



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:37 PM UTC

PDB ID : 3HOA / pdb_00003hoa
Title : Crystal structure of the Thermus thermophilus M32 carboxypeptidase
Authors : Lee, M.M.; Chan, M.K.
Deposited on : 2009-06-01
Resolution : 2.10 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

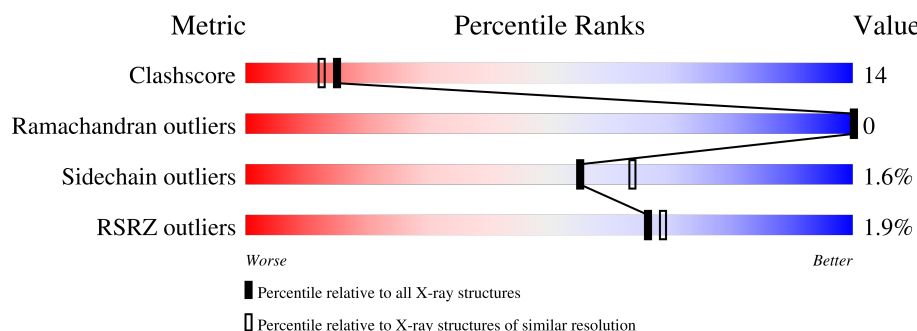
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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 $\leq 5\%$. 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	509	3% 71% 27% .
1	B	509	% 76% 23% .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8689 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 Thermostable carboxypeptidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	509	Total	C	N	O	S	0	0	0
			4108	2634	721	745	8			
1	B	509	Total	C	N	O	S	0	0	0
			4108	2634	721	745	8			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	232	Total	O	0	0
			232	232		

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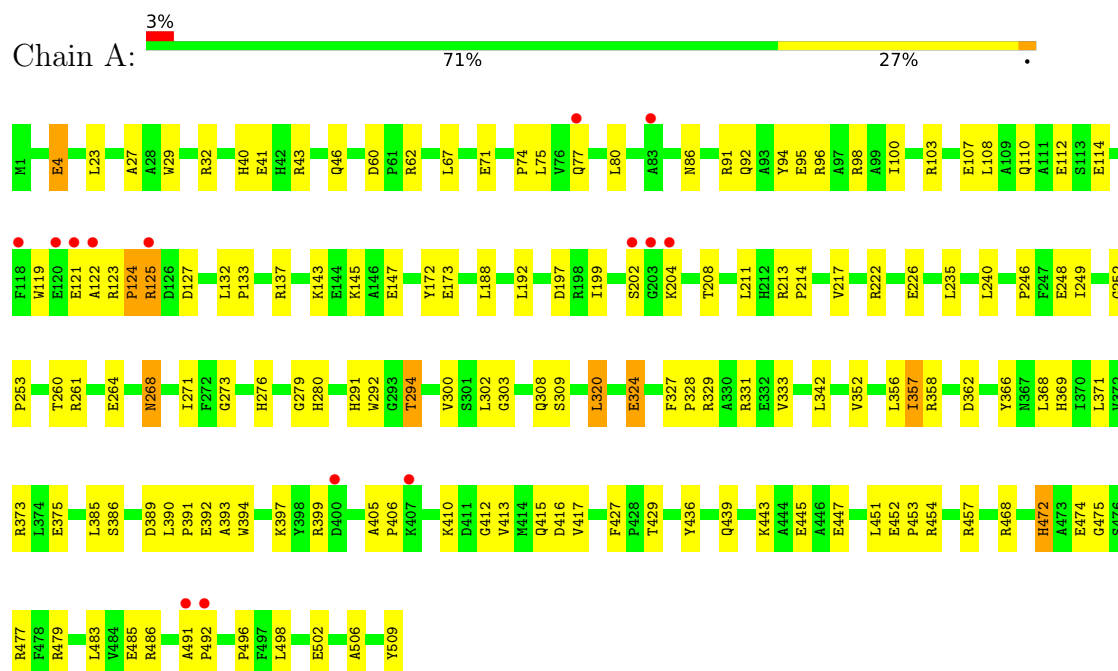
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	235	Total 235	O 235	0	0

