



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:53 AM UTC

PDB ID : 3IUM / pdb_00003ium
Title : apPEP_WTX opened state
Authors : Chiu, T.K.
Deposited on : 2009-08-31
Resolution : 2.25 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

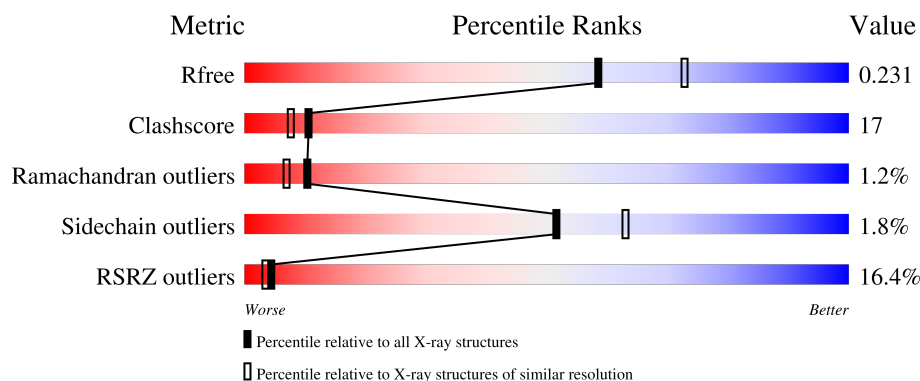
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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))
R_{free}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	693	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5440 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 Prolyl Endopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	668	5281	3353	913	1007	8	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q9X6R4
A	-1	SER	-	expression tag	UNP Q9X6R4
A	0	HIS	-	expression tag	UNP Q9X6R4
A	106	GLN	LYS	SEE REMARK 999	UNP Q9X6R4
A	325	GLN	HIS	SEE REMARK 999	UNP Q9X6R4
A	326	GLN	ARG	SEE REMARK 999	UNP Q9X6R4
A	334	SER	THR	SEE REMARK 999	UNP Q9X6R4
A	335	GLY	ALA	SEE REMARK 999	UNP Q9X6R4
A	348	ARG	PRO	SEE REMARK 999	UNP Q9X6R4
A	577	THR	ALA	SEE REMARK 999	UNP Q9X6R4

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

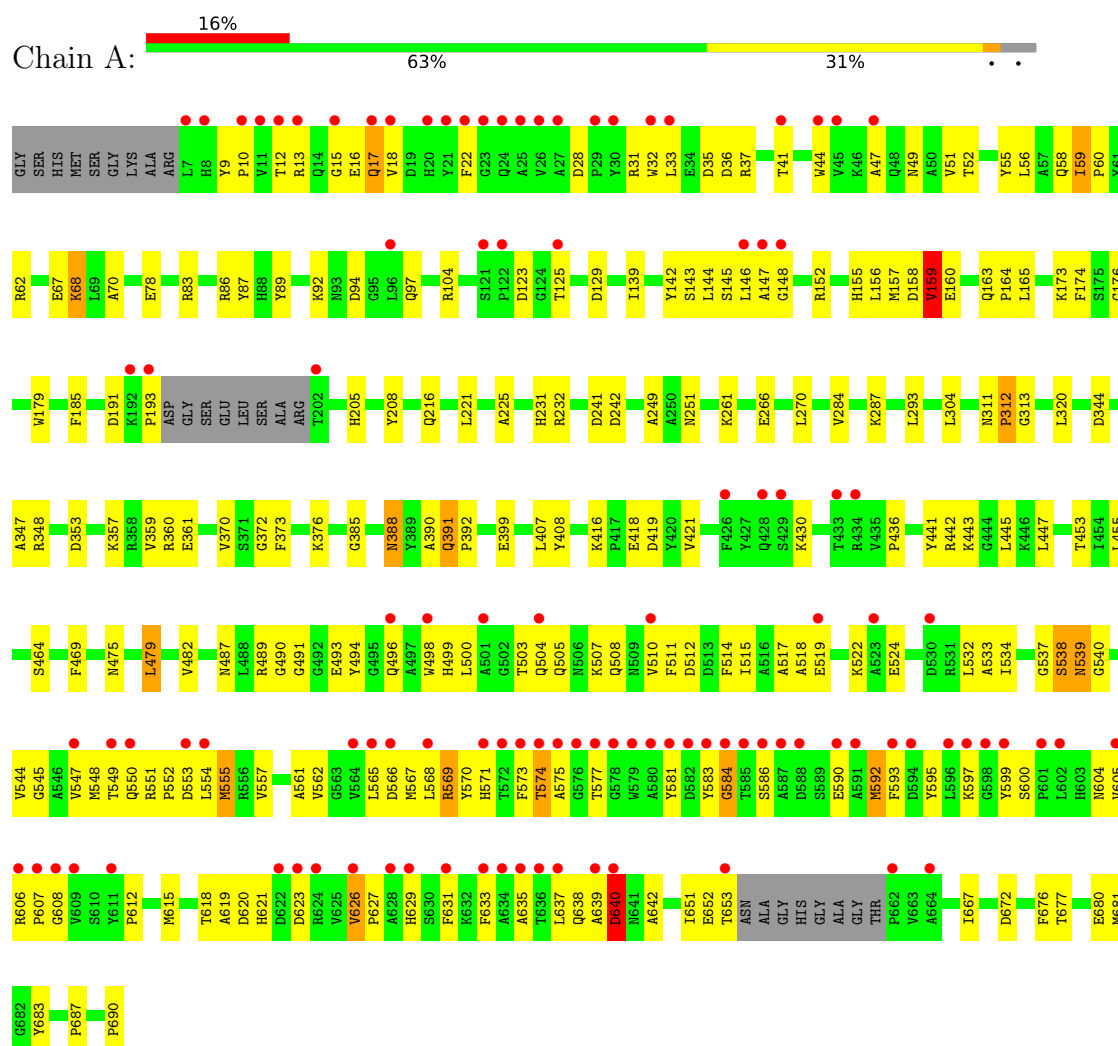
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	135	Total	O	0	0
			135	135		

