	0.55
1:A:42:GLU:HG3	1:A:45:LYS:HB3	1.87	0.55
1:A:13:LYS:O	1:A:17:GLU:HG3	2.07	0.55
1:A:44:ARG:NE	1:A:48:LEU:HD11	2.16	0.55
1:A:4:VAL:C	1:A:5:LEU:HG	2.28	0.54
1:A:42:GLU:HG3	1:A:45:LYS:CB	2.36	0.54
1:A:90:SER:HB2	1:A:151:ILE:O	2.08	0.54
1:A:210:MET:HG2	1:A:235:LYS:HG2	1.91	0.53
1:A:47:TYR:O	1:A:51:HIS:HD2	1.92	0.53
1:A:90:SER:OG	1:A:91:ASN:N	2.42	0.52
1:A:158:ARG:NH2	1:A:163:THR:HG23	2.13	0.51
1:A:148:GLU:HG3	1:A:149:PRO:HD2	1.92	0.51
1:A:134:LEU:O	1:A:136:GLU:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LYS:HD2	1:A:66:LYS:H	1.75	0.49
1:A:249:LYS:HE3	2:A:346:HOH:O	2.12	0.49
1:A:44:ARG:CG	1:A:44:ARG:HH11	2.25	0.49
1:A:44:ARG:HG3	1:A:44:ARG:HH11	1.76	0.49
1:A:42:GLU:O	1:A:46:GLU:HG3	2.12	0.48
1:A:224:SER:O	1:A:227:GLU:N	2.47	0.48
1:A:18:SER:HB3	1:A:23:LYS:HB2	1.95	0.48
1:A:235:LYS:HA	1:A:235:LYS:HD2	1.46	0.47
1:A:4:VAL:CG1	1:A:5:LEU:CD1	2.93	0.47
1:A:163:THR:H	1:A:166:GLN:NE2	2.10	0.47
1:A:121:ARG:H	1:A:121:ARG:HD2	1.79	0.46
1:A:215:PHE:HE2	1:A:256:ILE:HD13	1.78	0.46
1:A:44:ARG:HE	1:A:48:LEU:CD1	2.18	0.46
1:A:2:HIS:O	1:A:4:VAL:N	2.47	0.46
1:A:132:ASN:O	1:A:133:TRP:C	2.50	0.45
1:A:5:LEU:HD23	2:A:327:HOH:O	2.17	0.45
1:A:131:ARG:NH2	1:A:218:GLU:O	2.47	0.45
1:A:4:VAL:CG1	1:A:5:LEU:HG	2.47	0.45
1:A:215:PHE:CZ	1:A:256:ILE:CD1	3.00	0.44
1:A:289:SER:HB3	1:A:291:GLY:O	2.18	0.44
1:A:5:LEU:O	1:A:6:TYR:C	2.42	0.44
1:A:158:ARG:NH2	1:A:163:THR:CG2	2.77	0.44
1:A:138:HIS:HB3	1:A:139:PRO:CD	2.42	0.44
1:A:212:PHE:CE1	1:A:213:MET:HE2	2.54	0.43
1:A:236:LYS:HD3	1:A:236:LYS:N	2.17	0.43
1:A:248:ARG:HG3	1:A:249:LYS:HG2	2.00	0.43
1:A:215:PHE:CZ	1:A:256:ILE:HD13	2.54	0.43
1:A:13:LYS:HD3	1:A:17:GLU:OE2	2.18	0.43
1:A:121:ARG:HA	2:A:329:HOH:O	2.18	0.43
1:A:15:LEU:HA	1:A:15:LEU:HD23	1.76	0.42
1:A:210:MET:CG	1:A:235:LYS:HG2	2.48	0.42
1:A:103:LEU:HD13	2:A:341:HOH:O	2.20	0.42
1:A:134:LEU:O	1:A:135:LYS:C	2.57	0.42
1:A:121:ARG:HD2	1:A:121:ARG:N	2.35	0.42
1:A:186:ARG:HB3	1:A:193:GLU:OE2	2.20	0.42
1:A:215:PHE:CE2	1:A:256:ILE:CD1	3.00	0.42
1:A:6:TYR:CD2	1:A:7:ARG:N	2.88	0.41
1:A:145:SER:C	1:A:146:ARG:HG2	2.40	0.41
1:A:126:LEU:HA	1:A:126:LEU:HD23	1.72	0.41
1:A:3:GLN:NE2	1:A:116:ARG:HH21	2.16	0.41
1:A:36:TYR:CG	1:A:41:ARG:HB2	2.57	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	290/296 (98%)	275 (95%)	10 (3%)	5 (2%)	9 4

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	122	THR
1	A	135	LYS
1	A	292	LYS
1	A	158	ARG

5.3.2 Protein sidechains [i](#)

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	244/245 (100%)	205 (84%)	39 (16%)	2 1

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	VAL
1	A	2	HIS
1	A	5	LEU

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Mol	Chain	Res	Type
1	A	7	ARG
1	A	13	LYS
1	A	15	LEU
1	A	44	ARG
1	A	50	ARG
1	A	61	GLU
1	A	66	LYS
1	A	82	ASP
1	A	87	LEU
1	A	90	SER
1	A	91	ASN
1	A	103	LEU
1	A	110	ARG
1	A	121	ARG
1	A	124	SER
1	A	126	LEU
1	A	134	LEU
1	A	146	ARG
1	A	151	ILE
1	A	153	LYS
1	A	158	ARG
1	A	159	SER
1	A	165	GLU
1	A	175	ARG
1	A	184	GLN
1	A	188	LEU
1	A	213	MET
1	A	226	GLU
1	A	229	ARG
1	A	233	GLU
1	A	235	LYS
1	A	236	LYS
1	A	249	LYS
1	A	258	LEU
1	A	289	SER
1	A	290	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	51	HIS

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Mol	Chain	Res	Type
1	A	132	ASN
1	A	138	HIS
1	A	157	ASN
1	A	166	GLN
1	A	170	ASN
1	A	184	GLN
1	A	209	ASN
1	A	255	HIS
1	A	290	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
1	CSO	A	247	1	3,6,7	0.63	0	0,6,8	0.00	-

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
1	CSO	A	247	1	-	0/1/5/7	-

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.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.