Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:58 PM GMT

PDB ID	:	1RHS
Title	:	SULFUR-SUBSTITUTED RHODANESE
Authors	:	Zanotti, G.; Gliubich, F.; Colapietro, M.; Barba, L.
Deposited on	:	1997-07-16
Resolution	:	1.36 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

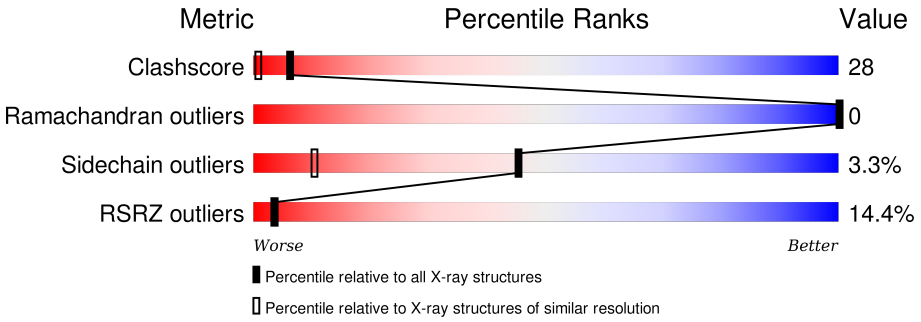
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.36 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	102246	2337 (1.40-1.32)
Ramachandran outliers	100387	2280 (1.40-1.32)
Sidechain outliers	100360	2279 (1.40-1.32)
RSRZ outliers	91569	2199 (1.40-1.32)

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 <=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	296	14% 72% 23%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2733 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 SULFUR-SUBSTITUTED RHODANESE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	0	0
			2326	1486	405	425	10			

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is water.

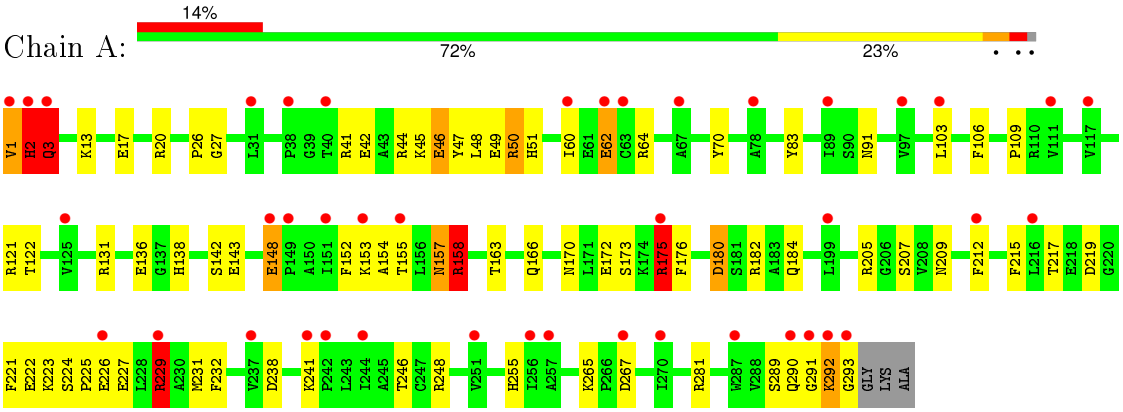
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	407	Total	O	0	0
			407	407		

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 (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: SULFUR-SUBSTITUTED RHODANESE

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	154.36Å 49.31Å 41.68Å 90.00° 99.81° 90.00°	Depositor
Resolution (Å)	25.00 – 1.36 28.52 – 1.31	Depositor EDS
% Data completeness (in resolution range)	74.0 (25.00-1.36) 66.4 (28.52-1.31)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	0.63 (at 1.30Å)	Xtriage
Refinement program	SHELXL-93	Depositor
R, R_{free}	0.169 , 0.229 0.203 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	5.8	Xtriage
Anisotropy	0.955	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.55 , 70.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	0 of 56060 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	2733	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CSS

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	1.33	10/2385 (0.4%)	1.66	38/3235 (1.2%)

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	A	1	6

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	17	GLU	CD-OE2	-6.95	1.18	1.25
1	A	148	GLU	CD-OE2	6.74	1.33	1.25
1	A	148	GLU	CB-CG	-6.01	1.40	1.52
1	A	175	ARG	CZ-NH1	5.95	1.40	1.33
1	A	148	GLU	CG-CD	-5.86	1.43	1.51
1	A	122	THR	CB-OG1	-5.55	1.32	1.43
1	A	3	GLN	CA-CB	-5.50	1.41	1.53
1	A	109	PRO	CA-CB	-5.29	1.43	1.53
1	A	207	SER	CB-OG	-5.22	1.35	1.42
1	A	83	TYR	CD2-CE2	-5.13	1.31	1.39