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: Prolyl Endopeptidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.47Å 100.08Å 155.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.75 – 2.25 38.75 – 2.25	Depositor EDS
% Data completeness (in resolution range)	96.5 (38.75-2.25) 98.3 (38.75-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 2.24Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.219 , 0.244 0.229 , 0.231	Depositor DCC
R_{free} test set	4373 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	50.7	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5440	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0/5414	0.93	28/7349 (0.4%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	311	ASN	CA-C-N	9.06	130.51	120.45
1	A	311	ASN	C-N-CA	9.06	130.51	120.45
1	A	59	ILE	CA-C-N	7.80	127.71	119.05
1	A	59	ILE	C-N-CA	7.80	127.71	119.05
1	A	320	LEU	N-CA-C	-7.68	103.88	113.55
1	A	176	GLY	N-CA-C	-7.16	101.27	112.58
1	A	312	PRO	N-CA-C	6.96	123.05	114.35
1	A	313	GLY	CA-C-N	6.41	126.63	119.32
1	A	313	GLY	C-N-CA	6.41	126.63	119.32
1	A	626	VAL	CA-C-N	6.36	126.85	119.47
1	A	626	VAL	C-N-CA	6.36	126.85	119.47
1	A	490	GLY	N-CA-C	-6.27	107.23	114.69
1	A	347	ALA	N-CA-C	6.23	119.28	110.50
1	A	539	ASN	N-CA-C	-5.99	104.08	111.75
1	A	159	VAL	N-CA-C	5.96	116.70	110.62
1	A	504	GLN	CB-CA-C	-5.84	109.29	117.23
1	A	399	GLU	CA-C-N	5.61	125.08	119.24
1	A	399	GLU	C-N-CA	5.61	125.08	119.24
1	A	479	LEU	N-CA-C	-5.39	106.48	113.16
1	A	284	VAL	N-CA-C	-5.31	106.99	111.56
1	A	584	GLY	N-CA-C	-5.28	103.07	112.58
1	A	532	LEU	N-CA-C	5.20	117.55	108.76
1	A	538	SER	CB-CA-C	-5.19	110.17	117.23
1	A	361	GLU	N-CA-C	-5.15	101.32	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	626	VAL	N-CA-C	5.15	114.62	108.96
1	A	179	TRP	N-CA-C	5.11	118.04	110.48
1	A	158	ASP	N-CA-C	-5.08	101.47	109.25
1	A	592	MSE	N-CA-C	-5.02	105.72	111.14

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	5281	0	5058	174	0
2	A	24	0	32	1	0
3	A	135	0	0	4	1
All	All	5440	0	5090	175	1

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 17.

