



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:47 PM UTC

PDB ID : 1ORB / pdb_00001orb
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (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

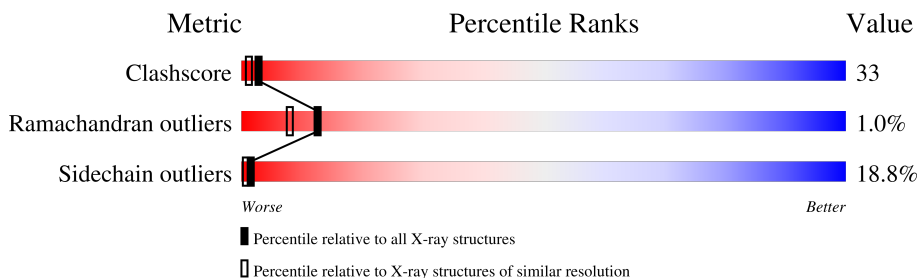
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

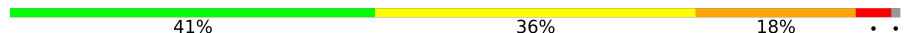
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	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	 41% 36% 18% . .

2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	293	2325	1486	405	425	9	0	0	0

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

- Molecule 3 is water.

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

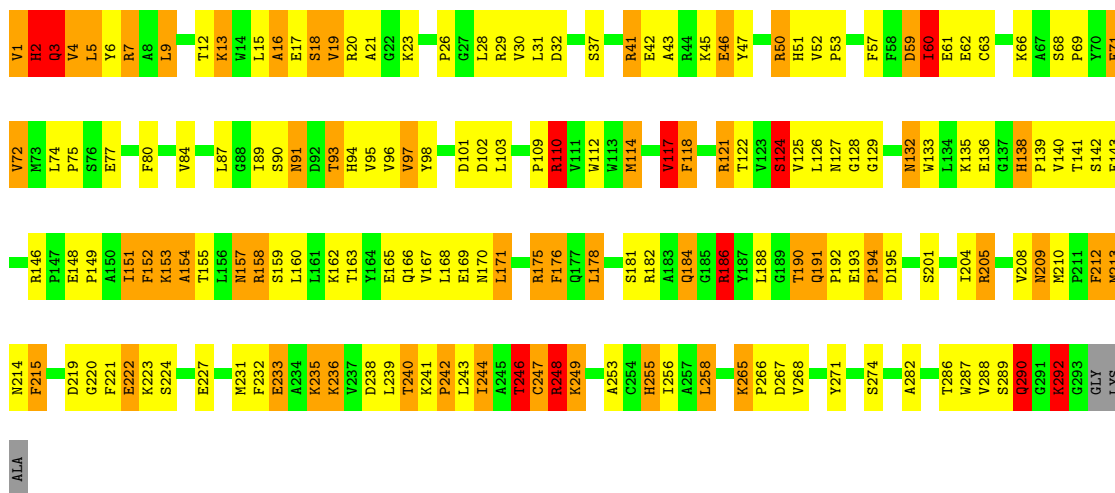
3 Residue-property plots

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. 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:  41% 36% 18%



4 Data and refinement statistics

Xtrriage (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.	Xtrriage
Total number of atoms	2430	wwPDB-VP
Average B, all atoms (Å ²)	41.0	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: 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	1.00	1/2392 (0.0%)	2.14	106/3246 (3.3%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	ASP	C-N	-5.65	1.26	1.34

