Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2024 – 11:51 AM EDT

PDB ID	:	1ORB
Title	:	ACTIVE SITE STRUCTURAL FEATURES FOR CHEMICALLY MODIFIED FORMS OF RHODANESE
Authors	:	Gliubich, F.; Gazerro, M.; Zanotti, G.; Delbono, S.; Berni, R.
Deposited on	:	1995-07-24
Resolution	:	2.00 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:

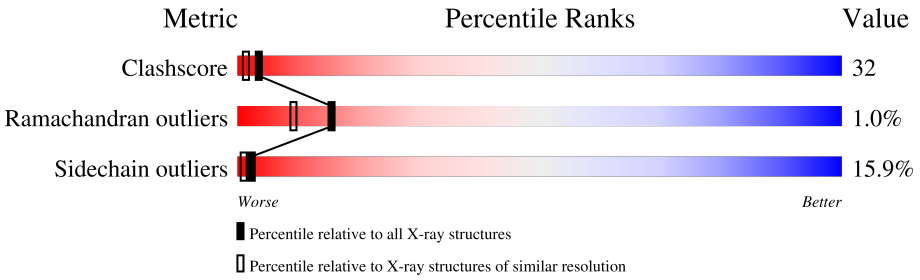
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.00 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 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	296	41% 40% 16%

2 Entry composition

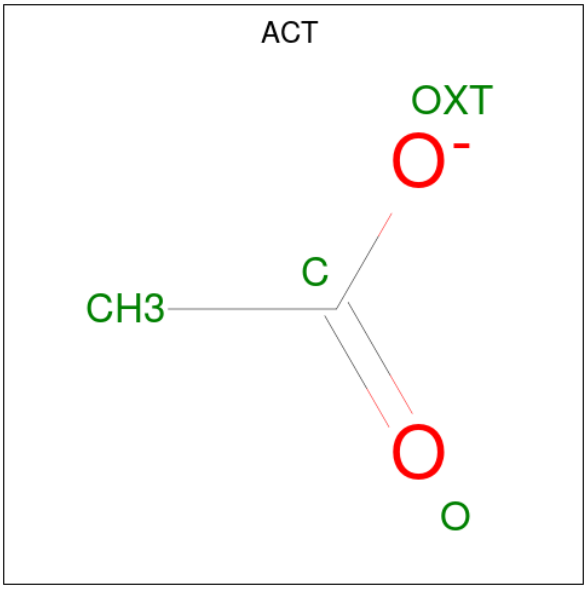
There are 3 unique types of molecules in this entry. The entry contains 2430 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CARBOXYMETHYLATED RHODANESE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	0	0
			2325	1486	405	425	9			

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	101	Total	O	0	0
			101	101		

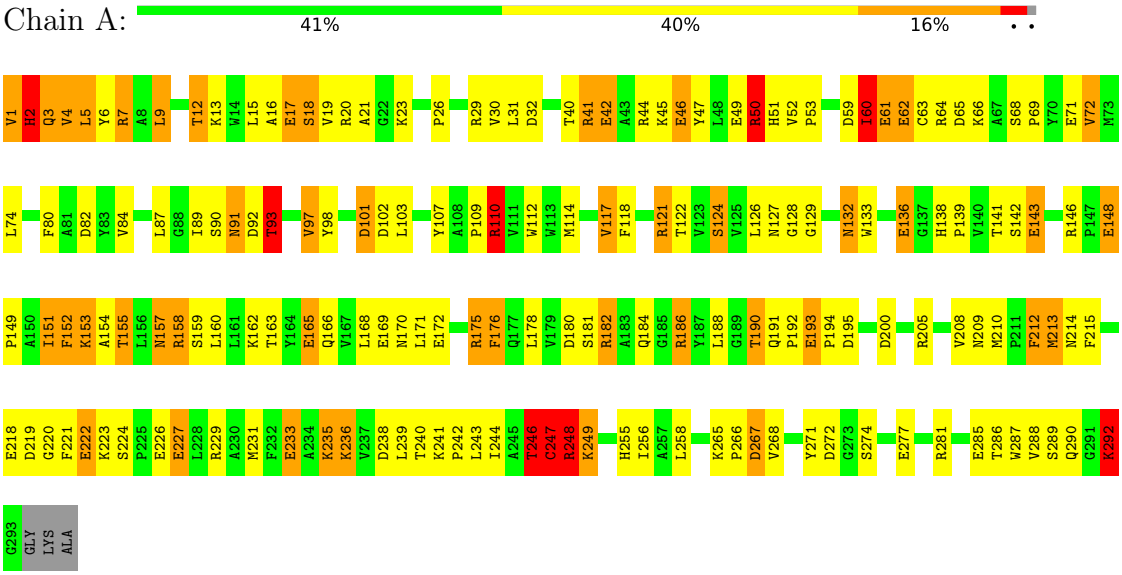
3 Residue-property plots (i)