All (175) 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:606:ARG:HH11	1:A:606:ARG:HB2	1.26	0.98
1:A:49:ASN:HD21	1:A:651:ILE:H	1.22	0.88
1:A:464:SER:HB2	1:A:493:GLU:HG3	1.54	0.87
1:A:606:ARG:HB2	1:A:606:ARG:NH1	1.92	0.84
1:A:508:GLN:HE22	1:A:550:GLN:HE22	1.27	0.82
1:A:193:PRO:HB3	1:A:216:GLN:HE21	1.47	0.79
1:A:555:MSE:HE2	1:A:612:PRO:HG3	1.64	0.79
1:A:221:LEU:HD21	1:A:225:ALA:HB2	1.68	0.75
1:A:56:LEU:HD21	1:A:615:MSE:HE1	1.69	0.74
1:A:388:ASN:C	1:A:388:ASN:HD22	1.96	0.74
1:A:584:GLY:HA3	1:A:592:MSE:HE3	1.68	0.74
1:A:139:ILE:HD12	1:A:165:LEU:HD22	1.71	0.72
1:A:574:THR:HG23	1:A:575:ALA:H	1.52	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:THR:O	1:A:577:THR:HG22	1.90	0.72
1:A:376:LYS:HE3	3:A:1052:HOH:O	1.92	0.69
2:A:701:GOL:H31	2:A:702:GOL:H32	1.76	0.66
1:A:104:ARG:NH1	1:A:159:VAL:HG13	2.11	0.64
1:A:565:LEU:HD13	1:A:633:PHE:CD2	2.34	0.63
1:A:17:GLN:O	1:A:28:ASP:HB3	1.99	0.62
1:A:155:HIS:HD2	3:A:1104:HOH:O	1.82	0.62
1:A:353:ASP:OD2	1:A:357:LYS:HB3	1.99	0.62
1:A:505:GLN:HA	1:A:595:TYR:CE2	2.35	0.61
1:A:67:GLU:HG3	3:A:1085:HOH:O	1.99	0.61
1:A:193:PRO:HD2	1:A:208:TYR:CE2	2.35	0.61
1:A:515:ILE:HG23	1:A:554:LEU:HD22	1.84	0.60
1:A:548:MSE:HA	1:A:555:MSE:HE1	1.83	0.59
1:A:388:ASN:ND2	1:A:390:ALA:H	2.01	0.59
1:A:407:LEU:HD23	1:A:408:TYR:N	2.18	0.59
1:A:261:LYS:HB2	1:A:270:LEU:HD23	1.85	0.58
1:A:436:PRO:HB2	1:A:487:ASN:HD22	1.68	0.58
1:A:586:SER:HB2	1:A:593:PHE:HD1	1.69	0.58
1:A:555:MSE:H	1:A:555:MSE:SE	2.37	0.57
1:A:266:GLU:HA	3:A:1130:HOH:O	2.04	0.57
1:A:232:ARG:H	1:A:251:ASN:HD22	1.52	0.57
1:A:620:ASP:OD2	1:A:653:THR:HA	2.05	0.57
1:A:416:LYS:HB3	1:A:418:GLU:OE1	2.05	0.56
1:A:505:GLN:HA	1:A:595:TYR:CD2	2.40	0.56
1:A:68:LYS:CD	1:A:690:PRO:HB2	2.36	0.55
1:A:565:LEU:HD13	1:A:633:PHE:CG	2.41	0.55
1:A:16:GLU:O	1:A:18:VAL:N	2.40	0.55
1:A:515:ILE:O	1:A:519:GLU:HG3	2.07	0.55
1:A:41:THR:O	1:A:44:TRP:HB3	2.07	0.55
1:A:605:VAL:HG11	1:A:637:LEU:HD23	1.89	0.54
1:A:607:PRO:HA	1:A:640:ASP:O	2.06	0.54
1:A:677:THR:O	1:A:681:MSE:HG3	2.07	0.54
1:A:68:LYS:HD3	1:A:690:PRO:HB2	1.89	0.54
1:A:545:GLY:HA2	1:A:548:MSE:CE	2.37	0.54
1:A:639:ALA:O	1:A:640:ASP:OD1	2.26	0.53
1:A:545:GLY:O	1:A:549:THR:HG23	2.08	0.53
1:A:36:ASP:O	1:A:37:ARG:HD3	2.09	0.53
1:A:606:ARG:HH11	1:A:606:ARG:CB	2.12	0.53
1:A:231:HIS:HA	1:A:251:ASN:HD21	1.74	0.52
1:A:567:MSE:HE1	1:A:583:TYR:CD1	2.44	0.52
1:A:16:GLU:O	1:A:18:VAL:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:GLN:HG3	1:A:164:PRO:HD2	1.91	0.52
1:A:551:ARG:C	1:A:553:ASP:H	2.17	0.52