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	205	ARG	NE-CZ-NH1	16.43	128.51	120.30
1	A	281	ARG	NE-CZ-NH1	-15.69	112.46	120.30
1	A	175	ARG	NE-CZ-NH2	15.36	127.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	148	GLU	CB-CG-CD	14.63	153.71	114.20
1	A	158	ARG	NE-CZ-NH2	13.59	127.09	120.30
1	A	20	ARG	NE-CZ-NH1	12.44	126.52	120.30
1	A	281	ARG	NE-CZ-NH2	12.25	126.42	120.30
1	A	175	ARG	NE-CZ-NH1	-11.76	114.42	120.30
1	A	158	ARG	NE-CZ-NH1	-11.62	114.49	120.30
1	A	205	ARG	CD-NE-CZ	11.00	139.00	123.60
1	A	20	ARG	NE-CZ-NH2	-10.28	115.16	120.30
1	A	182	ARG	NE-CZ-NH2	-9.10	115.75	120.30
1	A	205	ARG	NE-CZ-NH2	-8.73	115.94	120.30
1	A	1	VAL	CB-CA-C	8.54	127.63	111.40
1	A	148	GLU	OE1-CD-OE2	-8.24	113.41	123.30
1	A	219	ASP	CB-CG-OD1	7.90	125.41	118.30
1	A	64	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	A	62	GLU	OE1-CD-OE2	7.45	132.24	123.30
1	A	152	PHE	CB-CG-CD2	-7.35	115.66	120.80
1	A	70	TYR	CB-CG-CD2	-7.29	116.62	121.00
1	A	158	ARG	CD-NE-CZ	7.17	133.64	123.60
1	A	2	HIS	CB-CA-C	-6.86	96.67	110.40
1	A	3	GLN	N-CA-CB	6.63	122.53	110.60
1	A	44	ARG	CD-NE-CZ	6.39	132.54	123.60
1	A	219	ASP	CB-CG-OD2	-6.35	112.59	118.30
1	A	44	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	A	122	THR	CA-CB-OG1	5.64	120.84	109.00
1	A	221	PHE	CB-CG-CD2	-5.61	116.87	120.80
1	A	3	GLN	O-C-N	5.51	131.51	122.70
1	A	290	GLN	C-N-CA	-5.48	110.80	122.30
1	A	215	PHE	CB-CG-CD1	5.46	124.62	120.80
1	A	46	GLU	OE1-CD-OE2	-5.44	116.78	123.30
1	A	50	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	232	PHE	CB-CG-CD1	-5.32	117.07	120.80
1	A	180	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	A	205	ARG	NH1-CZ-NH2	-5.22	113.65	119.40
1	A	70	TYR	CB-CG-CD1	5.11	124.06	121.00
1	A	152	PHE	CB-CG-CD1	5.10	124.37	120.80

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1	VAL	CA

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	VAL	Peptide
1	A	131	ARG	Sidechain
1	A	158	ARG	Sidechain
1	A	175	ARG	Sidechain
1	A	229	ARG	Sidechain
1	A	248	ARG	Sidechain

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	2326	0	2262	128	9
2	A	407	0	0	56	8
All	All	2733	0	2262	128	10

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 28.