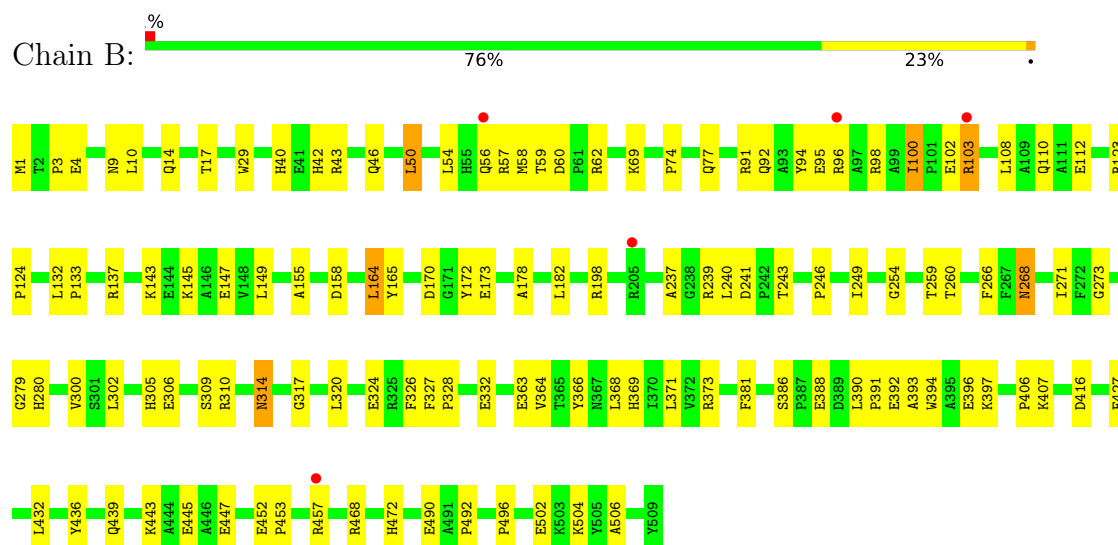
3 Residue-property plots [i](#)

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 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: Thermostable carboxypeptidase 1



• Molecule 1: Thermostable carboxypeptidase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.61Å 84.33Å 109.05Å 90.00° 93.75° 90.00°	Depositor
Resolution (Å)	19.98 – 2.10 19.98 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.9 (19.98-2.10) 99.6 (19.98-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.218 , 0.251 0.228 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 48.8	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8689	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: GOL

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	0.38	0/4226	0.87	12/5736 (0.2%)
1	B	0.39	0/4226	0.85	13/5736 (0.2%)
All	All	0.38	0/8452	0.86	25/11472 (0.2%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	300	VAL	N-CA-C	8.68	119.49	110.72
1	B	268	ASN	N-CA-C	7.73	119.34	111.07
1	A	324	GLU	N-CA-C	-7.49	103.13	111.82
1	B	324	GLU	N-CA-C	-7.20	103.44	111.71
1	A	506	ALA	N-CA-C	-7.04	103.65	111.82
1	B	300	VAL	N-CA-C	6.44	120.06	111.44
1	B	317	GLY	N-CA-C	6.41	121.80	113.27
1	B	314	ASN	N-CA-C	6.29	120.83	111.96
1	B	100	ILE	N-CA-C	6.02	113.04	107.56
1	A	125	ARG	N-CA-C	-5.91	100.66	110.17
1	B	364	VAL	N-CA-C	5.86	116.04	110.53
1	A	479	ARG	N-CA-C	-5.83	102.03	110.08
1	A	273	GLY	N-CA-C	-5.65	105.54	112.77
1	B	368	LEU	N-CA-C	-5.60	105.33	111.82
1	A	268	ASN	N-CA-C	5.58	120.53	111.37
1	B	506	ALA	N-CA-C	-5.49	105.29	111.28
1	B	271	ILE	N-CA-C	5.47	115.57	110.42
1	A	124	PRO	N-CA-C	-5.33	106.45	113.65
1	B	273	GLY	N-CA-C	-5.28	106.39	112.73
1	B	326	PHE	N-CA-C	5.27	119.87	113.38
1	B	40	HIS	N-CA-C	5.25	117.00	111.28
1	A	40	HIS	N-CA-C	5.14	116.58	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	LEU	N-CA-C	-5.12	105.88	111.82
1	A	271	ILE	N-CA-C	5.11	115.39	110.74
1	A	368	LEU	N-CA-C	-5.08	105.93	111.82

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	4108	0	3996	125	0
1	B	4108	0	3996	98	0
2	B	6	0	8	0	0
3	A	232	0	0	9	0
3	B	235	0	0	13	0
All	All	8689	0	8000	222	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 14.

