



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:16 AM UTC

PDB ID : 7PQO / pdb_00007pqo
Title : Catalytic fragment of MASP-1 in complex with P1 site mutant ecotin
Authors : Harmat, V.; Fodor, K.; Heja, D.
Deposited on : 2021-09-17
Resolution : 3.39 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

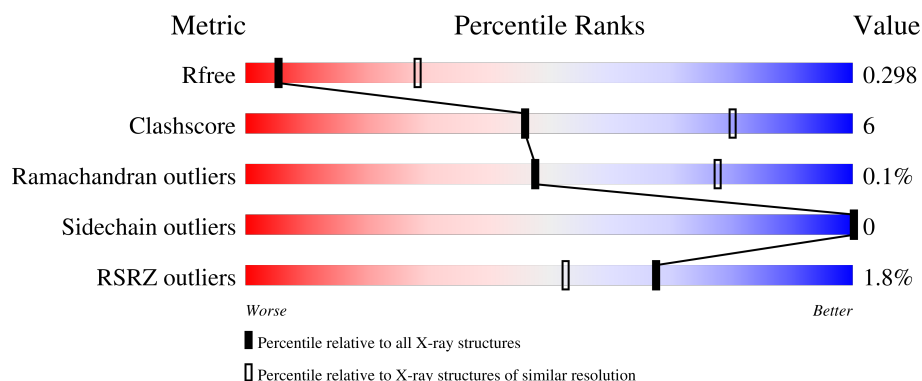
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.39 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	406	85% 13% .
1	B	406	4% 84% 11% 5%
1	C	406	2% 86% 11% .
2	I	162	% 68% 18% 14%
2	J	162	73% 12% 14%

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Mol	Chain	Length	Quality of chain
2	K	162	% 76% 10% 14%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11373 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 Mannan-binding lectin serine protease 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	393	Total	C	N	O	S	0	0	0
			2815	1773	477	540	25			
1	A	398	Total	C	N	O	S	0	0	0
			2841	1798	477	541	25			
1	B	385	Total	C	N	O	S	0	0	0
			2585	1621	438	503	23			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	294	ALA	-	expression tag	UNP P48740
C	295	SER	-	expression tag	UNP P48740
C	296	MET	-	expression tag	UNP P48740
C	297	THR	-	expression tag	UNP P48740
C	499	LYS	GLU	variant	UNP P48740
A	294	ALA	-	expression tag	UNP P48740
A	295	SER	-	expression tag	UNP P48740
A	296	MET	-	expression tag	UNP P48740
A	297	THR	-	expression tag	UNP P48740
A	499	LYS	GLU	variant	UNP P48740
B	294	ALA	-	expression tag	UNP P48740
B	295	SER	-	expression tag	UNP P48740
B	296	MET	-	expression tag	UNP P48740
B	297	THR	-	expression tag	UNP P48740
B	499	LYS	GLU	variant	UNP P48740

- Molecule 2 is a protein called Ecotin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	139	Total	C	N	O	S	0	0	0
			1043	665	172	201	5			

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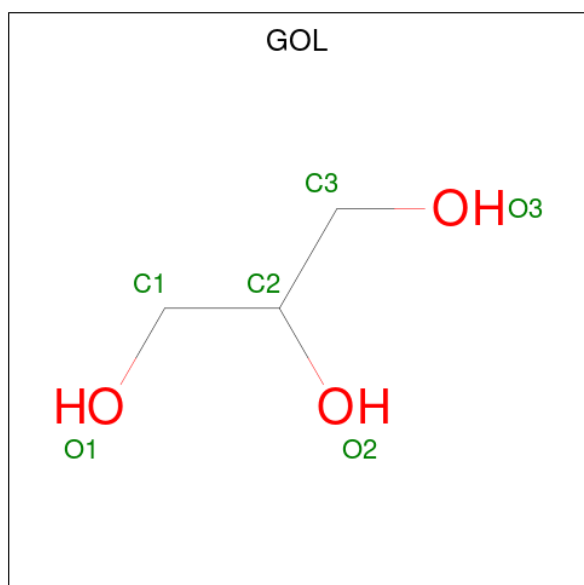
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	139	Total	C	N	O	S	0	0	0
			1026	656	167	198	5			
2	J	139	Total	C	N	O	S	0	0	0
			1020	654	172	189	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	84	ARG	MET	engineered mutation	UNP P23827
I	84	ARG	MET	engineered mutation	UNP P23827
J	84	ARG	MET	engineered mutation	UNP P23827

