



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 12:31 PM UTC

PDB ID : 9O5S / pdb_00009o5s
Title : minibinder-antigen complex BXMart1-3-MART1-HLA*A02
Authors : Xiang, X.; Jude, K.M.; Garcia, K.C.
Deposited on : 2025-04-10
Resolution : 2.27 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

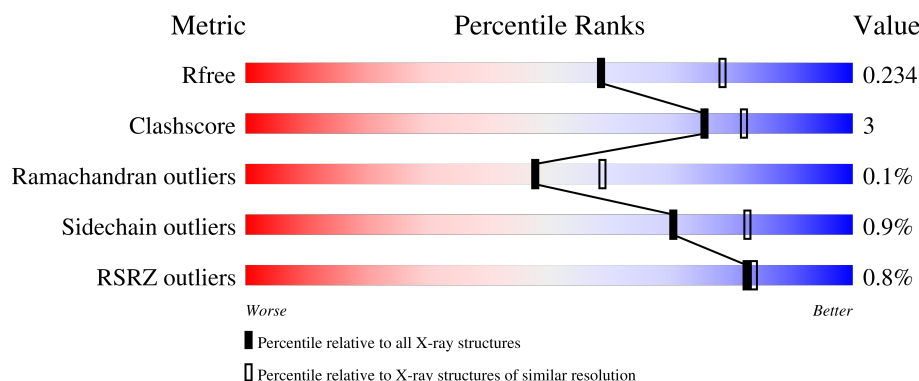
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

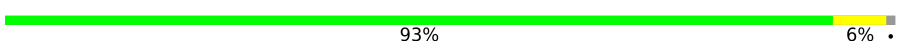
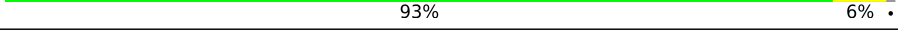
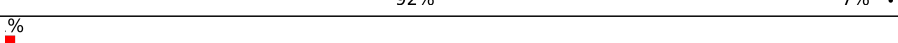
The reported resolution of this entry is 2.27 Å.

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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	279	 93% 6% .
1	C	279	 90% 8% .
1	H	279	 93% 6% .
1	L	279	 92% 7% .
2	B	99	 % 89% 11%

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Mol	Chain	Length	Quality of chain
2	D	99	 2% 89% 10%
2	I	99	 % 89% 10%
2	M	99	 % 93% 6%
3	E	10	 100%
3	J	10	 100%
3	N	10	 90% 10%
3	P	10	 90% 10%
4	F	117	 % 91% 9%
4	G	117	 % 88% 11%
4	K	117	 2% 91% 9%
4	O	117	 4% 92% 8%
5	Q	102	 82% 16%
5	R	102	 91% 9%
5	S	102	 % 92% 7%
5	T	102	 92% 7%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20183 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 HLA class I histocompatibility antigen, A alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	1	0
			2261	1413	413	426	9			
1	C	276	Total	C	N	O	S	0	1	0
			2264	1414	414	427	9			
1	H	276	Total	C	N	O	S	0	2	0
			2270	1417	415	429	9			
1	L	276	Total	C	N	O	S	0	2	0
			2268	1418	414	427	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP A5I8L1
C	0	MET	-	initiating methionine	UNP A5I8L1
H	0	MET	-	initiating methionine	UNP A5I8L1
L	0	MET	-	initiating methionine	UNP A5I8L1

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	1	0
			832	530	140	158	4			
2	D	99	Total	C	N	O	S	0	3	0
			843	537	143	159	4			
2	I	99	Total	C	N	O	S	0	1	0
			832	530	140	158	4			
2	M	99	Total	C	N	O	S	0	1	0
			832	530	140	158	4			

- Molecule 3 is a protein called Melanoma antigen recognized by T-cells 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	10	Total	C	N	O	0	0	0
			68	45	10	13			
3	E	10	Total	C	N	O	0	0	0
			68	45	10	13			
3	J	10	Total	C	N	O	0	0	0
			68	45	10	13			
3	N	10	Total	C	N	O	0	0	0
			68	45	10	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	2	LEU	ALA	engineered mutation	UNP Q16655
E	2	LEU	ALA	engineered mutation	UNP Q16655
J	2	LEU	ALA	engineered mutation	UNP Q16655
N	2	LEU	ALA	engineered mutation	UNP Q16655

