



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:26 PM UTC

PDB ID : 2ORA / pdb_00002ora
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

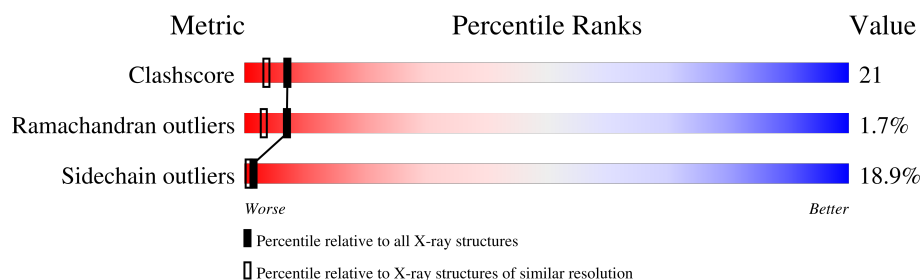
1 Overall quality at a glance

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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	296	

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
1	A	293	Total	C	N	O	S	0	0	0
			2326	1486	405	426	9			

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
2	A	81	Total	O	0	0
			81	81		

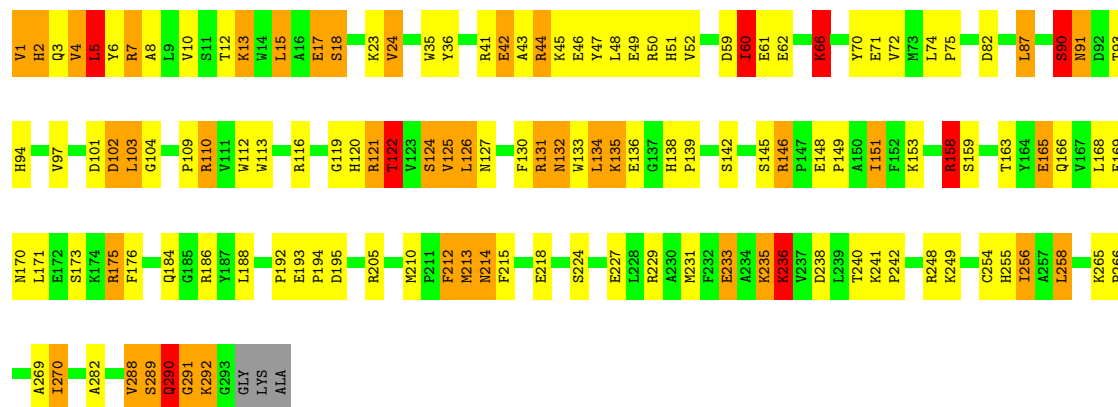
3 Residue-property plots

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. 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

Chain A: 



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

5.1 Standard geometry

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	0.97	1/2385 (0.0%)	1.92	64/3235 (2.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	291	GLY	C-N	5.22	1.41	1.33