All (128) 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:2:HIS:NE2	1:A:121:ARG:CD	1.81	1.41
1:A:2:HIS:NE2	1:A:121:ARG:HD2	1.11	1.38
1:A:229:ARG:CB	1:A:229:ARG:HH11	1.49	1.24
1:A:229:ARG:HB3	1:A:229:ARG:NH1	1.52	1.24
1:A:223:LYS:HB3	2:A:346:HOH:O	1.34	1.24
1:A:227:GLU:HB2	2:A:346:HOH:O	1.38	1.22
1:A:13:LYS:HA	2:A:671:HOH:O	1.40	1.21
1:A:2:HIS:CD2	2:A:461:HOH:O	1.88	1.20
1:A:292:LYS:H	1:A:293:GLY:HA3	1.00	1.15
1:A:153:LYS:HD2	1:A:153:LYS:C	1.49	1.14
1:A:2:HIS:CE1	1:A:121:ARG:HD2	1.82	1.12
1:A:47:TYR:HE2	2:A:446:HOH:O	1.31	1.12
1:A:50:ARG:N	2:A:462:HOH:O	1.83	1.09
1:A:46:GLU:HA	2:A:391:HOH:O	1.48	1.08
1:A:50:ARG:HG3	2:A:462:HOH:O	1.53	1.08
1:A:226:GLU:HA	1:A:229:ARG:HH12	0.95	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:LYS:CA	2:A:671:HOH:O	1.98	1.06
1:A:2:HIS:NE2	2:A:461:HOH:O	1.86	1.05
1:A:265:LYS:NZ	1:A:267:ASP:OD1	1.88	1.04
1:A:3:GLN:OE1	1:A:3:GLN:HA	1.43	1.03
1:A:46:GLU:CA	2:A:391:HOH:O	2.04	1.02
1:A:13:LYS:CB	2:A:671:HOH:O	2.06	1.02
1:A:170:ASN:HD22	1:A:175:ARG:HH11	1.09	0.99
1:A:2:HIS:NE2	1:A:121:ARG:NE	2.10	0.99
1:A:292:LYS:N	1:A:293:GLY:HA3	1.75	0.99
1:A:170:ASN:HB2	1:A:175:ARG:NH1	1.77	0.99
1:A:224:SER:N	2:A:346:HOH:O	1.96	0.96
1:A:2:HIS:CE1	1:A:121:ARG:CD	2.45	0.95
1:A:226:GLU:HA	1:A:229:ARG:NH1	1.80	0.95
1:A:103:LEU:CD1	2:A:658:HOH:O	2.13	0.94
1:A:292:LYS:H	1:A:293:GLY:CA	1.79	0.94
1:A:226:GLU:CA	1:A:229:ARG:HH12	1.80	0.93
1:A:217:THR:HG23	2:A:348:HOH:O	0.74	0.92
1:A:238:ASP:OD2	1:A:241:LYS:NZ	2.03	0.91
1:A:153:LYS:C	1:A:153:LYS:CD	2.40	0.91
1:A:173:SER:OG	1:A:175:ARG:HG2	1.72	0.90
1:A:170:ASN:HD21	1:A:176:PHE:H	1.11	0.89
1:A:49:GLU:HA	2:A:467:HOH:O	1.73	0.89
1:A:229:ARG:HB3	1:A:229:ARG:HH11	0.72	0.88
1:A:170:ASN:HB2	1:A:175:ARG:HH12	1.36	0.86
1:A:49:GLU:C	2:A:462:HOH:O	2.09	0.84
1:A:170:ASN:ND2	1:A:175:ARG:HH11	1.75	0.83
1:A:229:ARG:CB	1:A:229:ARG:NH1	2.24	0.82
1:A:153:LYS:O	1:A:153:LYS:HD2	1.79	0.81
1:A:49:GLU:CB	2:A:462:HOH:O	2.28	0.81
1:A:222:GLU:HG2	2:A:347:HOH:O	1.80	0.80
1:A:170:ASN:CB	1:A:175:ARG:NH1	2.44	0.80
1:A:175:ARG:HG3	1:A:175:ARG:HH11	1.46	0.79
1:A:26:PRO:C	2:A:411:HOH:O	2.19	0.79
1:A:91:ASN:HD21	1:A:153:LYS:H	1.27	0.79
1:A:142:SER:HB2	2:A:467:HOH:O	1.82	0.79
1:A:106:PHE:CE2	2:A:443:HOH:O	2.36	0.78
1:A:41:ARG:CB	2:A:380:HOH:O	2.31	0.77
1:A:163:THR:H	1:A:166:GLN:HE21	1.33	0.77
1:A:175:ARG:CG	1:A:175:ARG:HH11	1.98	0.76
1:A:103:LEU:HD13	2:A:658:HOH:O	1.80	0.75
1:A:2:HIS:CE1	1:A:121:ARG:NE	2.54	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:LEU:O	2:A:467:HOH:O	2.04	0.74
1:A:153:LYS:HD2	1:A:154:ALA:N	2.03	0.73
1:A:175:ARG:HG3	1:A:176:PHE:HD1	1.54	0.73
1:A:49:GLU:HB2	2:A:462:HOH:O	1.88	0.71
1:A:13:LYS:HB2	2:A:671:HOH:O	1.81	0.71
1:A:170:ASN:ND2	1:A:175:ARG:NH1	2.40	0.70