All (222) 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:125:ARG:HD2	1:A:127:ASP:HB2	1.48	0.93
1:B:164:LEU:HD11	1:B:381:PHE:HB3	1.58	0.85
1:A:43:ARG:HA	1:A:46:GLN:HE21	1.43	0.82
1:B:373:ARG:NH1	1:B:394:TRP:HH2	1.79	0.79
1:A:248:GLU:HG2	1:A:280:HIS:HB3	1.62	0.79
1:A:406:PRO:HG3	3:A:586:HOH:O	1.82	0.78
1:B:246:PRO:HB3	1:B:260:THR:HA	1.65	0.77
1:B:443:LYS:HE3	1:B:447:GLU:OE1	1.86	0.76
1:A:248:GLU:HG2	1:A:280:HIS:CB	2.16	0.76
1:B:94:TYR:CZ	1:B:98:ARG:HD2	2.22	0.74
1:B:239:ARG:HD3	1:B:241:ASP:OD2	1.86	0.74
1:A:294:THR:HG21	3:A:602:HOH:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:ARG:HH12	1:A:394:TRP:HH2	1.37	0.73
1:A:217:VAL:HG23	1:A:264:GLU:HG2	1.71	0.72
1:B:123:ARG:HB3	1:B:124:PRO:HD3	1.72	0.71
1:A:43:ARG:HE	1:A:46:GLN:HE22	1.38	0.71
1:A:329:ARG:NH1	1:A:333:VAL:HG23	2.06	0.70
1:A:443:LYS:HE3	1:A:447:GLU:OE1	1.92	0.70
1:B:43:ARG:HA	1:B:46:GLN:HE21	1.56	0.69
1:A:60:ASP:OD1	1:A:62:ARG:HD3	1.92	0.69
1:A:357:ILE:HD12	1:A:357:ILE:N	2.07	0.69
1:A:43:ARG:HE	1:A:46:GLN:NE2	1.91	0.68
1:B:43:ARG:HE	1:B:46:GLN:HE22	1.42	0.68
1:B:145:LYS:O	1:B:149:LEU:HD23	1.95	0.67
1:B:452:GLU:H	1:B:452:GLU:CD	2.03	0.67
1:A:173:GLU:HG2	1:A:429:THR:HG22	1.77	0.67
1:B:407:LYS:HD3	3:B:674:HOH:O	1.94	0.67
1:B:100:ILE:CD1	1:B:145:LYS:HE3	2.26	0.66
1:B:407:LYS:HD3	1:B:407:LYS:H	1.61	0.65
1:B:59:THR:HG22	1:B:59:THR:O	1.96	0.65
1:B:306:GLU:O	1:B:310:ARG:HG2	1.97	0.64
1:B:436:TYR:HE1	1:B:492:PRO:HB3	1.61	0.64
1:B:392:GLU:O	1:B:396:GLU:HG3	1.97	0.64
1:A:486:ARG:NH1	1:A:486:ARG:HB3	2.13	0.63
1:B:43:ARG:HE	1:B:46:GLN:NE2	1.96	0.63
1:B:164:LEU:HD12	1:B:165:TYR:N	2.14	0.63
1:B:310:ARG:HH21	1:B:314:ASN:HD21	1.45	0.63
1:A:74:PRO:HA	1:A:77:GLN:HG3	1.80	0.63
1:A:373:ARG:NH1	1:A:394:TRP:HH2	1.97	0.63
1:A:327:PHE:N	1:A:328:PRO:HD2	2.15	0.62
1:B:59:THR:HG23	1:B:98:ARG:HG2	1.82	0.61
1:A:80:LEU:HB3	1:A:477:ARG:HH21	1.64	0.61
1:A:452:GLU:CD	1:A:452:GLU:H	2.08	0.61
1:B:373:ARG:NE	3:B:568:HOH:O	2.33	0.61
1:A:389:ASP:HA	1:A:392:GLU:OE1	2.01	0.60
1:B:100:ILE:HD13	1:B:145:LYS:HE3	1.82	0.60
1:B:74:PRO:HA	1:B:77:GLN:HG3	1.83	0.60
1:A:385:LEU:HD23	1:A:386:SER:N	2.16	0.60
1:A:399:ARG:HG2	1:A:405:ALA:HB2	1.83	0.60
1:A:199:ILE:O	1:A:202:SER:HB3	2.01	0.60
1:A:329:ARG:HH12	1:A:333:VAL:HG23	1.66	0.60
1:B:496:PRO:HG2	3:B:513:HOH:O	2.01	0.60
1:A:197:ASP:HB3	3:A:512:HOH:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:LEU:HD22	1:B:54:LEU:HG	1.84	0.59
1:A:246:PRO:HB3	1:A:260:THR:HA	1.84	0.59
1:B:58:MET:HE3	3:B:723:HOH:O	2.01	0.58