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	VAL	N-CA-C	-18.87	94.41	113.47
1	A	5	LEU	O-C-N	-12.76	105.63	122.59
1	A	5	LEU	CA-C-N	-9.92	100.22	121.45
1	A	5	LEU	C-N-CA	-9.92	100.22	121.45
1	A	66	LYS	N-CA-CB	9.47	126.42	110.32
1	A	4	VAL	O-C-N	9.16	133.76	122.03
1	A	266	PRO	CB-CA-C	-8.85	100.09	110.00
1	A	24	VAL	N-CA-CB	8.35	119.63	110.53
1	A	269	ALA	CA-C-N	-7.60	113.76	123.19
1	A	269	ALA	C-N-CA	-7.60	113.76	123.19
1	A	93	THR	N-CA-C	7.24	120.99	110.28
1	A	125	VAL	N-CA-CB	-7.20	97.88	111.21
1	A	102	ASP	CA-CB-CG	-7.12	105.48	112.60
1	A	169	GLU	CB-CA-C	-7.07	99.06	110.79
1	A	60	ILE	CA-CB-CG2	6.98	122.36	110.50
1	A	110	ARG	NE-CZ-NH1	6.93	128.43	121.50
1	A	112	TRP	N-CA-C	-6.67	103.70	110.97
1	A	94	HIS	N-CA-C	-6.62	98.44	108.96
1	A	75	PRO	CA-C-N	-6.56	109.63	122.02
1	A	75	PRO	C-N-CA	-6.56	109.63	122.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	PHE	N-CA-C	6.53	119.24	111.33
1	A	194	PRO	CB-CA-C	-6.38	100.92	110.17
1	A	205	ARG	N-CA-CB	6.35	119.42	109.83
1	A	258	LEU	CB-CA-C	-6.34	100.89	110.90
1	A	214	ASN	CA-CB-CG	-6.24	106.36	112.60
1	A	74	LEU	CB-CA-C	-6.17	99.45	109.56
1	A	5	LEU	CB-CA-C	-6.12	98.25	110.42
1	A	122	THR	N-CA-CB	6.11	120.81	110.49
1	A	75	PRO	CB-CA-C	-6.05	101.57	111.56
1	A	132	ASN	CA-CB-CG	-6.04	106.56	112.60
1	A	265	LYS	CB-CA-C	-5.95	104.26	110.33
1	A	290	GLN	N-CA-C	-5.91	103.30	111.81
1	A	120	HIS	CB-CA-C	-5.88	101.38	110.78
1	A	110	ARG	CB-CG-CD	5.85	124.75	111.30
1	A	236	LYS	CA-CB-CG	-5.81	102.47	114.10
1	A	4	VAL	N-CA-CB	5.77	119.20	112.33
1	A	59	ASP	CA-CB-CG	5.76	118.36	112.60
1	A	288	VAL	N-CA-CB	-5.71	101.25	111.92
1	A	59	ASP	N-CA-CB	-5.70	101.85	110.35
1	A	70	TYR	CA-CB-CG	-5.61	103.80	113.90
1	A	282	ALA	N-CA-C	5.60	118.79	110.39
1	A	87	LEU	N-CA-C	-5.60	106.30	113.02
1	A	71	GLU	N-CA-C	5.41	118.36	109.76
1	A	62	GLU	CB-CG-CD	-5.39	103.43	112.60
1	A	1	VAL	CB-CA-C	5.36	121.59	111.40
1	A	119	GLY	N-CA-C	5.35	122.98	115.43
1	A	292	LYS	N-CA-C	5.35	122.19	110.80
1	A	18	SER	CA-C-O	5.34	126.11	119.97
1	A	90	SER	N-CA-CB	5.33	118.92	110.87
1	A	288	VAL	N-CA-C	5.32	117.43	108.81
1	A	110	ARG	CD-NE-CZ	5.31	131.83	124.40
1	A	24	VAL	N-CA-C	5.30	115.88	108.89
1	A	192	PRO	CB-CA-C	-5.30	102.49	110.17
1	A	131	ARG	NE-CZ-NH2	5.26	123.94	119.20
1	A	242	PRO	N-CA-CB	5.26	107.93	103.35
1	A	97	VAL	CB-CA-C	-5.26	102.40	110.50
1	A	256	ILE	CB-CA-C	-5.26	104.96	112.22
1	A	195	ASP	CB-CA-C	-5.23	104.17	111.80
1	A	104	GLY	N-CA-C	-5.19	107.72	113.79
1	A	270	ILE	N-CA-C	5.18	115.43	108.17
1	A	43	ALA	N-CA-C	5.11	117.25	111.11
1	A	258	LEU	CA-C-N	-5.09	113.06	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	258	LEU	C-N-CA	-5.09	113.06	120.29
1	A	127	ASN	CA-CB-CG	5.01	117.61	112.60

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	96	0
2	A	81	0	0	7	0
All	All	2407	0	2262	96	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 21.