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: CARBOXYMETHYLATED RHODANESE

Chain A:



4 Data and refinement statistics (i)

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 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (9.00-2.00)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.187 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2430	wwPDB-VP
Average B, all atoms (Å^2)	41.0	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: ACT

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	19/2392 (0.8%)	1.87	69/3246 (2.1%)

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	A	1	0

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	285	GLU	CD-OE2	6.64	1.32	1.25
1	A	193	GLU	CD-OE2	6.43	1.32	1.25
1	A	233	GLU	CD-OE1	5.98	1.32	1.25
1	A	136	GLU	CD-OE1	5.95	1.32	1.25
1	A	218	GLU	CD-OE1	5.87	1.32	1.25
1	A	169	GLU	CD-OE1	5.85	1.32	1.25
1	A	42	GLU	CD-OE2	5.76	1.31	1.25
1	A	17	GLU	CD-OE2	5.63	1.31	1.25
1	A	277	GLU	CD-OE2	5.62	1.31	1.25
1	A	226	GLU	CD-OE2	5.51	1.31	1.25
1	A	143	GLU	CD-OE2	5.46	1.31	1.25
1	A	165	GLU	CD-OE2	5.43	1.31	1.25
1	A	62	GLU	CD-OE2	5.39	1.31	1.25
1	A	148	GLU	CD-OE1	5.36	1.31	1.25
1	A	61	GLU	CD-OE2	5.24	1.31	1.25
1	A	49	GLU	CD-OE1	5.23	1.31	1.25
1	A	227	GLU	CD-OE2	5.19	1.31	1.25
1	A	222	GLU	CD-OE2	5.17	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	172	GLU	CD-OE2	5.03	1.31	1.25