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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

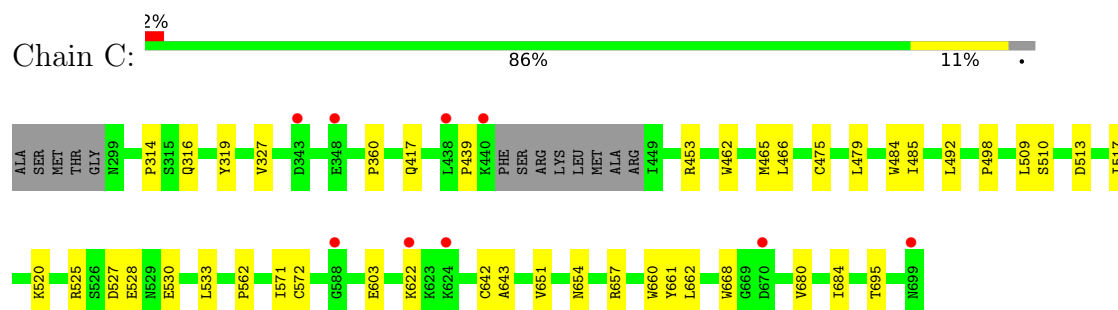
- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Na	0	0
			1	1		

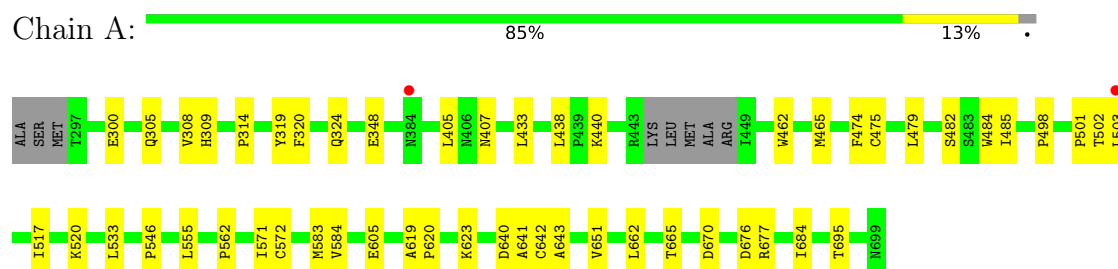
3 Residue-property plots [i](#)

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.

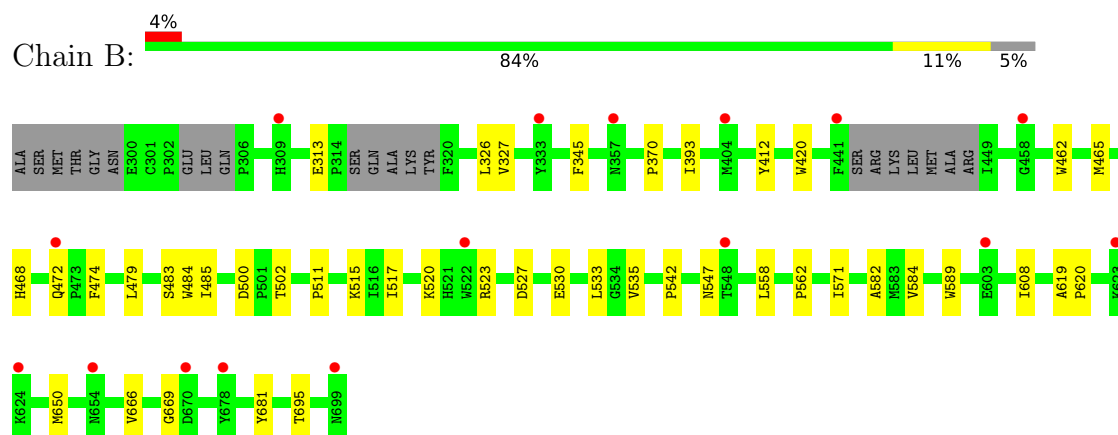
- Molecule 1: Mannan-binding lectin serine protease 1



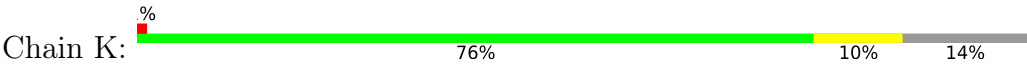
- Molecule 1: Mannan-binding lectin serine protease 1