1:A:13:ARG:HG3	1:A:13:ARG:HH11	1.74	0.52
1:A:35:ASP:O	1:A:41:THR:HG21	2.09	0.52
1:A:555:MSE:CE	1:A:612:PRO:HG3	2.37	0.52
1:A:548:MSE:HB2	1:A:555:MSE:CE	2.40	0.52
1:A:31:ARG:HA	1:A:31:ARG:HH11	1.73	0.52
1:A:651:ILE:HD12	1:A:651:ILE:N	2.25	0.52
1:A:416:LYS:HB2	1:A:419:ASP:OD2	2.10	0.51
1:A:28:ASP:OD2	1:A:31:ARG:NH1	2.43	0.51
1:A:407:LEU:HD23	1:A:407:LEU:C	2.34	0.51
1:A:537:GLY:HA2	1:A:561:ALA:O	2.10	0.51
1:A:508:GLN:NE2	1:A:550:GLN:HE22	2.01	0.51
1:A:676:PHE:O	1:A:680:GLU:HG2	2.10	0.51
1:A:683:TYR:CE1	1:A:687:PRO:HG3	2.46	0.51
1:A:123:ASP:OD1	1:A:125:THR:HG23	2.11	0.51
1:A:28:ASP:OD2	1:A:31:ARG:HB2	2.10	0.50
1:A:568:LEU:HD11	1:A:597:LYS:N	2.26	0.50
1:A:293:LEU:O	1:A:304:LEU:HD12	2.12	0.50
1:A:620:ASP:OD1	1:A:621:HIS:N	2.45	0.50
1:A:430:LYS:HD2	1:A:512:ASP:OD2	2.12	0.49
1:A:47:ALA:O	1:A:51:VAL:HG23	2.11	0.49
1:A:505:GLN:HE21	1:A:592:MSE:HA	1.77	0.49
1:A:13:ARG:HG3	1:A:13:ARG:NH1	2.28	0.49
1:A:78:GLU:HG3	1:A:92:LYS:HG2	1.95	0.49
1:A:555:MSE:SE	1:A:555:MSE:N	2.96	0.49
1:A:94:ASP:H	1:A:97:GLN:NE2	2.11	0.48
1:A:231:HIS:CG	1:A:249:ALA:HB1	2.48	0.48
1:A:442:ARG:HH11	1:A:442:ARG:HG2	1.79	0.48
1:A:522:LYS:HZ2	1:A:554:LEU:HD12	1.79	0.48
1:A:12:THR:HG21	1:A:635:ALA:HB1	1.96	0.47
1:A:464:SER:CB	1:A:493:GLU:HG3	2.36	0.47
1:A:22:PHE:HB3	1:A:590:GLU:OE2	2.15	0.47
1:A:538:SER:HA	1:A:562:VAL:O	2.15	0.47
1:A:55:TYR:O	1:A:58:GLN:HB3	2.14	0.47
1:A:87:TYR:CG	1:A:104:ARG:HD2	2.49	0.47
1:A:548:MSE:HB2	1:A:555:MSE:HE1	1.96	0.47
1:A:44:TRP:HZ3	1:A:631:PHE:CD1	2.33	0.47
1:A:12:THR:HG21	1:A:635:ALA:CB	2.45	0.47
1:A:52:THR:HG23	1:A:615:MSE:HE2	1.98	0.46
1:A:545:GLY:HA2	1:A:548:MSE:HE2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:LYS:NZ	1:A:554:LEU:HD12	2.31	0.46
1:A:599:TYR:C	1:A:599:TYR:CD1	2.92	0.46
1:A:445:LEU:C	1:A:445:LEU:HD23	2.40	0.46
1:A:104:ARG:HH12	1:A:159:VAL:HG13	1.80	0.46
1:A:49:ASN:HD21	1:A:651:ILE:N	2.03	0.46
1:A:193:PRO:HD2	1:A:208:TYR:CZ	2.50	0.46
1:A:15:GLY:O	1:A:16:GLU:HG3	2.16	0.46
1:A:599:TYR:O	1:A:600:SER:C	2.58	0.46
1:A:348:ARG:HH11	1:A:348:ARG:HG2	1.81	0.45
1:A:83:ARG:HG3	1:A:83:ARG:HH11	1.82	0.45
1:A:489:ARG:HA	1:A:498:TRP:CE2	2.51	0.45
1:A:388:ASN:ND2	1:A:391:GLN:H	2.14	0.45
1:A:618:THR:O	1:A:651:ILE:HA	2.17	0.45
1:A:626:VAL:HA	1:A:627:PRO:HD3	1.84	0.45
1:A:232:ARG:H	1:A:251:ASN:ND2	2.15	0.45
1:A:359:VAL:O	1:A:360:ARG:HB3	2.17	0.45
1:A:500:LEU:HA	1:A:503:THR:OG1	2.16	0.45
1:A:514:PHE:O	1:A:517:ALA:HB3	2.16	0.45
1:A:533:ALA:HB2	1:A:557:VAL:HB	1.99	0.45
1:A:565:LEU:H	1:A:629:HIS:HB3	1.82	0.44
1:A:571:HIS:C	1:A:573:PHE:H	2.24	0.44