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	248	ARG	NE-CZ-NH1	20.01	130.30	120.30
1	A	110	ARG	NE-CZ-NH2	-16.97	111.82	120.30
1	A	248	ARG	NE-CZ-NH2	-16.83	111.88	120.30
1	A	158	ARG	NE-CZ-NH1	13.29	126.94	120.30
1	A	110	ARG	NE-CZ-NH1	13.05	126.83	120.30
1	A	41	ARG	NE-CZ-NH2	-11.78	114.41	120.30
1	A	102	ASP	CB-CG-OD1	11.09	128.28	118.30
1	A	60	ILE	CB-CG1-CD1	10.13	142.27	113.90
1	A	102	ASP	CB-CG-OD2	-9.57	109.68	118.30
1	A	64	ARG	NE-CZ-NH1	9.34	124.97	120.30
1	A	248	ARG	CD-NE-CZ	8.89	136.05	123.60
1	A	41	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	A	200	ASP	CB-CG-OD2	-8.45	110.69	118.30
1	A	32	ASP	CB-CG-OD2	-8.17	110.94	118.30
1	A	158	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	A	2	HIS	N-CA-C	-7.81	89.91	111.00
1	A	107	TYR	CB-CG-CD1	-7.77	116.34	121.00
1	A	175	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	A	82	ASP	CB-CG-OD1	-7.54	111.51	118.30
1	A	110	ARG	CD-NE-CZ	7.53	134.14	123.60
1	A	4	VAL	N-CA-C	-7.50	90.75	111.00
1	A	92	ASP	CB-CG-OD1	-7.35	111.68	118.30
1	A	32	ASP	CB-CG-OD1	7.06	124.65	118.30
1	A	65	ASP	CB-CG-OD2	6.95	124.55	118.30
1	A	176	PHE	CB-CG-CD2	-6.90	115.97	120.80
1	A	40	THR	CA-CB-CG2	-6.88	102.77	112.40
1	A	65	ASP	CB-CG-OD1	-6.86	112.12	118.30
1	A	186	ARG	CD-NE-CZ	-6.86	114.00	123.60
1	A	107	TYR	CB-CG-CD2	6.63	124.98	121.00
1	A	200	ASP	CB-CG-OD1	6.59	124.23	118.30
1	A	97	VAL	CB-CA-C	-6.58	98.89	111.40
1	A	12	THR	CA-CB-CG2	-6.55	103.23	112.40
1	A	208	VAL	N-CA-CB	6.45	125.69	111.50
1	A	182	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	101	ASP	CB-CG-OD1	-6.32	112.61	118.30
1	A	82	ASP	CB-CG-OD2	6.21	123.89	118.30
1	A	176	PHE	CB-CG-CD1	6.20	125.14	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	50	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	A	272	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	A	229	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	2	HIS	C-N-CA	-5.96	106.80	121.70
1	A	132	ASN	CB-CA-C	5.92	122.23	110.40
1	A	5	LEU	N-CA-CB	5.87	122.14	110.40
1	A	246	THR	OG1-CB-CG2	5.80	123.34	110.00
1	A	93	THR	CA-CB-CG2	-5.79	104.29	112.40
1	A	101	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	195	ASP	CB-CG-OD2	5.77	123.50	118.30
1	A	152	PHE	CB-CG-CD2	-5.77	116.76	120.80
1	A	46	GLU	CG-CD-OE1	5.76	129.81	118.30
1	A	267	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	92	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	152	PHE	CB-CG-CD1	5.60	124.72	120.80
1	A	180	ASP	CB-CG-OD1	5.54	123.28	118.30
1	A	195	ASP	CB-CG-OD1	-5.50	113.35	118.30
1	A	64	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	A	267	ASP	CB-CG-OD1	-5.42	113.42	118.30
1	A	68	SER	CB-CA-C	-5.41	99.83	110.10
1	A	74	LEU	CB-CA-C	-5.34	100.05	110.20
1	A	9	LEU	CB-CA-C	-5.31	100.12	110.20
1	A	266	PRO	C-N-CA	-5.29	108.48	121.70
1	A	155	THR	CA-CB-CG2	-5.26	105.04	112.40
1	A	175	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	247	CYS	CA-CB-SG	-5.23	104.59	114.00
1	A	281	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	46	GLU	CG-CD-OE2	-5.17	107.97	118.30
1	A	153	LYS	C-N-CA	-5.15	108.83	121.70
1	A	222	GLU	CA-CB-CG	-5.14	102.08	113.40
1	A	21	ALA	C-N-CA	-5.09	111.61	122.30
1	A	212	PHE	CB-CG-CD2	-5.07	117.25	120.80

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	246	THR	CB

There are no planarity outliers.

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	2325	0	2262	147	0
2	A	4	0	2	1	0
3	A	101	0	0	19	0
All	All	2430	0	2264	147	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 32.