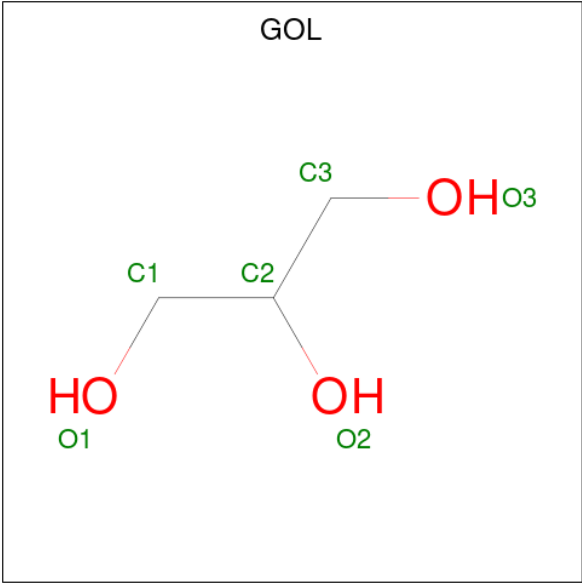
- Molecule 4 is a protein called antibody AD01.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	117	Total	C	N	O	S	0	0	0
			883	547	151	181	4			
4	F	117	Total	C	N	O	S	0	0	0
			883	547	151	181	4			
4	K	117	Total	C	N	O	S	0	0	0
			883	547	151	181	4			
4	O	117	Total	C	N	O	S	0	0	0
			883	547	151	181	4			

- Molecule 5 is a protein called BXMart1-3 minibinder.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	Q	102	Total	C	N	O	0	0	0
			852	529	156	167			
5	R	102	Total	C	N	O	0	0	0
			852	529	156	167			
5	S	102	Total	C	N	O	0	0	0
			852	529	156	167			
5	T	102	Total	C	N	O	0	1	0
			860	534	159	167			

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	G	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	H	1	Total	C	O	0	0
			6	3	3		
6	H	1	Total	C	O	0	0
			6	3	3		
6	H	1	Total	C	O	0	0
			6	3	3		
6	L	1	Total	C	O	0	0
			6	3	3		
6	L	1	Total	C	O	0	0
			6	3	3		
6	L	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	I	1	Total	C	O	0	0
			6	3	3		
6	I	1	Total	C	O	0	0
			6	3	3		
6	I	1	Total	C	O	0	0
			6	3	3		
6	I	1	Total	C	O	0	0
			6	3	3		
6	I	1	Total	C	O	0	0
			6	3	3		
6	I	1	Total	C	O	0	0
			6	3	3		
6	M	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	M	1	Total 6	C 3	O 3	0	0
6	M	1	Total 6	C 3	O 3	0	0
6	M	1	Total 6	C 3	O 3	0	0
6	M	1	Total 6	C 3	O 3	0	0
6	F	1	Total 6	C 3	O 3	0	0
6	K	1	Total 6	C 3	O 3	0	0
6	O	1	Total 6	C 3	O 3	0	0
6	O	1	Total 6	C 3	O 3	0	0
6	O	1	Total 6	C 3	O 3	0	0
6	O	1	Total 6	C 3	O 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	37	Total 37	O 37	0	0
7	B	39	Total 39	O 39	0	0
7	P	1	Total 1	O 1	0	0
7	G	11	Total 11	O 11	0	0
7	Q	4	Total 4	O 4	0	0
7	C	29	Total 29	O 29	0	0
7	H	26	Total 26	O 26	0	0
7	L	18	Total 18	O 18	0	0
7	D	22	Total 22	O 22	0	0

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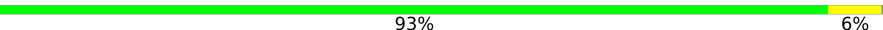
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	I	26	Total 26	O 26	0	0
7	M	26	Total 26	O 26	0	0
7	N	1	Total 1	O 1	0	0
7	F	14	Total 14	O 14	0	0
7	K	15	Total 15	O 15	0	0
7	O	16	Total 16	O 16	0	0
7	R	2	Total 2	O 2	0	0
7	S	3	Total 3	O 3	0	0
7	T	1	Total 1	O 1	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: HLA class I histocompatibility antigen, A alpha chain

Chain A: 



- Molecule 1: HLA class I histocompatibility antigen, A alpha chain

Chain C: 



- Molecule 1: HLA class I histocompatibility antigen, A alpha chain

Chain H: 