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	VAL	N-CA-C	-19.77	90.75	110.72
1	A	60	ILE	CB-CG1-CD1	13.56	142.27	113.80
1	A	2	HIS	N-CA-C	-12.83	89.91	109.41
1	A	2	HIS	CA-C-N	-9.63	106.80	122.11
1	A	2	HIS	C-N-CA	-9.63	106.80	122.11
1	A	248	ARG	NE-CZ-NH1	8.80	130.30	121.50
1	A	153	LYS	CA-C-N	-8.77	108.83	122.59
1	A	153	LYS	C-N-CA	-8.77	108.83	122.59
1	A	266	PRO	CA-C-N	-8.74	108.48	123.25
1	A	266	PRO	C-N-CA	-8.74	108.48	123.25
1	A	248	ARG	CD-NE-CZ	8.32	136.05	124.40
1	A	110	ARG	NE-CZ-NH2	-8.20	111.82	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	ARG	NE-CZ-NH2	-8.13	111.88	119.20
1	A	28	LEU	CA-C-N	7.94	134.19	123.00
1	A	28	LEU	C-N-CA	7.94	134.19	123.00
1	A	97	VAL	CB-CA-C	-7.87	98.89	110.62
1	A	125	VAL	N-CA-CB	-7.76	101.67	110.99
1	A	32	ASP	CA-C-N	-7.60	110.41	123.25
1	A	32	ASP	C-N-CA	-7.60	110.41	123.25
1	A	186	ARG	CD-NE-CZ	-7.43	114.00	124.40
1	A	19	VAL	N-CA-C	-7.33	103.19	110.30
1	A	69	PRO	CB-CA-C	-7.28	100.05	111.04
1	A	5	LEU	N-CA-CB	7.20	122.14	110.90
1	A	57	PHE	CA-C-N	-7.10	113.33	122.77
1	A	57	PHE	C-N-CA	-7.10	113.33	122.77
1	A	37	SER	O-C-N	7.03	127.14	121.38
1	A	246	THR	OG1-CB-CG2	7.02	123.34	109.30
1	A	110	ARG	CD-NE-CZ	6.96	134.14	124.40
1	A	60	ILE	N-CA-CB	6.92	119.12	110.47
1	A	132	ASN	CB-CA-C	6.89	122.23	110.79
1	A	208	VAL	N-CA-CB	6.66	125.69	111.91
1	A	16	ALA	CA-C-N	-6.64	110.72	120.28
1	A	16	ALA	C-N-CA	-6.64	110.72	120.28
1	A	71	GLU	N-CA-C	6.64	120.31	109.76
1	A	265	LYS	CB-CA-C	-6.61	104.49	110.44
1	A	102	ASP	CA-CB-CG	6.60	119.20	112.60
1	A	2	HIS	CA-C-O	-6.56	113.97	121.58
1	A	178	LEU	CA-C-N	-6.44	114.70	123.14
1	A	178	LEU	C-N-CA	-6.44	114.70	123.14
1	A	96	VAL	N-CA-CB	6.40	119.52	111.46
1	A	97	VAL	O-C-N	6.34	130.03	123.18
1	A	68	SER	CB-CA-C	-6.27	99.83	108.86
1	A	244	ILE	N-CA-CB	6.25	120.04	111.41
1	A	253	ALA	N-CA-C	-6.25	105.14	112.89
1	A	59	ASP	CA-C-N	6.23	129.32	120.53
1	A	59	ASP	C-N-CA	6.23	129.32	120.53
1	A	13	LYS	CA-C-N	6.22	128.94	120.54
1	A	13	LYS	C-N-CA	6.22	128.94	120.54
1	A	3	GLN	N-CA-C	6.20	117.29	108.74
1	A	258	LEU	CA-C-N	-6.13	111.59	120.29
1	A	258	LEU	C-N-CA	-6.13	111.59	120.29
1	A	74	LEU	CB-CA-C	-6.10	100.05	109.62
1	A	43	ALA	CA-C-N	-6.07	112.15	120.28
1	A	43	ALA	C-N-CA	-6.07	112.15	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	PHE	CA-CB-CG	-6.06	107.74	113.80
1	A	9	LEU	CB-CA-C	-6.05	100.12	110.16
1	A	222	GLU	CA-CB-CG	-6.01	102.08	114.10
1	A	4	VAL	N-CA-CB	6.00	119.58	110.58
1	A	266	PRO	CB-CA-C	-6.00	101.67	111.56
1	A	114	MET	CA-C-N	-5.94	112.71	120.44
1	A	114	MET	C-N-CA	-5.94	112.71	120.44
1	A	5	LEU	CB-CA-C	5.92	119.26	110.62
1	A	94	HIS	CA-C-O	-5.91	114.25	120.58
1	A	95	VAL	N-CA-C	5.81	117.12	108.23
1	A	194	PRO	CB-CA-C	-5.74	102.09	111.56
1	A	186	ARG	CA-CB-CG	-5.73	102.64	114.10
1	A	242	PRO	N-CA-CB	5.72	108.40	103.31
1	A	9	LEU	N-CA-C	5.68	117.67	108.41
1	A	75	PRO	CA-C-N	-5.62	110.74	122.03
1	A	75	PRO	C-N-CA	-5.62	110.74	122.03
1	A	59	ASP	N-CA-C	5.56	117.78	107.99
1	A	246	THR	CA-CB-OG1	5.56	117.94	109.60
1	A	176	PHE	N-CA-CB	-5.54	102.22	111.20
1	A	167	VAL	CA-C-O	5.54	126.28	119.58
1	A	46	GLU	N-CA-CB	-5.53	101.77	110.06
1	A	59	ASP	CB-CA-C	-5.52	101.92	111.30
1	A	138	HIS	CA-CB-CG	-5.51	108.29	113.80
1	A	255	HIS	N-CA-CB	5.50	119.37	110.40
1	A	118	PHE	O-C-N	5.50	129.21	122.34
1	A	158	ARG	NE-CZ-NH1	5.45	126.94	121.50
1	A	191	GLN	O-C-N	5.39	125.93	121.35
1	A	209	ASN	N-CA-C	5.38	117.49	108.73
1	A	290	GLN	N-CA-C	-5.38	104.19	111.55
1	A	140	VAL	N-CA-CB	5.34	121.44	112.47
1	A	215	PHE	CB-CA-C	-5.34	100.40	110.01
1	A	152	PHE	N-CA-C	-5.33	101.25	109.52
1	A	110	ARG	NE-CZ-NH1	5.33	126.83	121.50
1	A	41	ARG	NE-CZ-NH2	-5.32	114.41	119.20
1	A	59	ASP	O-C-N	-5.31	115.93	122.68
1	A	75	PRO	CB-CA-C	-5.30	102.82	111.56
1	A	195	ASP	N-CA-C	5.25	118.83	111.90
1	A	110	ARG	CB-CA-C	-5.24	102.66	110.88
1	A	204	ILE	CA-C-N	-5.19	112.79	120.94
1	A	204	ILE	C-N-CA	-5.19	112.79	120.94
1	A	175	ARG	N-CA-C	5.19	119.32	112.89
1	A	124	SER	CA-C-N	5.19	129.47	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	SER	C-N-CA	5.19	129.47	122.93
1	A	21	ALA	CA-C-N	-5.17	111.61	120.87
1	A	21	ALA	C-N-CA	-5.17	111.61	120.87
1	A	248	ARG	N-CA-CB	5.16	119.00	110.33
1	A	253	ALA	CA-C-O	5.13	125.68	119.31
1	A	117	VAL	CA-C-N	-5.11	114.10	122.54
1	A	117	VAL	C-N-CA	-5.11	114.10	122.54
1	A	282	ALA	N-CA-C	5.08	117.17	110.36
1	A	154	ALA	CA-C-N	-5.04	113.86	122.33
1	A	154	ALA	C-N-CA	-5.04	113.86	122.33