All (96) 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:O	1:A:44:ARG:HD2	1.82	0.80
1:A:122:THR:N	2:A:329:HOH:O	2.17	0.78
1:A:290:GLN:NE2	1:A:290:GLN:HA	1.99	0.77
1:A:212:PHE:CE1	1:A:213:MET:HE3	2.19	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
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:ND2	1:A:91:ASN:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:A:290:GLN:HE21	1.57	0.68
1:A:4:VAL:HG12	1:A:5:LEU:CD1	2.25	0.67
1:A:158:ARG:HH22	1:A:163:THR:CG2	2.06	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:44:ARG:HD2	1:A:44:ARG:C	2.22	0.64
1:A:3:GLN:HE22	1:A:116:ARG:HH21	1.45	0.64
1:A:101:ASP:OD2	1:A:103:LEU:HB2	1.97	0.64
1:A:170:ASN:ND2	1:A:176:PHE:H	1.98	0.61
1:A:165:GLU:H	1:A:165:GLU:CD	2.07	0.60
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:52:VAL:HG22	1:A:133:TRP:CE2	2.37	0.59
1:A:4:VAL:C	1:A:5:LEU:HG	2.28	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:4:VAL:HG13	1:A:5:LEU:HG	1.86	0.56
1:A:49:GLU:O	1:A:142:SER:HB3	2.05	0.56
1:A:44:ARG:HG3	1:A:44:ARG:NH1	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: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:214:ASN:HB3	1:A:231:MET:HE3	1.91	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
1:A:132:ASN:O	1:A:133:TRP:C	2.50	0.51
1:A:66:LYS:HD2	1:A:66:LYS:H	1.75	0.49
1:A:44:ARG:HG3	1:A:44:ARG:HH11	1.76	0.49
1:A:44:ARG:HH11	1:A:44:ARG:CG	2.25	0.49
1:A:249:LYS:HE3	2:A:346:HOH:O	2.12	0.49
1:A:42:GLU:O	1:A:46:GLU:HG3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:SER:O	1:A:227:GLU:N	2.47	0.48
1:A:5:LEU:O	1:A:6:TYR:C	2.42	0.48
1:A:18:SER:HB3	1:A:23:LYS:HB2	1.95	0.48
1:A:4:VAL:CG1	1:A:5:LEU:CD1	2.93	0.47
1:A:134:LEU:O	1:A:135:LYS:C	2.57	0.47
1:A:235:LYS:HA	1:A:235:LYS:HD2	1.46	0.47
1:A:163:THR:H	1:A:166:GLN:NE2	2.10	0.47
1:A:212:PHE:CD1	1:A:213:MET:HE3	2.50	0.46
1:A:121:ARG:HD2	1:A:121:ARG:H	1.79	0.46
1:A:215:PHE:HE2	1:A:256:ILE:HD13	1.78	0.46
1:A:145:SER:C	1:A:146:ARG:HG2	2.40	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:5:LEU:HD23	2:A:327:HOH:O	2.17	0.45
1:A:4:VAL:CG1	1:A:5:LEU:HG	2.47	0.45
1:A:131:ARG:NH2	1:A:218:GLU:O	2.47	0.45
1:A:8:ALA:C	1:A:124:SER:HB3	2.42	0.44
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: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:236:LYS:N	1:A:236:LYS:HD3	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:HD23	1:A:15:LEU:HA	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: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:51:HIS:O	1:A:52:VAL:C	2.63	0.41
1:A:126:LEU:HD23	1:A:126:LEU:HA	1.72	0.41
1:A:3:GLN:NE2	1:A:116:ARG:HH21	2.16	0.41
1:A:238:ASP:OD1	1:A:240:THR:OG1	2.29	0.41
1:A:130:PHE:O	1:A:131:ARG:C	2.64	0.40
1:A:36:TYR:CG	1:A:41:ARG:HB2	2.57	0.40

There are no symmetry-related clashes.

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	290/296 (98%)	275 (95%)	10 (3%)	5 (2%)	7 3

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

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%)	198 (81%)	46 (19%)	1 1

All (46) 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
1	A	7	ARG
1	A	10	VAL
1	A	12	THR

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Mol	Chain	Res	Type
1	A	13	LYS
1	A	15	LEU
1	A	17	GLU
1	A	24	VAL
1	A	42	GLU
1	A	44	ARG
1	A	50	ARG
1	A	60	ILE
1	A	61	GLU
1	A	66	LYS
1	A	72	VAL
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	125	VAL
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	229	ARG
1	A	233	GLU
1	A	235	LYS
1	A	236	LYS
1	A	258	LEU
1	A	288	VAL
1	A	289	SER
1	A	290	GLN

Sometimes 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
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 ⓘ

There are no RNA molecules in this entry.

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

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	0.61	0	1,6,8	0.47	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
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 oligosaccharides 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.