- Molecule 1: HLA class I histocompatibility antigen, A alpha chain

Chain L: 

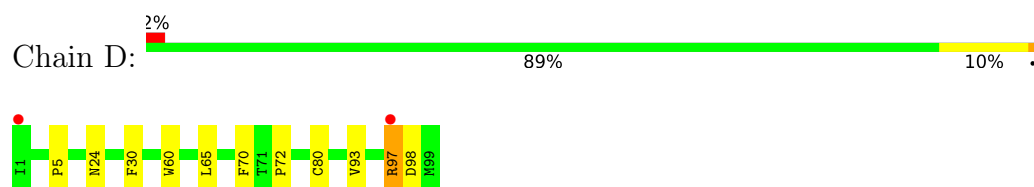


- Molecule 2: Beta-2-microglobulin

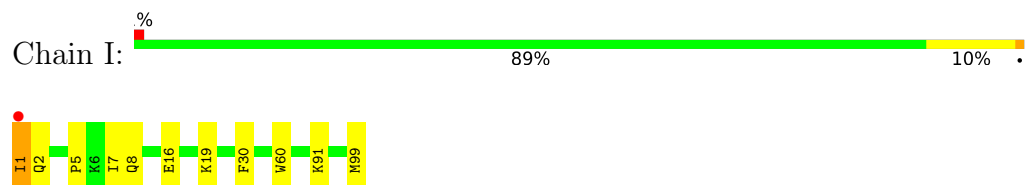
Chain B: 



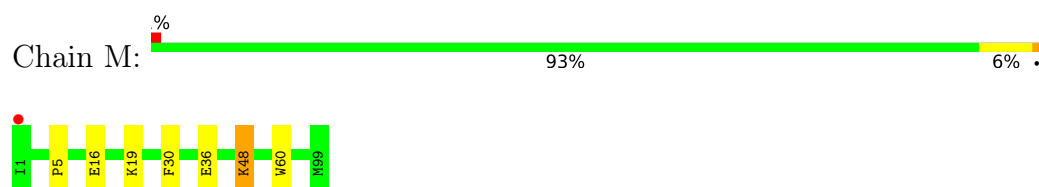
- Molecule 2: Beta-2-microglobulin



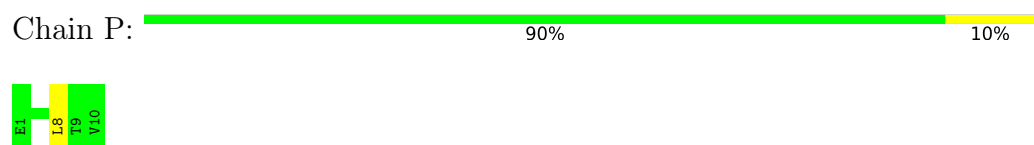
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



- Molecule 3: Melanoma antigen recognized by T-cells 1



- Molecule 3: Melanoma antigen recognized by T-cells 1



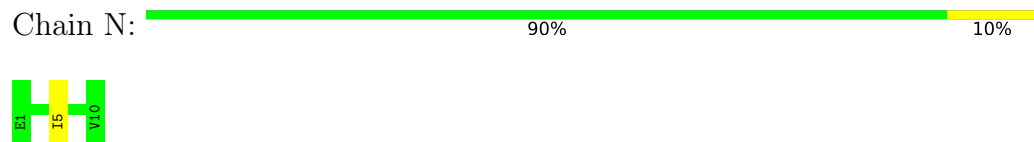
There are no outlier residues recorded for this chain.

- Molecule 3: Melanoma antigen recognized by T-cells 1

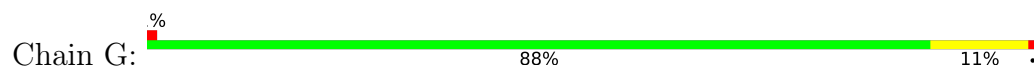


There are no outlier residues recorded for this chain.