1:B:439:GLN:NE2	1:B:490:GLU:HG3	2.17	0.58
1:A:122:ALA:O	1:A:125:ARG:O	2.21	0.58
1:B:164:LEU:HD12	1:B:164:LEU:C	2.28	0.58
1:A:143:LYS:O	1:A:147:GLU:HG3	2.03	0.58
1:A:204:LYS:HD2	1:A:509:TYR:C	2.29	0.58
1:A:468:ARG:HE	1:A:472:HIS:HD2	1.52	0.58
1:A:121:GLU:HG2	1:A:125:ARG:NH2	2.19	0.57
1:B:439:GLN:HE21	1:B:490:GLU:HG3	1.70	0.57
1:B:98:ARG:NE	3:B:548:HOH:O	2.37	0.57
1:A:94:TYR:CZ	1:A:98:ARG:HD2	2.40	0.57
1:A:96:ARG:HG3	1:A:96:ARG:HH11	1.69	0.57
1:A:67:LEU:O	1:A:71:GLU:HG3	2.05	0.56
1:B:132:LEU:HB3	1:B:133:PRO:HD3	1.88	0.56
1:A:110:GLN:O	1:A:114:GLU:HG3	2.04	0.56
1:B:143:LYS:O	1:B:147:GLU:HG3	2.05	0.56
1:A:86:ASN:OD1	1:A:294:THR:HG23	2.05	0.56
1:B:388:GLU:CD	1:B:388:GLU:H	2.14	0.56
1:A:291:HIS:O	1:A:294:THR:HB	2.04	0.56
1:A:399:ARG:NH1	1:A:405:ALA:HB3	2.21	0.56
1:A:217:VAL:CG2	1:A:264:GLU:HG2	2.36	0.55
1:B:94:TYR:CE1	1:B:98:ARG:HD2	2.40	0.55
1:A:393:ALA:O	1:A:397:LYS:HG2	2.07	0.55
1:B:74:PRO:HA	1:B:77:GLN:HE21	1.72	0.55
1:A:32:ARG:HD2	3:A:559:HOH:O	2.06	0.55
1:B:60:ASP:OD1	1:B:62:ARG:HD3	2.07	0.55
1:A:172:TYR:HB3	1:A:302:LEU:HD12	1.89	0.55
1:B:102:GLU:HG3	1:B:103:ARG:HE	1.71	0.55
1:B:327:PHE:N	1:B:328:PRO:HD2	2.21	0.55
1:A:222:ARG:O	1:A:226:GLU:HG3	2.07	0.55
1:A:125:ARG:HD2	1:A:127:ASP:CB	2.30	0.54
1:A:320:LEU:HD22	1:A:324:GLU:HG3	1.89	0.54
1:B:96:ARG:HG3	1:B:96:ARG:HH11	1.72	0.54
1:A:100:ILE:HD13	1:A:145:LYS:HE3	1.89	0.53
1:B:468:ARG:HE	1:B:472:HIS:HD2	1.57	0.52
1:A:213:ARG:HB3	1:A:214:PRO:HD2	1.91	0.52
1:B:373:ARG:HH12	1:B:394:TRP:HH2	1.56	0.52
1:A:110:GLN:NE2	1:A:137:ARG:HH22	2.08	0.52
1:A:373:ARG:NH1	1:A:394:TRP:CH2	2.77	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:LEU:HD13	1:B:371:LEU:C	2.35	0.52
1:A:452:GLU:N	1:A:453:PRO:HD2	2.24	0.52
1:A:108:LEU:O	1:A:112:GLU:HG3	2.10	0.52
1:A:276:HIS:NE2	3:A:510:HOH:O	2.34	0.52
1:B:243:THR:HG21	1:B:259:THR:OG1	2.11	0.51
1:A:324:GLU:HG2	1:A:342:LEU:HD21	1.91	0.51
1:A:373:ARG:CZ	3:A:593:HOH:O	2.58	0.51
1:A:279:GLY:HA3	1:A:309:SER:HA	1.93	0.51
1:A:123:ARG:HB3	1:A:124:PRO:HD3	1.92	0.51
1:B:96:ARG:NH2	1:B:170:ASP:OD1	2.43	0.51
1:B:108:LEU:O	1:B:112:GLU:HG3	2.10	0.51
1:A:86:ASN:CG	1:A:294:THR:HG23	2.36	0.51
1:A:92:GLN:HE21	1:A:96:ARG:NH1	2.08	0.51
1:A:103:ARG:O	1:A:107:GLU:HG3	2.11	0.50
1:A:352:VAL:HG13	1:A:362:ASP:OD2	2.12	0.50
1:B:279:GLY:HA3	1:B:309:SER:HA	1.92	0.50
1:B:504:LYS:HE3	3:B:722:HOH:O	2.10	0.50
1:A:261:ARG:HG2	1:A:261:ARG:HH11	1.77	0.50
1:A:253:PRO:HD3	1:A:292:TRP:CD1	2.47	0.50
1:A:173:GLU:OE2	1:A:303:GLY:N	2.32	0.50