1:A:70:ALA:HA	1:A:667:ILE:HD13	1.98	0.44
1:A:205:HIS:HB2	1:A:232:ARG:O	2.18	0.44
1:A:419:ASP:HB3	1:A:442:ARG:NH1	2.33	0.44
1:A:489:ARG:HA	1:A:498:TRP:NE1	2.33	0.44
1:A:421:VAL:HG23	1:A:443:LYS:HB2	1.98	0.44
1:A:548:MSE:HE3	1:A:633:PHE:CE2	2.52	0.44
1:A:89:TYR:CE1	1:A:104:ARG:HD3	2.52	0.44
1:A:145:SER:HB3	1:A:152:ARG:CZ	2.48	0.44
1:A:500:LEU:HD21	1:A:581:TYR:OH	2.18	0.44
1:A:193:PRO:HB3	1:A:216:GLN:NE2	2.24	0.43
1:A:511:PHE:O	1:A:515:ILE:HG13	2.18	0.43
1:A:566:ASP:O	1:A:570:TYR:HB3	2.17	0.43
1:A:567:MSE:HE1	1:A:583:TYR:CG	2.54	0.43
1:A:32:TRP:H	1:A:32:TRP:CD1	2.36	0.43
1:A:453:THR:OG1	1:A:482:VAL:HB	2.18	0.43
1:A:489:ARG:O	1:A:510:VAL:HG22	2.18	0.43
1:A:507:LYS:NZ	1:A:539:ASN:HD21	2.16	0.43
1:A:129:ASP:HB3	1:A:143:SER:OG	2.19	0.43
1:A:59:ILE:HA	1:A:60:PRO:HD3	1.70	0.43
1:A:565:LEU:HD12	1:A:629:HIS:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:THR:O	1:A:577:THR:HG23	2.17	0.43
1:A:619:ALA:HA	1:A:652:GLU:HB2	2.01	0.43
1:A:191:ASP:C	1:A:193:PRO:HD3	2.44	0.42
1:A:534:ILE:CD1	1:A:544:VAL:HG13	2.48	0.42
1:A:475:ASN:O	1:A:479:LEU:HG	2.19	0.42
1:A:344:ASP:OD1	1:A:494:TYR:OH	2.30	0.42
1:A:545:GLY:HA2	1:A:548:MSE:HE3	2.00	0.42
1:A:144:LEU:HD12	1:A:155:HIS:CE1	2.54	0.42
1:A:533:ALA:CB	1:A:557:VAL:HB	2.50	0.42
1:A:370:VAL:HA	1:A:385:GLY:O	2.20	0.42
1:A:372:GLY:O	1:A:373:PHE:HB2	2.20	0.42
1:A:491:GLY:O	1:A:498:TRP:HD1	2.03	0.42
1:A:514:PHE:HD2	1:A:547:VAL:HG21	1.84	0.42
1:A:569:ARG:HB2	1:A:569:ARG:NH1	2.34	0.42
1:A:86:ARG:HH21	1:A:160:GLU:CD	2.28	0.42
1:A:142:TYR:CE2	1:A:157:MSE:HE3	2.54	0.42
1:A:146:LEU:O	1:A:148:GLY:N	2.52	0.42
1:A:9:TYR:HB3	1:A:638:GLN:NE2	2.35	0.41
1:A:62:ARG:HD2	1:A:672:ASP:OD1	2.20	0.41
1:A:87:TYR:HB3	1:A:104:ARG:HG3	2.01	0.41
1:A:392:PRO:HA	1:A:469:PHE:CG	2.55	0.41
1:A:455:LEU:HG	1:A:514:PHE:CE1	2.56	0.41
1:A:68:LYS:HD2	1:A:690:PRO:HB2	2.01	0.41
1:A:569:ARG:HA	1:A:571:HIS:CE1	2.56	0.41
1:A:156:LEU:HD21	1:A:185:PHE:CE2	2.56	0.41
1:A:499:HIS:O	1:A:503:THR:HG23	2.20	0.41
1:A:561:ALA:O	1:A:562:VAL:C	2.63	0.41
1:A:548:MSE:HE3	1:A:633:PHE:CZ	2.56	0.41
1:A:570:TYR:OH	1:A:583:TYR:HB2	2.21	0.41
1:A:584:GLY:HA3	1:A:592:MSE:CE	2.45	0.41
1:A:608:GLY:H	1:A:642:ALA:HB2	1.86	0.41
1:A:33:LEU:C	1:A:35:ASP:H	2.30	0.40
1:A:441:TYR:HB3	1:A:482:VAL:HG22	2.02	0.40
1:A:447:LEU:HD22	1:A:524:GLU:O	2.21	0.40
1:A:538:SER:C	1:A:540:GLY:N	2.78	0.40
1:A:241:ASP:O	1:A:242:ASP:HB2	2.20	0.40
1:A:584:GLY:CA	1:A:592:MSE:HE3	2.46	0.40
1:A:173:LYS:O	1:A:174:PHE:C	2.64	0.40
1:A:518:ALA:HB3	1:A:554:LEU:HD21	2.04	0.40