- Molecule 3: Melanoma antigen recognized by T-cells 1

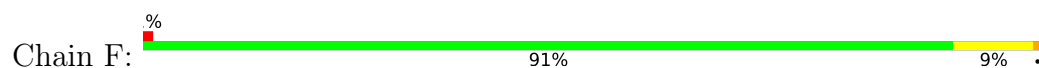


- Molecule 4: antibody AD01

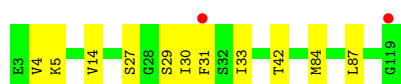




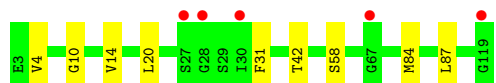
- Molecule 4: antibody AD01



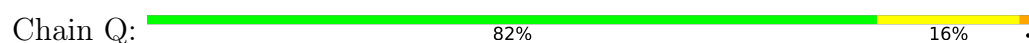
- Molecule 4: antibody AD01



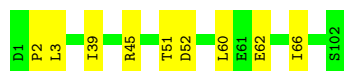
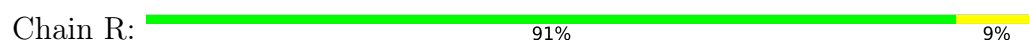
- Molecule 4: antibody AD01



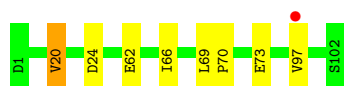
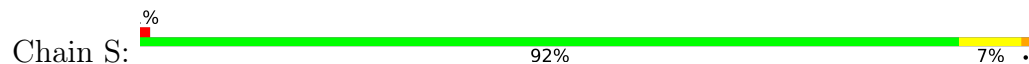
- Molecule 5: BXMart1-3 minibinder



- Molecule 5: BXMart1-3 minibinder



- Molecule 5: BXMart1-3 minibinder



- Molecule 5: BXMart1-3 minibinder





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	87.95Å 95.86Å 99.13Å 89.72° 69.93° 73.90°	Depositor
Resolution (Å)	48.12 – 2.27 48.12 – 2.27	Depositor EDS
% Data completeness (in resolution range)	90.8 (48.12-2.27) 90.8 (48.12-2.27)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.207 , 0.234 0.207 , 0.234	Depositor DCC
R_{free} test set	1994 reflections (1.35%)	wwPDB-VP
Wilson B-factor (Å ²)	52.7	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20183	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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	0.08	0/2330	0.26	0/3163
1	C	0.08	0/2330	0.24	0/3163
1	H	0.09	0/2336	0.26	0/3171
1	L	0.08	0/2337	0.25	0/3173
2	B	0.12	0/858	0.30	0/1160
2	D	0.11	0/875	0.29	0/1182
2	I	0.11	0/858	0.29	0/1160
2	M	0.10	0/858	0.28	0/1160
3	E	0.07	0/67	0.16	0/90
3	J	0.06	0/67	0.18	0/90
3	N	0.08	0/67	0.19	0/90
3	P	0.09	0/67	0.23	0/90
4	F	0.10	0/899	0.31	0/1215
4	G	0.13	0/899	0.34	0/1215
4	K	0.11	0/899	0.30	0/1215
4	O	0.11	0/899	0.33	0/1215
5	Q	0.10	0/862	0.29	0/1161
5	R	0.12	0/862	0.30	0/1161
5	S	0.09	0/862	0.26	0/1161
5	T	0.13	0/873	0.30	0/1175
All	All	0.10	0/20105	0.28	0/27210

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

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	2261	0	2116	12	0
1	C	2264	0	2115	14	0
1	H	2270	0	2119	12	0
1	L	2268	0	2124	11	0
2	B	832	0	799	9	0
2	D	843	0	817	6	0
2	I	832	0	799	9	0
2	M	832	0	799	5	0
3	E	68	0	79	0	0
3	J	68	0	79	0	0
3	N	68	0	79	2	0
3	P	68	0	79	1	0
4	F	883	0	847	6	0
4	G	883	0	847	10	0
4	K	883	0	847	6	0
4	O	883	0	847	6	0
5	Q	852	0	873	13	0
5	R	852	0	873	5	0
5	S	852	0	873	5	0
5	T	860	0	886	5	0
6	A	36	0	48	1	0
6	B	48	0	64	2	0
6	C	18	0	24	0	0
6	D	12	0	16	0	0
6	F	6	0	8	1	0
6	G	6	0	8	0	0
6	H	18	0	24	1	0
6	I	48	0	64	3	0
6	K	6	0	8	1	0
6	L	18	0	24	0	0
6	M	30	0	40	0	0
6	O	24	0	32	2	0
7	A	37	0	0	0	0
7	B	39	0	0	0	0
7	C	29	0	0	0	0
7	D	22	0	0	0	0
7	F	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	11	0	0	0	0
7	H	26	0	0	0	0
7	I	26	0	0	1	0
7	K	15	0	0	0	0
7	L	18	0	0	0	0
7	M	26	0	0	2	0
7	N	1	0	0	0	0
7	O	16	0	0	0	0
7	P	1	0	0	0	0
7	Q	4	0	0	0	0
7	R	2	0	0	0	0
7	S	3	0	0	0	0
7	T	1	0	0	0	0
All	All	20183	0	19257	119	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 3.