1:B:173:GLU:HG2	1:B:432:LEU:CD1	2.42	0.49
1:A:235:LEU:N	1:A:235:LEU:HD12	2.28	0.49
1:A:373:ARG:NE	3:A:593:HOH:O	2.45	0.49
1:A:454:ARG:HG3	1:A:454:ARG:HH11	1.78	0.49
1:B:102:GLU:HG2	1:B:103:ARG:HH21	1.77	0.49
1:B:328:PRO:O	1:B:332:GLU:HG3	2.12	0.49
1:B:436:TYR:CE1	1:B:492:PRO:HB3	2.45	0.49
1:A:486:ARG:NH2	3:A:722:HOH:O	2.46	0.49
1:B:373:ARG:NH1	1:B:394:TRP:CH2	2.70	0.49
1:A:486:ARG:CB	1:A:486:ARG:HH11	2.26	0.48
1:A:329:ARG:HH12	1:A:333:VAL:CG2	2.24	0.48
1:A:439:GLN:HG2	1:A:496:PRO:HG2	1.96	0.48
1:B:172:TYR:HB3	1:B:302:LEU:HD12	1.93	0.48
1:B:237:ALA:HB1	1:B:254:GLY:HA2	1.96	0.48
1:B:406:PRO:HG3	3:B:515:HOH:O	2.13	0.48
1:A:110:GLN:HE21	1:A:137:ARG:HH22	1.62	0.47
1:B:1:MET:HE1	1:B:9:ASN:HD22	1.80	0.47
1:A:41:GLU:HG3	3:A:645:HOH:O	2.14	0.47
1:A:373:ARG:HG2	1:A:373:ARG:HH11	1.79	0.47
1:B:62:ARG:HD2	3:B:617:HOH:O	2.15	0.47
1:B:92:GLN:HE21	1:B:96:ARG:CZ	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:LYS:HD3	1:B:407:LYS:N	2.29	0.47
1:A:358:ARG:HD3	1:A:373:ARG:HE	1.80	0.47
1:B:10:LEU:O	1:B:14:GLN:HG2	2.14	0.47
1:B:373:ARG:HD3	1:B:427:PHE:CZ	2.50	0.47
1:B:59:THR:O	1:B:59:THR:CG2	2.62	0.47
1:A:357:ILE:N	1:A:357:ILE:CD1	2.76	0.47
1:B:100:ILE:HD11	1:B:145:LYS:HE3	1.97	0.46
1:A:4:GLU:HA	1:A:75:LEU:HD11	1.97	0.46
1:A:121:GLU:HG2	1:A:125:ARG:HH21	1.79	0.46
1:B:110:GLN:NE2	1:B:137:ARG:HH22	2.14	0.46
1:A:331:ARG:HG3	1:A:331:ARG:HH11	1.81	0.46
1:A:394:TRP:CE3	1:A:413:VAL:HG12	2.50	0.46
1:B:239:ARG:NH2	3:B:603:HOH:O	2.49	0.46
1:A:445:GLU:HG2	1:A:451:LEU:HG	1.98	0.45
1:A:371:LEU:HD23	1:A:371:LEU:O	2.17	0.45
1:B:1:MET:HG2	1:B:69:LYS:HE2	1.98	0.45
1:B:373:ARG:HD3	1:B:427:PHE:CE1	2.52	0.45
1:B:29:TRP:HB2	1:B:249:ILE:HG21	1.98	0.45
1:B:56:GLN:NE2	3:B:626:HOH:O	2.50	0.45
1:B:373:ARG:CZ	1:B:416:ASP:OD2	2.64	0.45
1:A:119:TRP:C	1:A:121:GLU:H	2.25	0.45
1:A:252:GLY:HA3	1:B:42:HIS:CD2	2.51	0.45
1:A:92:GLN:HE21	1:A:96:ARG:CZ	2.30	0.45
1:B:314:ASN:HB3	1:B:363:GLU:OE2	2.17	0.45
1:A:320:LEU:HD22	1:A:324:GLU:CG	2.47	0.45
1:A:399:ARG:CG	1:A:405:ALA:HB2	2.47	0.45
1:B:178:ALA:O	1:B:182:LEU:HG	2.17	0.45
1:B:386:SER:HB2	1:B:388:GLU:OE1	2.17	0.45
1:A:356:LEU:HB2	1:A:357:ILE:HD12	1.99	0.45
1:B:468:ARG:HA	1:B:472:HIS:HB2	1.99	0.45
1:A:366:TYR:O	1:A:369:HIS:HB2	2.18	0.44
1:A:453:PRO:O	1:A:457:ARG:HG3	2.17	0.44
1:B:1:MET:HE1	1:B:9:ASN:ND2	2.32	0.44
1:B:445:GLU:OE2	1:B:452:GLU:OE2	2.35	0.44
1:B:453:PRO:O	1:B:457:ARG:HG3	2.17	0.44
1:A:132:LEU:HB3	1:A:133:PRO:HD3	1.98	0.44
1:A:173:GLU:CG	1:A:429:THR:HG22	2.44	0.44
1:A:329:ARG:NH1	1:A:333:VAL:CG2	2.76	0.44