All (1) 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)
3:A:1114:HOH:O	3:A:1115:HOH:O[4_476]	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	662/693 (96%)	608 (92%)	46 (7%)	8 (1%)	10 7

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	604	ASN
1	A	569	ARG
1	A	574	THR
1	A	147	ALA
1	A	10	PRO
1	A	640	ASP
1	A	552	PRO

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	549/556 (99%)	539 (98%)	10 (2%)	51 63

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	LYS
1	A	159	VAL
1	A	287	LYS
1	A	312	PRO
1	A	388	ASN
1	A	391	GLN
1	A	496	GLN
1	A	555	MSE
1	A	623	ASP
1	A	640	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	A	24	GLN
1	A	49	ASN
1	A	53	GLN
1	A	74	ASN
1	A	88	HIS
1	A	97	GLN
1	A	155	HIS
1	A	251	ASN
1	A	274	GLN
1	A	316	HIS
1	A	326	GLN
1	A	388	ASN
1	A	451	ASN
1	A	487	ASN
1	A	505	GLN
1	A	509	ASN
1	A	539	ASN
1	A	550	GLN
1	A	603	HIS
1	A	645	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](#)

4 ligands are 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	A	704	-	5,5,5	0.43	0	5,5,5	0.25	0
2	GOL	A	702	-	5,5,5	0.37	0	5,5,5	0.34	0
2	GOL	A	703	-	5,5,5	0.47	0	5,5,5	0.33	0
2	GOL	A	701	-	5,5,5	0.29	0	5,5,5	0.32	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	A	704	-	-	0/4/4/4	-
2	GOL	A	702	-	-	0/4/4/4	-
2	GOL	A	703	-	-	0/4/4/4	-
2	GOL	A	701	-	-	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.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	702	GOL	1	0
2	A	701	GOL	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 ⓘ