The worst 5 of 119 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)
2:B:2:GLN:HG3	6:H:303:GOL:H32	1.74	0.70
4:F:42:THR:HG23	6:F:201:GOL:H11	1.75	0.67
1:H:230:LEU:HD22	1:H:243:LYS:HE3	1.81	0.63
1:C:230:LEU:HD22	1:C:243:LYS:HE3	1.82	0.62
5:Q:70:PRO:HB2	5:Q:73:GLU:OE1	2.00	0.62

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	275/279 (99%)	267 (97%)	8 (3%)	0	100	100
1	C	275/279 (99%)	265 (96%)	10 (4%)	0	100	100
1	H	276/279 (99%)	267 (97%)	9 (3%)	0	100	100
1	L	276/279 (99%)	267 (97%)	9 (3%)	0	100	100
2	B	98/99 (99%)	98 (100%)	0	0	100	100
2	D	100/99 (101%)	100 (100%)	0	0	100	100
2	I	98/99 (99%)	98 (100%)	0	0	100	100
2	M	98/99 (99%)	98 (100%)	0	0	100	100
3	E	8/10 (80%)	8 (100%)	0	0	100	100
3	J	8/10 (80%)	8 (100%)	0	0	100	100
3	N	8/10 (80%)	8 (100%)	0	0	100	100
3	P	8/10 (80%)	8 (100%)	0	0	100	100
4	F	115/117 (98%)	112 (97%)	2 (2%)	1 (1%)	14	15
4	G	115/117 (98%)	111 (96%)	3 (3%)	1 (1%)	14	15
4	K	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
4	O	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
5	Q	100/102 (98%)	99 (99%)	1 (1%)	0	100	100
5	R	100/102 (98%)	99 (99%)	1 (1%)	0	100	100
5	S	100/102 (98%)	99 (99%)	1 (1%)	0	100	100
5	T	101/102 (99%)	100 (99%)	1 (1%)	0	100	100
All	All	2389/2428 (98%)	2336 (98%)	51 (2%)	2 (0%)	48	59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	G	29	SER
4	F	30	ILE

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	233/235 (99%)	233 (100%)	0	100	100
1	C	233/235 (99%)	231 (99%)	2 (1%)	70	82
1	H	234/235 (100%)	233 (100%)	1 (0%)	84	91
1	L	234/235 (100%)	231 (99%)	3 (1%)	61	76
2	B	95/94 (101%)	95 (100%)	0	100	100
2	D	97/94 (103%)	94 (97%)	3 (3%)	35	50
2	I	95/94 (101%)	94 (99%)	1 (1%)	65	79
2	M	95/94 (101%)	94 (99%)	1 (1%)	65	79
3	E	7/7 (100%)	7 (100%)	0	100	100
3	J	7/7 (100%)	7 (100%)	0	100	100
3	N	7/7 (100%)	7 (100%)	0	100	100
3	P	7/7 (100%)	7 (100%)	0	100	100
4	F	97/97 (100%)	96 (99%)	1 (1%)	68	81
4	G	97/97 (100%)	96 (99%)	1 (1%)	68	81
4	K	97/97 (100%)	96 (99%)	1 (1%)	68	81
4	O	97/97 (100%)	97 (100%)	0	100	100
5	Q	95/95 (100%)	93 (98%)	2 (2%)	47	63
5	R	95/95 (100%)	94 (99%)	1 (1%)	65	79
5	S	95/95 (100%)	94 (99%)	1 (1%)	65	79
5	T	96/95 (101%)	95 (99%)	1 (1%)	68	81
All	All	2113/2112 (100%)	2094 (99%)	19 (1%)	70	82

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	F	30	ILE
5	S	20	VAL
5	T	20	VAL
5	R	51	THR
1	L	223	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	197	HIS

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Mol	Chain	Res	Type
2	D	13	HIS
5	S	44	ASN
2	M	13	HIS
1	C	72	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](#)