All (147) 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:CD2	1:A:121:ARG:HG3	2.05	0.91
1:A:170:ASN:HD21	1:A:176:PHE:H	1.12	0.87
1:A:141:THR:HG22	1:A:143:GLU:H	1.39	0.86
1:A:109:PRO:HG2	1:A:255:HIS:CE1	2.11	0.85
1:A:148:GLU:HG3	1:A:149:PRO:HD2	1.60	0.84
1:A:238:ASP:OD1	1:A:240:THR:HB	1.79	0.81
1:A:128:GLY:HA2	1:A:220:GLY:O	1.83	0.78
1:A:2:HIS:ND1	1:A:3:GLN:N	2.33	0.76
1:A:91:ASN:HB3	3:A:343:HOH:O	1.86	0.76
1:A:50:ARG:HD2	3:A:373:HOH:O	1.85	0.76
1:A:158:ARG:HH12	1:A:166:GLN:NE2	1.84	0.75
1:A:158:ARG:HH12	1:A:166:GLN:HE22	1.35	0.74
1:A:1:VAL:HG12	1:A:3:GLN:HE22	1.53	0.74
1:A:2:HIS:CG	1:A:121:ARG:HG3	2.23	0.74
1:A:52:VAL:HG22	1:A:133:TRP:CE2	2.24	0.72
1:A:168:LEU:O	1:A:171:LEU:HB2	1.89	0.72
1:A:248:ARG:HG3	1:A:249:LYS:N	2.03	0.71
1:A:2:HIS:CE1	1:A:121:ARG:HG3	2.26	0.70
1:A:41:ARG:HD2	1:A:46:GLU:OE2	1.90	0.70
1:A:222:GLU:HG3	1:A:223:LYS:N	2.05	0.70
1:A:151:ILE:HD13	1:A:152:PHE:N	2.07	0.69
1:A:91:ASN:ND2	1:A:91:ASN:H	1.91	0.69
1:A:1:VAL:HG12	1:A:3:GLN:NE2	2.07	0.69
1:A:2:HIS:NE2	1:A:121:ARG:HG3	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:VAL:HG13	1:A:5:LEU:HD12	1.73	0.68
1:A:71:GLU:OE1	1:A:248:ARG:HD2	1.93	0.68
1:A:42:GLU:HG2	3:A:358:HOH:O	1.93	0.68
1:A:91:ASN:H	1:A:91:ASN:HD22	1.41	0.68
1:A:29:ARG:HG3	1:A:89:ILE:HG13	1.78	0.65
1:A:247:CYS:HB3	2:A:297:ACT:OXT	1.95	0.65
1:A:246:THR:HG23	1:A:271:TYR:CD2	2.32	0.64
1:A:118:PHE:HB3	1:A:154:ALA:HB1	1.80	0.64
1:A:132:ASN:ND2	3:A:305:HOH:O	2.29	0.63
1:A:214:ASN:HB2	3:A:340:HOH:O	1.98	0.63
1:A:224:SER:OG	1:A:227:GLU:HG3	1.98	0.63
1:A:163:THR:H	1:A:166:GLN:HE21	1.46	0.63
1:A:117:VAL:HG23	1:A:160:LEU:HB2	1.80	0.63
1:A:90:SER:H	1:A:93:THR:CG2	2.12	0.62
1:A:6:TYR:CE1	1:A:122:THR:HG22	2.35	0.61
1:A:194:PRO:O	1:A:248:ARG:NH2	2.30	0.60
1:A:215:PHE:HB2	3:A:397:HOH:O	2.02	0.60
1:A:248:ARG:HG3	1:A:249:LYS:HG2	1.81	0.60
1:A:170:ASN:ND2	1:A:176:PHE:H	1.90	0.60
1:A:255:HIS:HD2	3:A:397:HOH:O	1.85	0.59
1:A:20:ARG:CZ	3:A:348:HOH:O	2.50	0.58
1:A:141:THR:HG22	1:A:142:SER:N	2.19	0.57
1:A:152:PHE:HE1	1:A:154:ALA:HB2	1.70	0.56
1:A:41:ARG:NH1	1:A:46:GLU:OE1	2.37	0.56
1:A:60:ILE:H	1:A:60:ILE:CD1	2.19	0.55
1:A:186:ARG:HB3	1:A:193:GLU:OE2	2.06	0.55
1:A:148:GLU:CG	1:A:149:PRO:HD2	2.33	0.55
1:A:191:GLN:HB3	1:A:192:PRO:HD2	1.88	0.55
1:A:246:THR:HG23	1:A:271:TYR:HD2	1.71	0.55
1:A:42:GLU:HG3	1:A:45:LYS:HB3	1.90	0.54
1:A:184:GLN:HG3	1:A:188:LEU:CD1	2.38	0.54
1:A:138:HIS:HB3	1:A:139:PRO:HD2	1.88	0.54
1:A:178:LEU:HD23	3:A:396:HOH:O	2.08	0.54
1:A:3:GLN:HB3	1:A:5:LEU:C	2.28	0.54
1:A:15:LEU:O	1:A:19:VAL:HG23	2.08	0.53
1:A:60:ILE:H	1:A:60:ILE:HD13	1.73	0.53
1:A:4:VAL:C	1:A:5:LEU:HD12	2.29	0.53
1:A:246:THR:CG2	1:A:274:SER:HA	2.40	0.52
1:A:190:THR:HG22	1:A:191:GLN:HG2	1.92	0.52
1:A:246:THR:HG22	1:A:274:SER:HA	1.92	0.52
1:A:7:ARG:O	1:A:124:SER:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:GLU:OE1	1:A:138:HIS:HE1	1.93	0.51
1:A:212:PHE:CE1	1:A:213:MET:HE2	2.45	0.51
1:A:233:GLU:O	1:A:236:LYS:HD3	2.10	0.51
1:A:110:ARG:NH1	3:A:352:HOH:O	2.44	0.51
1:A:239:LEU:O	1:A:265:LYS:HD2	2.11	0.51
1:A:224:SER:O	1:A:227:GLU:N	2.44	0.51
1:A:20:ARG:NH2	3:A:348:HOH:O	2.44	0.50
1:A:184:GLN:HE21	1:A:209:ASN:HD22	1.58	0.50