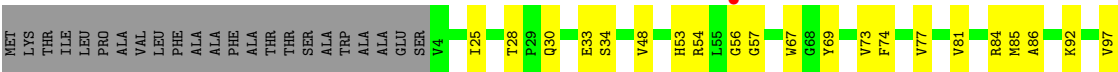
- Molecule 1: Mannan-binding lectin serine protease 1



- Molecule 2: Ecotin



● Molecule 2: Ecotin



● Molecule 2: Ecotin



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	251.07Å 251.07Å 211.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.60 – 3.39 39.60 – 3.39	Depositor EDS
% Data completeness (in resolution range)	96.3 (39.60-3.39) 79.6 (39.60-3.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.74 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.257 , 0.297 0.259 , 0.298	Depositor DCC
R_{free} test set	2261 reflections (2.68%)	wwPDB-VP
Wilson B-factor (Å ²)	93.4	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 133.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11373	wwPDB-VP
Average B, all atoms (Å ²)	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NA

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	0.11	0/2919	0.32	0/4002
1	B	0.10	0/2655	0.33	0/3653
1	C	0.12	0/2892	0.32	0/3966
2	I	0.09	0/1048	0.28	0/1436
2	J	0.08	0/1042	0.30	0/1429
2	K	0.09	0/1065	0.28	0/1457
All	All	0.11	0/11621	0.31	0/15943

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

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	2841	0	2440	36	0
1	B	2585	0	2035	27	0
1	C	2815	0	2411	28	0
2	I	1026	0	931	22	0
2	J	1020	0	934	16	0
2	K	1043	0	967	11	0
3	A	18	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	6	0	8	1	0
3	I	12	0	16	0	0
3	K	6	0	8	1	0
4	C	1	0	0	0	0
All	All	11373	0	9774	122	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 6.