1:B:452:GLU:N	1:B:453:PRO:HD2	2.33	0.44
1:B:3:PRO:HG2	1:B:4:GLU:OE1	2.17	0.44
1:A:468:ARG:HD2	1:A:472:HIS:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:LEU:HD13	1:A:268:ASN:OD1	2.18	0.44
1:A:498:LEU:O	1:A:502:GLU:HG3	2.17	0.44
1:B:92:GLN:NE2	1:B:96:ARG:CZ	2.81	0.44
1:B:137:ARG:NH2	3:B:540:HOH:O	2.33	0.43
1:B:373:ARG:CZ	3:B:568:HOH:O	2.65	0.43
1:B:393:ALA:O	1:B:397:LYS:HG2	2.17	0.43
1:A:486:ARG:NH1	1:A:486:ARG:CB	2.81	0.43
1:A:392:GLU:CD	1:A:392:GLU:H	2.26	0.43
1:A:308:GLN:OE1	1:A:472:HIS:HE1	2.02	0.43
1:A:436:TYR:HE1	1:A:492:PRO:HB3	1.83	0.43
1:A:454:ARG:HG3	1:A:454:ARG:NH1	2.34	0.43
1:B:17:THR:OG1	1:B:57:ARG:HD3	2.17	0.43
1:A:320:LEU:O	1:A:324:GLU:HG3	2.18	0.43
1:A:188:LEU:O	1:A:192:LEU:HG	2.19	0.43
1:A:390:LEU:N	1:A:391:PRO:CD	2.82	0.43
1:B:452:GLU:HB2	1:B:453:PRO:CD	2.49	0.43
1:B:94:TYR:O	1:B:98:ARG:HG3	2.19	0.42
1:B:96:ARG:HG3	1:B:96:ARG:NH1	2.33	0.42
1:B:310:ARG:NH2	3:B:582:HOH:O	2.52	0.42
1:A:96:ARG:HG3	1:A:96:ARG:NH1	2.33	0.42
1:B:155:ALA:HB3	1:B:158:ASP:OD2	2.19	0.42
1:A:485:GLU:HG2	1:A:491:ALA:HA	2.02	0.42
1:B:198:ARG:HH12	1:B:502:GLU:HG2	1.85	0.42
1:A:29:TRP:HB2	1:A:249:ILE:HG21	2.01	0.42
1:B:91:ARG:O	1:B:95:GLU:HG2	2.20	0.42
1:A:373:ARG:CZ	1:A:416:ASP:OD2	2.67	0.42
1:A:235:LEU:N	1:A:235:LEU:CD1	2.83	0.42
1:A:412:GLY:O	1:A:415:GLN:HG2	2.20	0.42
1:A:373:ARG:HD3	1:A:427:PHE:CE1	2.55	0.42
1:A:91:ARG:O	1:A:95:GLU:HG2	2.20	0.41
1:A:27:ALA:HB1	1:A:43:ARG:HD2	2.03	0.41
1:A:124:PRO:HA	1:A:410:LYS:HE2	2.01	0.41
1:A:119:TRP:C	1:A:121:GLU:N	2.78	0.41
1:A:327:PHE:N	1:A:328:PRO:CD	2.83	0.41
1:B:280:HIS:ND1	1:B:305:HIS:ND1	2.61	0.41
1:B:366:TYR:O	1:B:369:HIS:HB2	2.20	0.41
1:B:390:LEU:HB2	1:B:391:PRO:HD3	2.02	0.41
1:A:119:TRP:CZ3	1:A:417:VAL:HB	2.56	0.41
1:A:375:GLU:OE1	1:A:397:LYS:HD2	2.21	0.41
1:A:474:GLU:O	1:A:475:GLY:C	2.63	0.41
1:A:331:ARG:HG3	1:A:331:ARG:NH1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:LEU:HD23	1:A:386:SER:O	2.20	0.41
1:A:92:GLN:HE21	1:A:96:ARG:NH2	2.19	0.40
1:A:123:ARG:C	1:A:125:ARG:N	2.77	0.40
1:B:266:PHE:CZ	1:B:268:ASN:HB2	2.56	0.40
1:A:373:ARG:HD3	1:A:427:PHE:CZ	2.56	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	507/509 (100%)	495 (98%)	12 (2%)	0	100	100
1	B	507/509 (100%)	494 (97%)	13 (3%)	0	100	100
All	All	1014/1018 (100%)	989 (98%)	25 (2%)	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	412/412 (100%)	404 (98%)	8 (2%)	50	58
1	B	412/412 (100%)	407 (99%)	5 (1%)	63	72
All	All	824/824 (100%)	811 (98%)	13 (2%)	55	64