1:A:27:GLY:N	2:A:411:HOH:O	2.26	0.69
1:A:175:ARG:HG3	1:A:176:PHE:CD1	2.27	0.68
1:A:46:GLU:CB	2:A:391:HOH:O	2.38	0.68
1:A:170:ASN:HD22	1:A:175:ARG:NH1	1.87	0.67
1:A:41:ARG:HB3	2:A:380:HOH:O	1.94	0.67
1:A:175:ARG:NH1	1:A:175:ARG:HG3	2.09	0.67
1:A:170:ASN:ND2	1:A:176:PHE:H	1.90	0.66
1:A:103:LEU:HD11	2:A:658:HOH:O	1.84	0.66
1:A:27:GLY:N	2:A:636:HOH:O	2.24	0.65
1:A:50:ARG:CB	2:A:462:HOH:O	2.45	0.65
1:A:106:PHE:CD2	2:A:443:HOH:O	2.46	0.65
1:A:47:TYR:O	1:A:51:HIS:HD2	1.80	0.65
1:A:227:GLU:OE1	2:A:346:HOH:O	2.15	0.65
1:A:291:GLY:N	1:A:292:LYS:HA	2.11	0.64
1:A:170:ASN:HD22	1:A:175:ARG:CG	2.11	0.64
1:A:106:PHE:O	1:A:255:HIS:HE1	1.82	0.63
1:A:153:LYS:HE2	1:A:155:THR:OG1	1.99	0.63
1:A:289:SER:O	1:A:292:LYS:HA	1.99	0.63
1:A:222:GLU:CG	2:A:347:HOH:O	2.43	0.62
1:A:138:HIS:HD2	2:A:448:HOH:O	1.83	0.62
1:A:142:SER:CB	2:A:467:HOH:O	2.45	0.59
1:A:157:ASN:HD22	1:A:157:ASN:C	2.05	0.58
1:A:223:LYS:C	2:A:346:HOH:O	2.37	0.57
1:A:2:HIS:CE1	2:A:461:HOH:O	2.44	0.55
1:A:222:GLU:HB3	2:A:347:HOH:O	2.07	0.55
1:A:229:ARG:HB2	1:A:229:ARG:NH1	2.19	0.54
1:A:170:ASN:HD22	1:A:175:ARG:HG2	1.71	0.54
1:A:173:SER:OG	1:A:175:ARG:CG	2.52	0.54
1:A:175:ARG:NH1	1:A:176:PHE:HD1	2.06	0.54
1:A:212:PHE:HZ	2:A:443:HOH:O	1.91	0.53
1:A:136:GLU:OE1	1:A:138:HIS:HE1	1.91	0.52
1:A:225:PRO:O	1:A:229:ARG:NH1	2.42	0.52
1:A:170:ASN:HD22	1:A:175:ARG:HG3	1.74	0.52
1:A:229:ARG:HB2	1:A:229:ARG:CZ	2.41	0.51
1:A:292:LYS:N	1:A:293:GLY:CA	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:HIS:CD2	1:A:121:ARG:HE	2.29	0.50
1:A:46:GLU:HB3	2:A:391:HOH:O	2.07	0.50
1:A:153:LYS:CE	1:A:155:THR:OG1	2.60	0.50
1:A:175:ARG:NH1	1:A:176:PHE:CD1	2.80	0.49
1:A:231:MET:N	2:A:397:HOH:O	2.27	0.49
1:A:46:GLU:O	2:A:391:HOH:O	2.20	0.48
1:A:222:GLU:CB	2:A:347:HOH:O	2.62	0.47
1:A:289:SER:HB3	1:A:292:LYS:O	2.13	0.47
1:A:143:GLU:HB3	2:A:452:HOH:O	2.14	0.47
1:A:106:PHE:HE2	2:A:443:HOH:O	1.87	0.47
1:A:50:ARG:CG	2:A:462:HOH:O	2.28	0.46
1:A:26:PRO:HB2	2:A:411:HOH:O	2.15	0.46
1:A:217:THR:CG2	2:A:348:HOH:O	1.64	0.46
1:A:291:GLY:H	1:A:292:LYS:HA	1.78	0.46
1:A:170:ASN:ND2	1:A:175:ARG:HG3	2.30	0.46
1:A:158:ARG:NH2	1:A:166:GLN:HE22	2.14	0.45
1:A:13:LYS:HG3	2:A:671:HOH:O	2.17	0.44
1:A:170:ASN:CG	1:A:175:ARG:NH1	2.71	0.44
1:A:238:ASP:OD2	1:A:241:LYS:CE	2.65	0.44
1:A:180:ASP:HA	1:A:246:THR:O	2.18	0.43
1:A:170:ASN:ND2	1:A:175:ARG:CG	2.80	0.43
1:A:27:GLY:CA	2:A:411:HOH:O	2.65	0.43
1:A:238:ASP:CG	1:A:241:LYS:HZ1	2.10	0.43
1:A:62:GLU:HG3	2:A:694:HOH:O	2.19	0.43
1:A:2:HIS:NE2	1:A:121:ARG:CB	2.82	0.42
1:A:292:LYS:HG2	1:A:292:LYS:O	2.15	0.41
1:A:184:GLN:HA	1:A:209:ASN:HD21	1.86	0.41
1:A:223:LYS:CA	2:A:346:HOH:O	2.60	0.41
1:A:26:PRO:HB2	2:A:636:HOH:O	2.20	0.40
1:A:175:ARG:H	1:A:175:ARG:HG2	1.58	0.40