All (122) 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:B:502:THR:OG1	2:I:34:SER:HB2	1.91	0.71
1:B:468:HIS:O	1:B:515:LYS:NZ	2.31	0.64
1:A:502:THR:HG21	2:J:34:SER:HB2	1.80	0.63
1:A:498:PRO:HB2	2:I:97:VAL:HA	1.79	0.62
1:B:533:LEU:HD11	1:B:562:PRO:HB3	1.83	0.61
1:A:503:LEU:HG	1:A:546:PRO:HG3	1.83	0.61
2:K:41:LEU:HB2	2:K:126:LYS:HB2	1.82	0.60
1:B:465:MET:HE2	1:B:517:ILE:HD12	1.84	0.60
1:A:300:GLU:HA	1:A:320:PHE:HA	1.83	0.60
2:I:74:PHE:HB3	2:I:119:THR:HG22	1.83	0.59
2:I:25:ILE:HB	2:I:115:ILE:HB	1.85	0.59
1:B:547:ASN:O	2:J:54:ARG:HD2	2.03	0.58
1:A:665:THR:HG23	1:A:684:ILE:HD11	1.86	0.58
1:C:417:GLN:OE1	1:C:417:GLN:N	2.37	0.57
1:C:520:LYS:NZ	1:C:525:ARG:O	2.34	0.57
1:B:483:SER:HA	1:B:558:LEU:HD12	1.87	0.56
1:C:465:MET:HE2	1:C:517:ILE:HD12	1.86	0.56
1:A:465:MET:HE2	1:A:517:ILE:HD12	1.85	0.56
1:A:474:PHE:HA	2:I:86:ALA:HB3	1.88	0.56
1:B:584:VAL:HG11	1:B:650:MET:HE3	1.89	0.54
1:A:670:ASP:HA	2:I:81:VAL:HG12	1.88	0.54
1:B:517:ILE:HG21	1:B:520:LYS:HD2	1.89	0.53
1:C:571:ILE:HG12	1:C:662:LEU:HB2	1.90	0.53
1:C:651:VAL:HG12	1:C:662:LEU:HA	1.91	0.52
1:B:582:ALA:HB3	1:B:608:ILE:HD12	1.90	0.52
2:K:74:PHE:HB3	2:K:119:THR:HG22	1.92	0.51
1:C:484:TRP:CD2	1:C:695:THR:HG22	2.46	0.51
1:C:517:ILE:HG21	1:C:520:LYS:HD2	1.92	0.51
1:C:453:ARG:NH2	1:C:603:GLU:OE2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:VAL:HG12	1:A:662:LEU:HA	1.94	0.50
1:C:527:ASP:OD1	1:C:530:GLU:HG3	2.12	0.50
1:A:484:TRP:CD2	1:A:695:THR:HG22	2.47	0.49
2:K:21:LYS:HE3	2:K:23:GLN:NE2	2.27	0.49
1:C:316:GLN:HB3	1:C:319:TYR:CE2	2.47	0.49
1:B:313:GLU:CB	1:B:326:LEU:H	2.26	0.49
2:I:77:VAL:HG21	2:I:120:PRO:HG2	1.95	0.48
1:C:642:CYS:SG	1:C:643:ALA:N	2.84	0.48
2:K:47:GLU:HA	2:K:94:LYS:HA	1.96	0.48
1:A:517:ILE:HG21	1:A:520:LYS:HD2	1.94	0.48
1:C:622:LYS:HB3	2:K:57:GLY:H	1.79	0.48
1:A:475:CYS:SG	2:I:85:MET:HG3	2.54	0.48
1:C:533:LEU:HD11	1:C:562:PRO:HB3	1.95	0.47
1:C:572:CYS:HB2	1:C:661:TYR:HA	1.96	0.47
1:B:619:ALA:N	1:B:620:PRO:HD2	2.30	0.47
2:J:48:VAL:HB	2:J:53:HIS:NE2	2.29	0.47
1:B:484:TRP:CD2	1:B:695:THR:HG22	2.50	0.47
2:K:70:ASP:OD2	3:K:901:GOL:O3	2.27	0.47
1:A:498:PRO:O	2:I:98:THR:OG1	2.31	0.47
1:A:533:LEU:HD11	1:A:562:PRO:HB3	1.96	0.47
1:A:555:LEU:HD13	1:A:695:THR:HG23	1.96	0.47
1:B:370:PRO:HG3	1:B:420:TRP:CE2	2.49	0.47
2:J:41:LEU:HB2	2:J:126:LYS:HB2	1.96	0.47
1:B:669:GLY:HA3	2:J:84:ARG:NH2	2.30	0.47
1:A:623:LYS:HA	1:A:623:LYS:HD2	1.64	0.46
1:A:482:SER:O	1:A:562:PRO:HD2	2.15	0.46
1:A:571:ILE:HG12	1:A:662:LEU:HB2	1.98	0.46
2:J:47:GLU:HA	2:J:94:LYS:HA	1.98	0.46
2:J:67:TRP:HB3	2:J:69:TYR:CD1	2.50	0.46
1:C:510:SER:OG	1:C:513:ASP:OD2	2.33	0.46
1:C:439:PRO:HG3	1:C:660:TRP:HE1	1.80	0.46
1:C:462:TRP:CE2	1:C:571:ILE:HD13	2.51	0.45
2:K:48:VAL:HB	2:K:53:HIS:NE2	2.32	0.45
1:C:498:PRO:HB2	2:K:97:VAL:HA	1.99	0.45
2:I:67:TRP:HB3	2:I:69:TYR:CD1	2.52	0.45
1:B:527:ASP:OD1	1:B:530:GLU:HG3	2.16	0.44
2:I:48:VAL:HB	2:I:53:HIS:NE2	2.32	0.44