45 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	$\# Z > 2$
6	GOL	A	303	-	5,5,5	0.34	0	5,5,5	0.41	0
6	GOL	H	303	-	5,5,5	0.41	0	5,5,5	0.33	0
6	GOL	M	104	-	5,5,5	0.33	0	5,5,5	0.42	0
6	GOL	B	105	-	5,5,5	0.36	0	5,5,5	0.36	0
6	GOL	B	108	-	5,5,5	0.33	0	5,5,5	0.40	0
6	GOL	C	301	-	5,5,5	0.34	0	5,5,5	0.39	0
6	GOL	A	305	-	5,5,5	0.34	0	5,5,5	0.31	0
6	GOL	A	302	-	5,5,5	0.33	0	5,5,5	0.45	0
6	GOL	I	107	-	5,5,5	0.33	0	5,5,5	0.46	0
6	GOL	L	303	-	5,5,5	0.33	0	5,5,5	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	B	104	-	5,5,5	0.34	0	5,5,5	0.40	0
6	GOL	H	301	-	5,5,5	0.35	0	5,5,5	0.44	0
6	GOL	M	103	-	5,5,5	0.34	0	5,5,5	0.40	0
6	GOL	M	105	-	5,5,5	0.33	0	5,5,5	0.33	0
6	GOL	D	101	-	5,5,5	0.33	0	5,5,5	0.42	0
6	GOL	C	302	-	5,5,5	0.33	0	5,5,5	0.43	0
6	GOL	L	301	-	5,5,5	0.34	0	5,5,5	0.38	0
6	GOL	O	204	-	5,5,5	0.36	0	5,5,5	0.37	0
6	GOL	L	302	-	5,5,5	0.34	0	5,5,5	0.41	0
6	GOL	D	102	-	5,5,5	0.34	0	5,5,5	0.44	0
6	GOL	I	108	-	5,5,5	0.36	0	5,5,5	0.33	0
6	GOL	M	101	-	5,5,5	0.34	0	5,5,5	0.50	0
6	GOL	M	102	-	5,5,5	0.35	0	5,5,5	0.22	0
6	GOL	I	103	-	5,5,5	0.34	0	5,5,5	0.39	0
6	GOL	I	106	-	5,5,5	0.33	0	5,5,5	0.41	0
6	GOL	B	103	-	5,5,5	0.33	0	5,5,5	0.40	0
6	GOL	K	201	-	5,5,5	0.35	0	5,5,5	0.45	0
6	GOL	I	101	-	5,5,5	0.34	0	5,5,5	0.62	0
6	GOL	I	102	-	5,5,5	0.33	0	5,5,5	0.39	0
6	GOL	B	106	-	5,5,5	0.34	0	5,5,5	0.45	0
6	GOL	G	201	-	5,5,5	0.34	0	5,5,5	0.40	0
6	GOL	A	306	-	5,5,5	0.34	0	5,5,5	0.46	0
6	GOL	F	201	-	5,5,5	0.35	0	5,5,5	0.40	0
6	GOL	H	302	-	5,5,5	0.35	0	5,5,5	0.41	0
6	GOL	O	201	-	5,5,5	0.34	0	5,5,5	0.43	0
6	GOL	B	102	-	5,5,5	0.34	0	5,5,5	0.39	0
6	GOL	B	101	-	5,5,5	0.34	0	5,5,5	0.39	0
6	GOL	I	104	-	5,5,5	0.32	0	5,5,5	0.45	0
6	GOL	C	303	-	5,5,5	0.35	0	5,5,5	0.39	0
6	GOL	A	301	-	5,5,5	0.35	0	5,5,5	0.45	0
6	GOL	B	107	-	5,5,5	0.33	0	5,5,5	0.38	0
6	GOL	I	105	-	5,5,5	0.33	0	5,5,5	0.42	0
6	GOL	O	203	-	5,5,5	0.34	0	5,5,5	0.40	0
6	GOL	A	304	-	5,5,5	0.34	0	5,5,5	0.43	0
6	GOL	O	202	-	5,5,5	0.35	0	5,5,5	0.39	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
6	GOL	A	303	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	H	303	-	-	4/4/4/4	-
6	GOL	M	104	-	-	0/4/4/4	-
6	GOL	B	105	-	-	0/4/4/4	-
6	GOL	B	108	-	-	0/4/4/4	-
6	GOL	C	301	-	-	2/4/4/4	-
6	GOL	A	305	-	-	2/4/4/4	-
6	GOL	A	302	-	-	2/4/4/4	-
6	GOL	I	107	-	-	2/4/4/4	-
6	GOL	L	303	-	-	1/4/4/4	-
6	GOL	B	104	-	-	4/4/4/4	-
6	GOL	H	301	-	-	2/4/4/4	-
6	GOL	M	103	-	-	2/4/4/4	-
6	GOL	M	105	-	-	2/4/4/4	-
6	GOL	D	101	-	-	0/4/4/4	-
6	GOL	C	302	-	-	4/4/4/4	-
6	GOL	L	301	-	-	2/4/4/4	-
6	GOL	O	204	-	-	0/4/4/4	-
6	GOL	L	302	-	-	1/4/4/4	-
6	GOL	D	102	-	-	4/4/4/4	-
6	GOL	I	108	-	-	2/4/4/4	-
6	GOL	M	101	-	-	2/4/4/4	-
6	GOL	M	102	-	-	4/4/4/4	-
6	GOL	I	103	-	-	2/4/4/4	-
6	GOL	I	106	-	-	4/4/4/4	-
6	GOL	B	103	-	-	0/4/4/4	-
6	GOL	K	201	-	-	4/4/4/4	-
6	GOL	I	101	-	-	2/4/4/4	-
6	GOL	I	102	-	-	4/4/4/4	-
6	GOL	B	106	-	-	0/4/4/4	-
6	GOL	G	201	-	-	0/4/4/4	-
6	GOL	A	306	-	-	2/4/4/4	-
6	GOL	F	201	-	-	0/4/4/4	-
6	GOL	H	302	-	-	1/4/4/4	-
6	GOL	O	201	-	-	4/4/4/4	-
6	GOL	B	102	-	-	4/4/4/4	-
6	GOL	B	101	-	-	0/4/4/4	-
6	GOL	I	104	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	C	303	-	-	4/4/4/4	-
6	GOL	A	301	-	-	2/4/4/4	-
6	GOL	B	107	-	-	0/4/4/4	-
6	GOL	I	105	-	-	0/4/4/4	-
6	GOL	O	203	-	-	2/4/4/4	-
6	GOL	A	304	-	-	2/4/4/4	-
6	GOL	O	202	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 85 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	301	GOL	C1-C2-C3-O3
6	A	302	GOL	C1-C2-C3-O3
6	A	302	GOL	O2-C2-C3-O3
6	A	304	GOL	O1-C1-C2-C3
6	A	305	GOL	C1-C2-C3-O3