1:A:158:ARG:HB2	3:A:345:HOH:O	2.12	0.49
1:A:42:GLU:O	1:A:46:GLU:HB2	2.12	0.49
1:A:1:VAL:CG1	1:A:3:GLN:HE22	2.21	0.49
1:A:3:GLN:HB2	1:A:6:TYR:HA	1.93	0.49
1:A:97:VAL:HG12	1:A:98:TYR:N	2.27	0.49
1:A:2:HIS:ND1	1:A:121:ARG:HB2	2.28	0.49
1:A:15:LEU:HB3	1:A:133:TRP:HZ3	1.78	0.49
1:A:243:LEU:HD22	1:A:268:VAL:HG13	1.95	0.49
1:A:246:THR:CG2	1:A:271:TYR:HD2	2.24	0.49
1:A:20:ARG:NE	3:A:348:HOH:O	2.46	0.48
1:A:236:LYS:HD3	1:A:236:LYS:N	2.17	0.48
1:A:170:ASN:HD21	1:A:176:PHE:N	1.95	0.48
1:A:121:ARG:NH2	3:A:344:HOH:O	2.46	0.47
1:A:246:THR:HG23	1:A:271:TYR:HB3	1.96	0.47
1:A:118:PHE:C	1:A:155:THR:O	2.53	0.47
1:A:162:LYS:HA	1:A:166:GLN:NE2	2.29	0.47
1:A:240:THR:HG22	1:A:241:LYS:HG2	1.97	0.47
1:A:1:VAL:HB	1:A:3:GLN:OE1	2.13	0.47
1:A:157:ASN:C	1:A:157:ASN:HD22	2.17	0.47
1:A:9:LEU:HD22	1:A:127:ASN:HB2	1.97	0.47
1:A:47:TYR:O	1:A:51:HIS:HD2	1.98	0.46
1:A:121:ARG:HD2	3:A:376:HOH:O	2.15	0.46
1:A:141:THR:HG22	1:A:142:SER:H	1.80	0.46
1:A:151:ILE:HD12	1:A:151:ILE:HG23	1.70	0.46
1:A:26:PRO:O	1:A:93:THR:HB	2.15	0.45
1:A:2:HIS:CE1	1:A:121:ARG:CG	2.98	0.45
1:A:52:VAL:HG22	1:A:133:TRP:CZ2	2.52	0.45
1:A:90:SER:O	1:A:93:THR:HG23	2.15	0.45
1:A:133:TRP:CE2	1:A:138:HIS:HB2	2.52	0.45
1:A:235:LYS:HA	1:A:235:LYS:HD2	1.69	0.45
1:A:52:VAL:O	1:A:53:PRO:C	2.55	0.45
1:A:128:GLY:O	1:A:132:ASN:HB2	2.17	0.45
1:A:221:PHE:HZ	3:A:305:HOH:O	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:HIS:ND1	1:A:121:ARG:CB	2.80	0.45
1:A:4:VAL:CG1	1:A:5:LEU:N	2.80	0.44
1:A:138:HIS:HB3	1:A:139:PRO:CD	2.46	0.44
1:A:267:ASP:OD1	1:A:267:ASP:N	2.50	0.44
1:A:62:GLU:O	1:A:66:LYS:HE3	2.17	0.44
1:A:18:SER:O	1:A:23:LYS:HB2	2.17	0.44
1:A:236:LYS:HD3	1:A:236:LYS:HA	1.20	0.44
1:A:91:ASN:ND2	1:A:91:ASN:N	2.57	0.43
1:A:205:ARG:HG3	1:A:286:THR:O	2.17	0.43
1:A:162:LYS:HG3	1:A:244:ILE:HG12	1.99	0.43
1:A:60:ILE:HG22	1:A:72:VAL:CG1	2.49	0.43
1:A:182:ARG:HG3	1:A:247:CYS:SG	2.58	0.43
1:A:16:ALA:O	1:A:17:GLU:C	2.57	0.43
1:A:231:MET:HE1	3:A:340:HOH:O	2.19	0.43
1:A:215:PHE:CE2	1:A:256:ILE:HD13	2.54	0.42
1:A:246:THR:CG2	1:A:271:TYR:CD2	2.98	0.42
1:A:101:ASP:OD2	1:A:103:LEU:HB2	2.19	0.42
1:A:90:SER:H	1:A:93:THR:HG21	1.82	0.42
1:A:233:GLU:HG3	1:A:236:LYS:HE2	2.01	0.42
1:A:184:GLN:CG	1:A:188:LEU:CD1	2.98	0.42
1:A:118:PHE:O	1:A:155:THR:N	2.30	0.42
1:A:212:PHE:CE1	1:A:213:MET:CE	3.03	0.42
1:A:6:TYR:CD2	1:A:7:ARG:N	2.88	0.42
1:A:103:LEU:HA	3:A:332:HOH:O	2.19	0.41
1:A:30:VAL:O	1:A:31:LEU:HD23	2.20	0.41
1:A:287:TRP:C	1:A:288:VAL:HG13	2.41	0.41
1:A:132:ASN:O	1:A:133:TRP:C	2.58	0.41
1:A:80:PHE:O	1:A:84:VAL:HG22	2.20	0.41
1:A:110:ARG:O	1:A:114:MET:HG3	2.20	0.41
1:A:219:ASP:HB2	3:A:350:HOH:O	2.19	0.41
1:A:148:GLU:HG3	1:A:149:PRO:CD	2.41	0.41
1:A:157:ASN:C	1:A:157:ASN:ND2	2.74	0.41
1:A:176:PHE:CD2	1:A:242:PRO:HB2	2.56	0.41
1:A:181:SER:HA	1:A:210:MET:O	2.21	0.41
1:A:292:LYS:HD2	1:A:292:LYS:HA	1.61	0.41
1:A:184:GLN:HG3	1:A:188:LEU:HD11	2.03	0.40
1:A:2:HIS:ND1	1:A:121:ARG:HG3	2.36	0.40
1:A:151:ILE:HD13	1:A:151:ILE:C	2.41	0.40
1:A:59:ASP:HB3	1:A:62:GLU:HB2	2.02	0.40
1:A:238:ASP:OD2	1:A:241:LYS:HG3	2.22	0.40
1:A:112:TRP:CH2	1:A:258:LEU:HA	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	291/296 (98%)	270 (93%)	18 (6%)	3 (1%)	15 9