All (10) 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:172:GLU:OE2	1:A:172:GLU:OE2[2_657]	0.93	1.27
1:A:42:GLU:CG	2:A:527:HOH:O[4_557]	1.01	1.19
1:A:45:LYS:CB	2:A:663:HOH:O[4_557]	1.07	1.13
1:A:42:GLU:CB	2:A:527:HOH:O[4_557]	1.36	0.84
1:A:45:LYS:CG	2:A:663:HOH:O[4_557]	1.36	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:GLU:CD	2:A:527:HOH:O[4_557]	1.49	0.71
1:A:45:LYS:CD	2:A:663:HOH:O[4_557]	1.67	0.53
2:A:533:HOH:O	2:A:668:HOH:O[1_554]	2.00	0.20
1:A:42:GLU:OE1	2:A:527:HOH:O[4_557]	2.14	0.06
1:A:172:GLU:CD	1:A:172:GLU:OE2[2_657]	2.18	0.02

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%)	277 (96%)	13 (4%)	0	100 100

There are no Ramachandran outliers to report.

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%)	236 (97%)	8 (3%)	45 10

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	HIS
1	A	3	GLN
1	A	60	ILE

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Mol	Chain	Res	Type
1	A	148	GLU
1	A	157	ASN
1	A	158	ARG
1	A	229	ARG
1	A	292	LYS

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	51	HIS
1	A	91	ASN
1	A	132	ASN
1	A	138	HIS
1	A	157	ASN
1	A	166	GLN
1	A	170	ASN
1	A	191	GLN
1	A	209	ASN
1	A	255	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)

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	CSS	A	247	1	4,6,7	0.83	0	3,6,8	0.90	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	CSS	A	247	1	-	0/1/5/7	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.

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

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^{th} 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	292/296 (98%)	1.44	42 (14%) 3 3	11, 16, 26, 114	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	VAL	26.6
1	A	2	HIS	14.8
1	A	293	GLY	14.6
1	A	291	GLY	12.7
1	A	292	LYS	10.3
1	A	175	ARG	4.1
1	A	290	GLN	4.1
1	A	38	PRO	3.3
1	A	60	ILE	3.1
1	A	242	PRO	3.0
1	A	148	GLU	2.9
1	A	3	GLN	2.8
1	A	256	ILE	2.7
1	A	257	ALA	2.7
1	A	229	ARG	2.6
1	A	267	ASP	2.6
1	A	111	VAL	2.6
1	A	89	ILE	2.5
1	A	125	VAL	2.5
1	A	212	PHE	2.5
1	A	97	VAL	2.5
1	A	67	ALA	2.4
1	A	270	ILE	2.4
1	A	151	ILE	2.4
1	A	117	VAL	2.3
1	A	199	LEU	2.3
1	A	149	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	287	TRP	2.2
1	A	78	ALA	2.2
1	A	237	VAL	2.2
1	A	241	LYS	2.2
1	A	31	LEU	2.2
1	A	226	GLU	2.2
1	A	63	CYS	2.1
1	A	40	THR	2.1
1	A	155	THR	2.1
1	A	62	GLU	2.1
1	A	251	VAL	2.1
1	A	103	LEU	2.1
1	A	216	LEU	2.1
1	A	244	ILE	2.1
1	A	153	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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^{th} 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(Å^2)	Q<0.9
1	CSS	A	247	7/8	0.99	0.11	-	11,11,12,13	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.