There are no ring outliers.

10 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	303	GOL	1	0
6	B	108	GOL	1	0
6	O	204	GOL	1	0
6	I	108	GOL	1	0
6	K	201	GOL	1	0
6	I	101	GOL	2	0
6	F	201	GOL	1	0
6	A	301	GOL	1	0
6	B	107	GOL	1	0
6	O	202	GOL	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	276/279 (98%)	-0.13	1 (0%) 88 89	45, 71, 132, 171	1 (0%)
1	C	276/279 (98%)	-0.08	1 (0%) 88 89	39, 81, 134, 165	1 (0%)
1	H	276/279 (98%)	-0.03	1 (0%) 88 89	36, 76, 128, 164	2 (0%)
1	L	276/279 (98%)	-0.07	1 (0%) 88 89	42, 80, 133, 163	2 (0%)
2	B	99/99 (100%)	-0.32	1 (1%) 79 81	42, 53, 78, 91	1 (1%)
2	D	99/99 (100%)	-0.17	2 (2%) 65 66	43, 64, 88, 113	3 (3%)
2	I	99/99 (100%)	-0.32	1 (1%) 79 81	45, 59, 84, 104	1 (1%)
2	M	99/99 (100%)	-0.26	1 (1%) 79 81	45, 60, 79, 113	1 (1%)
3	E	10/10 (100%)	0.33	0 100 100	73, 76, 80, 80	0
3	J	10/10 (100%)	0.07	0 100 100	73, 75, 80, 83	0
3	N	10/10 (100%)	0.10	0 100 100	73, 80, 84, 87	0
3	P	10/10 (100%)	-0.09	0 100 100	64, 68, 75, 80	0
4	F	117/117 (100%)	-0.18	1 (0%) 81 82	47, 65, 100, 125	0
4	G	117/117 (100%)	-0.20	1 (0%) 81 82	44, 64, 108, 152	0
4	K	117/117 (100%)	-0.14	2 (1%) 69 70	47, 65, 109, 163	0
4	O	117/117 (100%)	-0.10	5 (4%) 40 41	43, 63, 137, 174	0
5	Q	102/102 (100%)	0.06	0 100 100	71, 100, 140, 168	0
5	R	102/102 (100%)	0.16	0 100 100	80, 112, 161, 178	0
5	S	102/102 (100%)	0.20	1 (0%) 79 81	88, 124, 160, 184	0
5	T	102/102 (100%)	0.16	0 100 100	71, 121, 154, 170	1 (0%)
All	All	2416/2428 (99%)	-0.08	19 (0%) 82 84	36, 74, 138, 184	13 (0%)