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

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	150	0
2	A	4	0	2	1	0
3	A	101	0	0	18	0
All	All	2430	0	2264	150	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 33.

All (150) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:212:PHE:CE1	1:A:213:MET:HE3	2.27	0.68
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:212:PHE:CD1	1:A:213:MET:HE3	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:4:VAL:C	1:A:5:LEU:HD12	2.29	0.58
1:A:20:ARG:CZ	3:A:348:HOH:O	2.50	0.58
1:A:3:GLN:HB3	1:A:5:LEU:C	2.28	0.57
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: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: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:118:PHE:C	1:A:155:THR:O	2.53	0.52
1:A:7:ARG:O	1:A:124:SER:HB3	2.10	0.52
1:A:136:GLU:OE1	1:A:138:HIS:HE1	1.93	0.51
1:A:157:ASN:C	1:A:157:ASN:HD22	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:52:VAL:O	1:A:53:PRO:C	2.55	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:287:TRP:C	1:A:288:VAL:HG13	2.41	0.46
1:A:132:ASN:O	1:A:133:TRP:C	2.58	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:157:ASN:C	1:A:157:ASN:ND2	2.74	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:128:GLY:O	1:A:132:ASN:HB2	2.17	0.45
1:A:151:ILE:HD13	1:A:151:ILE:C	2.41	0.45
1:A:221:PHE:HZ	3:A:305:HOH:O	1.99	0.45
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:16:ALA:O	1:A:17:GLU:C	2.57	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:191:GLN:O	1:A:201:SER:OG	2.34	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: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:290:GLN:NE2	1:A:290:GLN:C	2.79	0.40
1:A:2:HIS:ND1	1:A:121:ARG:HG3	2.36	0.40
1:A:59:ASP:HB3	1:A:62:GLU:HB2	2.02	0.40
1:A:231:MET:O	1:A:232:PHE:C	2.63	0.40
1:A:238:ASP:OD2	1:A:241:LYS:HG3	2.22	0.40
1:A:2:HIS:ND1	1:A:2:HIS:C	2.79	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%)	12 8

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%)	199 (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	3	GLN
1	A	7	ARG
1	A	12	THR
1	A	13	LYS
1	A	18	SER
1	A	50	ARG
1	A	60	ILE
1	A	61	GLU
1	A	63	CYS
1	A	72	VAL
1	A	77	GLU
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	135	LYS

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Mol	Chain	Res	Type
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	169	GLU
1	A	171	LEU
1	A	175	ARG
1	A	184	GLN
1	A	186	ARG
1	A	190	THR
1	A	205	ARG
1	A	213	MET
1	A	233	GLU
1	A	235	LYS
1	A	236	LYS
1	A	240	THR
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
1	A	166	GLN
1	A	170	ASN
1	A	184	GLN
1	A	191	GLN
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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	0.86	0	3,3,3	1.33	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.