2:J:48:VAL:HB	2:J:53:HIS:HE2	1.83	0.44
1:B:479:LEU:HA	1:B:485:ILE:HD13	1.99	0.44
1:C:662:LEU:HG	1:C:684:ILE:HD12	1.99	0.44
1:A:619:ALA:N	1:A:620:PRO:HD2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:57:GLY:HA3	2:K:74:PHE:CZ	2.53	0.44
1:A:501:PRO:HG3	2:I:54:ARG:CZ	2.48	0.44
2:I:28:THR:O	2:I:109:TYR:OH	2.27	0.44
1:C:492:LEU:HA	1:C:509:LEU:HD12	2.00	0.44
1:A:642:CYS:O	2:I:84:ARG:HB3	2.18	0.43
1:B:474:PHE:HA	2:J:86:ALA:HB3	1.98	0.43
1:A:642:CYS:SG	1:A:643:ALA:N	2.86	0.43
1:B:327:VAL:HG12	1:B:345:PHE:HB3	2.00	0.43
2:I:53:HIS:O	2:I:54:ARG:NE	2.49	0.43
2:K:53:HIS:O	2:K:54:ARG:NH1	2.52	0.43
1:A:405:LEU:HD13	1:A:433:LEU:HD11	2.01	0.43
1:A:462:TRP:CE2	1:A:571:ILE:HD13	2.54	0.43
1:A:324:GLN:HB3	1:A:348:GLU:HG2	2.01	0.43
1:B:511:PRO:HB3	1:B:535:VAL:HG12	2.01	0.43
2:I:57:GLY:HA3	2:I:74:PHE:CZ	2.54	0.43
1:B:462:TRP:CE2	1:B:571:ILE:HD13	2.54	0.42
1:B:393:ILE:N	1:B:412:TYR:O	2.46	0.42
2:I:73:VAL:HG22	2:I:118:TYR:HB2	2.00	0.42
1:A:583:MET:HE3	1:A:605:GLU:HG2	2.00	0.42
2:I:56:GLY:O	2:I:77:VAL:HA	2.20	0.42
1:C:479:LEU:HA	1:C:485:ILE:HD13	2.00	0.42
1:B:666:VAL:HA	1:B:681:TYR:CD2	2.55	0.42
1:A:584:VAL:O	1:A:605:GLU:HA	2.20	0.42
1:A:438:LEU:O	1:A:440:LYS:NZ	2.53	0.42
1:A:479:LEU:HA	1:A:485:ILE:HD13	2.01	0.42
1:A:571:ILE:HG13	1:A:572:CYS:N	2.35	0.42
2:I:130:TRP:CZ2	2:J:132:ALA:HB2	2.55	0.42
2:J:53:HIS:O	2:J:54:ARG:NE	2.53	0.42
1:C:668:TRP:CH2	1:C:680:VAL:HG21	2.55	0.41
1:B:500:ASP:CG	2:J:128:ARG:HH12	2.28	0.41
2:K:25:ILE:HB	2:K:115:ILE:HB	2.02	0.41
1:A:308:VAL:HG12	1:A:309:HIS:ND1	2.35	0.41
1:C:439:PRO:HD3	1:C:660:TRP:CD1	2.55	0.41
2:I:30:GLN:HB2	2:I:33:GLU:HG2	2.01	0.41
2:I:48:VAL:O	2:I:92:LYS:HA	2.20	0.41
1:A:640:ASP:OD1	1:A:641:ALA:N	2.53	0.41
2:J:48:VAL:O	2:J:92:LYS:HA	2.20	0.41
1:C:466:LEU:HD12	1:C:475:CYS:HB3	2.03	0.41
1:C:654:ASN:HB3	1:C:657:ARG:HB3	2.03	0.41
1:B:472:GLN:HB3	2:J:88:PRO:HB3	2.02	0.41
1:A:305:GLN:OE1	1:A:305:GLN:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:57:GLY:HA3	2:J:74:PHE:CZ	2.55	0.41
1:B:523:ARG:HG3	1:B:589:TRP:HB3	2.03	0.41
1:C:327:VAL:HG11	1:C:360:PRO:HG2	2.03	0.41
1:C:528:GLU:OE2	3:C:701:GOL:O3	2.38	0.41
1:A:405:LEU:C	1:A:407:ASN:H	2.29	0.41
1:B:542:PRO:HB2	2:I:113:LEU:HD11	2.02	0.41
2:J:77:VAL:HG21	2:J:120:PRO:HG2	2.02	0.41
1:C:571:ILE:HG13	1:C:572:CYS:N	2.36	0.40
1:A:314:PRO:O	1:A:319:TYR:OH	2.36	0.40
1:A:676:ASP:O	1:A:677:ARG:HG3	2.21	0.40
1:B:547:ASN:OD1	1:B:547:ASN:N	2.54	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	394/406 (97%)	376 (95%)	18 (5%)	0	100	100
1	B	377/406 (93%)	358 (95%)	19 (5%)	0	100	100
1	C	389/406 (96%)	369 (95%)	19 (5%)	1 (0%)	36	65
2	I	137/162 (85%)	131 (96%)	6 (4%)	0	100	100
2	J	137/162 (85%)	131 (96%)	6 (4%)	0	100	100
2	K	137/162 (85%)	131 (96%)	6 (4%)	0	100	100
All	All	1571/1704 (92%)	1496 (95%)	74 (5%)	1 (0%)	48	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	314	PRO