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1	ILE	3.2
2	M	1	ILE	3.1
4	G	119	GLY	3.1
2	D	1	ILE	3.0
2	I	1	ILE	2.8

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
6	GOL	I	106	6/6	0.67	0.21	61,80,89,98	0
6	GOL	I	108	6/6	0.69	0.13	68,82,85,91	0
6	GOL	L	301	6/6	0.71	0.14	95,107,110,111	0
6	GOL	D	102	6/6	0.71	0.17	96,98,101,105	0
6	GOL	B	105	6/6	0.72	0.16	81,87,98,102	0
6	GOL	A	306	6/6	0.77	0.10	93,102,104,106	0
6	GOL	O	203	6/6	0.77	0.10	85,90,95,100	0
6	GOL	O	204	6/6	0.78	0.15	66,78,86,88	0
6	GOL	C	301	6/6	0.79	0.10	83,91,97,100	0
6	GOL	M	101	6/6	0.79	0.14	85,96,102,102	0
6	GOL	I	107	6/6	0.80	0.12	77,90,93,93	0
6	GOL	B	106	6/6	0.81	0.15	78,85,88,93	0
6	GOL	B	107	6/6	0.82	0.08	82,86,93,95	0
6	GOL	H	302	6/6	0.82	0.11	91,93,99,100	0
6	GOL	I	101	6/6	0.83	0.14	55,75,83,85	0
6	GOL	I	102	6/6	0.83	0.13	83,84,91,92	0
6	GOL	M	103	6/6	0.83	0.10	76,87,91,96	0
6	GOL	O	201	6/6	0.83	0.12	59,77,87,89	0
6	GOL	B	102	6/6	0.83	0.11	80,85,92,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	GOL	A	304	6/6	0.83	0.11	87,94,97,102	0
6	GOL	B	108	6/6	0.84	0.10	74,79,88,92	0
6	GOL	O	202	6/6	0.84	0.12	75,83,91,91	0
6	GOL	M	102	6/6	0.84	0.12	66,74,81,87	0
6	GOL	A	303	6/6	0.84	0.09	68,82,86,88	0
6	GOL	H	301	6/6	0.85	0.14	71,80,87,94	0
6	GOL	A	305	6/6	0.86	0.14	62,79,83,90	0
6	GOL	D	101	6/6	0.87	0.12	74,76,81,86	0
6	GOL	C	303	6/6	0.87	0.10	76,80,85,85	0
6	GOL	B	104	6/6	0.88	0.11	72,73,85,94	0
6	GOL	I	104	6/6	0.88	0.08	70,78,80,95	0
6	GOL	C	302	6/6	0.89	0.10	62,75,80,91	0
6	GOL	I	103	6/6	0.89	0.12	86,89,93,97	0
6	GOL	A	301	6/6	0.89	0.09	68,83,94,105	0
6	GOL	M	104	6/6	0.89	0.12	81,83,90,90	0
6	GOL	B	103	6/6	0.90	0.10	74,79,83,86	0
6	GOL	K	201	6/6	0.90	0.09	75,78,89,91	0
6	GOL	L	302	6/6	0.90	0.10	71,73,83,89	0
6	GOL	B	101	6/6	0.91	0.11	70,75,83,86	0
6	GOL	H	303	6/6	0.91	0.09	68,76,86,97	0
6	GOL	G	201	6/6	0.92	0.09	60,83,86,89	0
6	GOL	L	303	6/6	0.92	0.10	83,84,94,99	0
6	GOL	A	302	6/6	0.93	0.10	63,75,83,88	0
6	GOL	M	105	6/6	0.93	0.09	81,82,90,92	0
6	GOL	F	201	6/6	0.93	0.08	73,83,93,97	0
6	GOL	I	105	6/6	0.93	0.09	65,72,82,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.