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	129	GLY
1	A	247	CYS
1	A	292	LYS

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	245/246 (100%)	206 (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	3	GLN
1	A	7	ARG
1	A	12	THR

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Mol	Chain	Res	Type
1	A	13	LYS
1	A	18	SER
1	A	44	ARG
1	A	50	ARG
1	A	60	ILE
1	A	61	GLU
1	A	63	CYS
1	A	69	PRO
1	A	72	VAL
1	A	87	LEU
1	A	91	ASN
1	A	93	THR
1	A	110	ARG
1	A	117	VAL
1	A	121	ARG
1	A	124	SER
1	A	126	LEU
1	A	146	ARG
1	A	151	ILE
1	A	153	LYS
1	A	157	ASN
1	A	159	SER
1	A	165	GLU
1	A	175	ARG
1	A	190	THR
1	A	213	MET
1	A	235	LYS
1	A	236	LYS
1	A	246	THR
1	A	248	ARG
1	A	249	LYS
1	A	289	SER
1	A	290	GLN
1	A	292	LYS

Sometimes 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	132	ASN
1	A	138	HIS
1	A	157	ASN

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Mol	Chain	Res	Type
1	A	166	GLN
1	A	170	ASN
1	A	191	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

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

1 ligand 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	$\#\|Z\| > 2$
2	ACT	A	297	1	3,3,3	0.81	0	3,3,3	1.34	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	297	ACT	1	0

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.