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	660/693 (95%)	0.78	108 (16%) 4 3	30, 56, 95, 95	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	21	TYR	5.9
1	A	576	GLY	5.8
1	A	33	LEU	5.5
1	A	29	PRO	5.2
1	A	27	ALA	5.1
1	A	575	ALA	4.9
1	A	26	VAL	4.9
1	A	202	THR	4.9
1	A	30	TYR	4.5
1	A	11	VAL	4.3
1	A	662	PRO	4.2
1	A	25	ALA	4.1
1	A	147	ALA	4.1
1	A	32	TRP	4.1
1	A	7	LEU	4.1
1	A	577	THR	3.9
1	A	15	GLY	3.8
1	A	20	HIS	3.8
1	A	599	TYR	3.7
1	A	587	ALA	3.7
1	A	554	LEU	3.7
1	A	594	ASP	3.7
1	A	581	TYR	3.7
1	A	593	PHE	3.5
1	A	653	THR	3.5
1	A	637	LEU	3.4
1	A	586	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	584	GLY	3.4
1	A	193	PRO	3.4
1	A	591	ALA	3.4
1	A	96	LEU	3.3
1	A	568	LEU	3.3
1	A	573	PHE	3.3
1	A	596	LEU	3.3
1	A	192	LYS	3.3
1	A	22	PHE	3.3
1	A	45	VAL	3.2
1	A	609	VAL	3.2
1	A	122	PRO	3.2
1	A	640	ASP	3.1
1	A	121	SER	3.1
1	A	583	TYR	3.1
1	A	578	GLY	3.1
1	A	41	THR	3.0
1	A	574	THR	3.0
1	A	607	PRO	3.0
1	A	605	VAL	3.0
1	A	635	ALA	2.9
1	A	18	VAL	2.8
1	A	564	VAL	2.8
1	A	23	GLY	2.8
1	A	547	VAL	2.8
1	A	148	GLY	2.8
1	A	580	ALA	2.8
1	A	549	THR	2.8
1	A	12	THR	2.7
1	A	572	THR	2.7
1	A	602	LEU	2.7
1	A	631	PHE	2.7
1	A	601	PRO	2.7
1	A	44	TRP	2.7
1	A	579	TRP	2.7
1	A	606	ARG	2.7
1	A	504	GLN	2.7
1	A	428	GLN	2.6
1	A	550	GLN	2.6
1	A	17	GLN	2.6
1	A	608	GLY	2.6
1	A	24	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	553	ASP	2.6
1	A	611	TYR	2.6
1	A	8	HIS	2.6
1	A	598	GLY	2.5
1	A	496	GLN	2.5
1	A	565	LEU	2.5
1	A	585	THR	2.5
1	A	434	ARG	2.5
1	A	125	THR	2.4
1	A	588	ASP	2.4
1	A	433	THR	2.4
1	A	628	ALA	2.4
1	A	571	HIS	2.4
1	A	623	ASP	2.4
1	A	636	THR	2.4
1	A	519	GLU	2.4
1	A	590	GLU	2.4
1	A	597	LYS	2.3
1	A	639	ALA	2.3
1	A	501	ALA	2.3
1	A	523	ALA	2.3
1	A	146	LEU	2.3
1	A	530	ASP	2.2
1	A	626	VAL	2.2
1	A	633	PHE	2.2
1	A	624	ARG	2.2
1	A	47	ALA	2.2
1	A	582	ASP	2.2
1	A	622	ASP	2.2
1	A	429	SER	2.2
1	A	13	ARG	2.1
1	A	10	PRO	2.1
1	A	498	TRP	2.1
1	A	634	ALA	2.1
1	A	629	HIS	2.1
1	A	510	VAL	2.1
1	A	426	PHE	2.1
1	A	664	ALA	2.0
1	A	566	ASP	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	A	703	6/6	0.67	0.21	79,88,92,93	0
2	GOL	A	702	6/6	0.74	0.23	74,78,81,82	0
2	GOL	A	701	6/6	0.82	0.20	64,74,77,83	0
2	GOL	A	704	6/6	0.84	0.19	72,80,83,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.