5.3.2 Protein sidechains ⓘ

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	263/355 (74%)	263 (100%)	0	100	100
1	B	214/355 (60%)	214 (100%)	0	100	100
1	C	265/355 (75%)	265 (100%)	0	100	100
2	I	97/139 (70%)	97 (100%)	0	100	100
2	J	95/139 (68%)	95 (100%)	0	100	100
2	K	103/139 (74%)	103 (100%)	0	100	100
All	All	1037/1482 (70%)	1037 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	521	HIS
1	A	529	ASN
1	A	551	ASN
1	A	615	GLN
1	B	529	ASN
1	B	543	GLN
1	B	687	ASN
2	I	30	GLN
2	J	23	GLN
2	J	30	GLN
2	J	138	ASN

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](#)

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 for Mogul analysis.

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	$\# Z > 2$
3	GOL	A	701	-	5,5,5	0.95	0	5,5,5	1.06	0
3	GOL	I	202	-	5,5,5	0.92	0	5,5,5	1.09	0
3	GOL	K	901	-	5,5,5	0.94	0	5,5,5	1.07	0
3	GOL	A	702	-	5,5,5	0.96	0	5,5,5	1.06	0
3	GOL	C	701	-	5,5,5	0.94	0	5,5,5	1.06	0
3	GOL	I	201	-	5,5,5	0.93	0	5,5,5	1.06	0
3	GOL	A	703	-	5,5,5	0.91	0	5,5,5	1.12	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
3	GOL	A	701	-	-	0/4/4/4	-
3	GOL	I	202	-	-	0/4/4/4	-
3	GOL	K	901	-	-	0/4/4/4	-
3	GOL	A	702	-	-	0/4/4/4	-
3	GOL	C	701	-	-	0/4/4/4	-
3	GOL	I	201	-	-	0/4/4/4	-
3	GOL	A	703	-	-	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 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	901	GOL	1	0
3	C	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	398/406 (98%)	0.12	2 (0%) 87 78	71, 122, 188, 258	0
1	B	385/406 (94%)	0.31	16 (4%) 40 29	103, 157, 210, 262	0
1	C	393/406 (96%)	0.08	9 (2%) 61 46	68, 123, 194, 228	0
2	I	139/162 (85%)	-0.15	1 (0%) 84 73	83, 120, 163, 204	0
2	J	139/162 (85%)	-0.03	0 100 100	97, 136, 181, 199	0
2	K	139/162 (85%)	-0.01	1 (0%) 84 73	82, 115, 163, 193	0
All	All	1593/1704 (93%)	0.11	29 (1%) 67 53	68, 133, 195, 262	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	441	PHE	5.3
1	C	622	LYS	4.9
1	C	440	LYS	3.7
1	B	548	THR	3.6
2	K	103	ASP	3.6
1	B	654	ASN	3.5
1	B	670	ASP	2.9
1	B	699	ASN	2.9
1	B	333	TYR	2.7
1	C	348	GLU	2.7
1	C	670	ASP	2.7
1	C	343	ASP	2.5
1	C	624	LYS	2.5
1	B	603	GLU	2.4
1	C	438	LEU	2.4
1	B	458	GLY	2.3
1	B	678	TYR	2.3
1	A	384	ASN	2.3
1	B	623	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	624	LYS	2.3
1	B	472	GLN	2.2
1	B	404	MET	2.2
2	I	56	GLY	2.2
1	C	699	ASN	2.1
1	B	309	HIS	2.1
1	B	357	ASN	2.1
1	B	522	TRP	2.1
1	A	503	LEU	2.0
1	C	588	GLY	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(Å ²)	Q<0.9
3	GOL	A	703	6/6	0.28	0.16	142,147,155,157	0
4	NA	C	702	1/1	0.58	0.21	159,159,159,159	0
3	GOL	C	701	6/6	0.64	0.19	150,157,166,173	0
3	GOL	I	202	6/6	0.69	0.14	128,143,148,150	0
3	GOL	K	901	6/6	0.69	0.16	124,134,144,150	0
3	GOL	A	701	6/6	0.70	0.15	148,165,179,184	0
3	GOL	I	201	6/6	0.83	0.08	161,166,173,176	0
3	GOL	A	702	6/6	0.84	0.11	131,141,144,148	0

6.5 Other polymers [i](#)

There are no such residues in this entry.