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	208	THR
1	A	240	LEU
1	A	294	THR
1	A	320	LEU
1	A	357	ILE
1	A	472	HIS
1	A	483	LEU
1	B	50	LEU
1	B	103	ARG
1	B	164	LEU
1	B	240	LEU
1	B	320	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	92	GLN
1	A	110	GLN
1	A	245	HIS
1	A	291	HIS
1	A	346	HIS
1	A	472	HIS
1	B	8	GLN
1	B	9	ASN
1	B	46	GLN
1	B	56	GLN
1	B	77	GLN
1	B	92	GLN
1	B	110	GLN
1	B	442	GLN
1	B	472	HIS

5.3.3 RNA ⓘ

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	GOL	B	510	-	5,5,5	0.23	0	5,5,5	0.35	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
2	GOL	B	510	-	-	0/4/4/4	-

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.

5.7 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](#)

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, 95th 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	509/509 (100%)	0.41	14 (2%) 55 57	7, 21, 35, 52	0
1	B	509/509 (100%)	0.16	5 (0%) 79 81	8, 18, 30, 40	0
All	All	1018/1018 (100%)	0.28	19 (1%) 66 69	7, 19, 33, 52	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	203	GLY	4.0
1	A	125	ARG	2.9
1	A	407	LYS	2.7
1	B	457	ARG	2.7
1	B	205	ARG	2.6
1	A	204	LYS	2.6
1	A	121	GLU	2.5
1	A	122	ALA	2.5
1	A	118	PHE	2.4
1	A	492	PRO	2.4
1	B	103	ARG	2.3
1	B	56	GLN	2.2
1	A	400	ASP	2.2
1	A	491	ALA	2.2
1	A	77	GLN	2.2
1	A	202	SER	2.2
1	B	96	ARG	2.1
1	A	120	GLU	2.0
1	A	83	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [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. The B-factors column lists the minimum, median, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	B	510	6/6	0.75	0.20	36,37,38,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.