



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:31 PM UTC

PDB ID : 3C2X / pdb_00003c2x
Title : Crystal structure of peptidoglycan recognition protein at 1.8Å resolution
Authors : Sharma, P.; Singh, N.; Sinha, M.; Sharma, S.; Perbandt, M.; Betzel, C.; Kaur, P.; Srinivasan, A.; Singh, T.P.
Deposited on : 2008-01-26
Resolution : 1.83 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

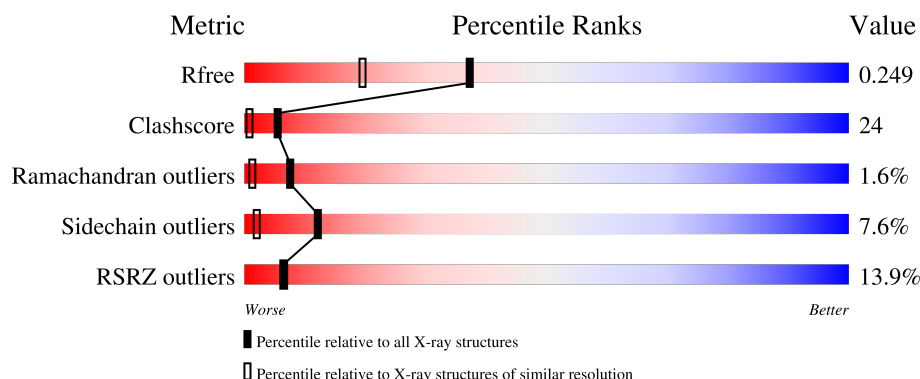
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.83 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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	171	8% 70% 23% 6%
1	B	171	26% 53% 34% 9%
1	C	171	7% 71% 23% 5%
1	D	171	15% 59% 33% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	175	-	-	X	-
2	GOL	D	504	-	-	X	-
2	GOL	D	507	-	-	X	-

2 Entry composition [i](#)

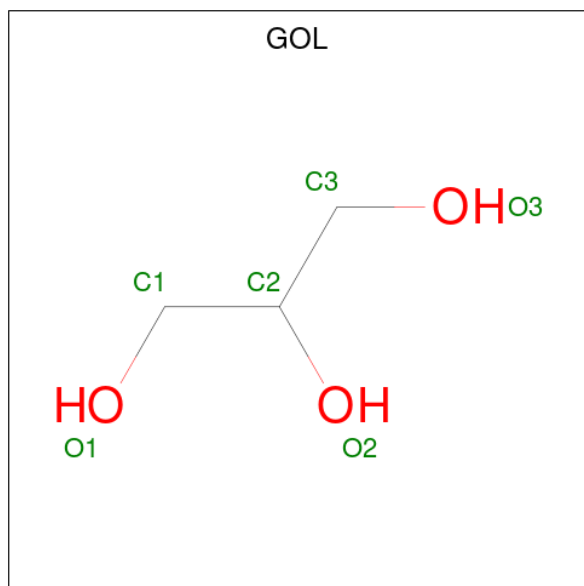
There are 5 unique types of molecules in this entry. The entry contains 6180 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Peptidoglycan recognition protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	171	Total	C	N	O	S	0	0	0
			1337	834	254	241	8			
1	B	171	Total	C	N	O	S	0	0	0
			1337	834	254	241	8			
1	C	171	Total	C	N	O	S	0	0	0
			1337	834	254	241	8			
1	D	171	Total	C	N	O	S	0	0	0
			1337	834	254	241	8			

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



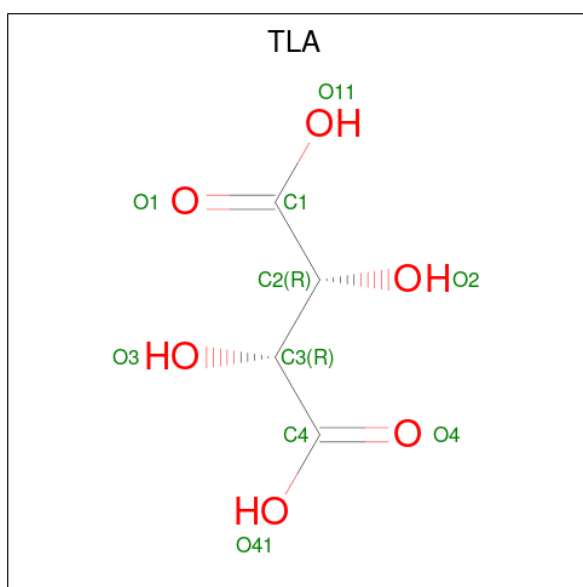
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		

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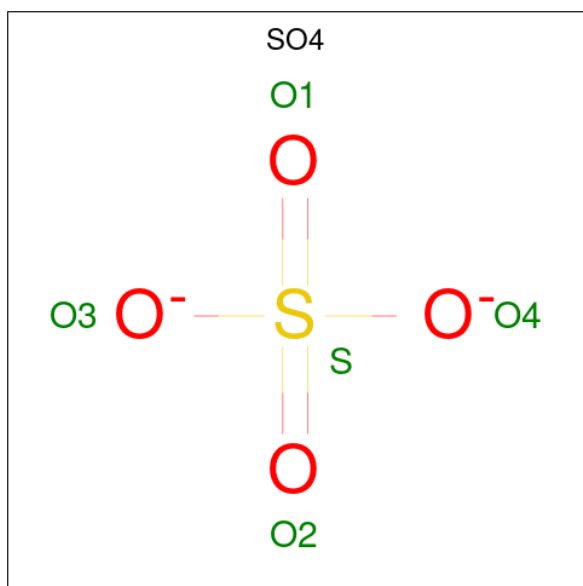
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total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

- Molecule 3 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			10	4	6		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	O	S	0	0
			5	4	1		

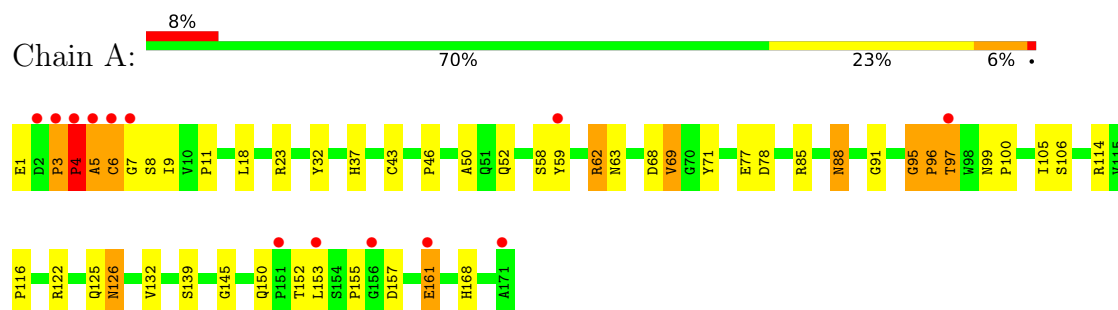
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	172	Total	O	0	0
			172	172		
5	B	162	Total	O	0	0
			162	162		
5	C	235	Total	O	0	0
			235	235		
5	D	170	Total	O	0	0
			170	170		

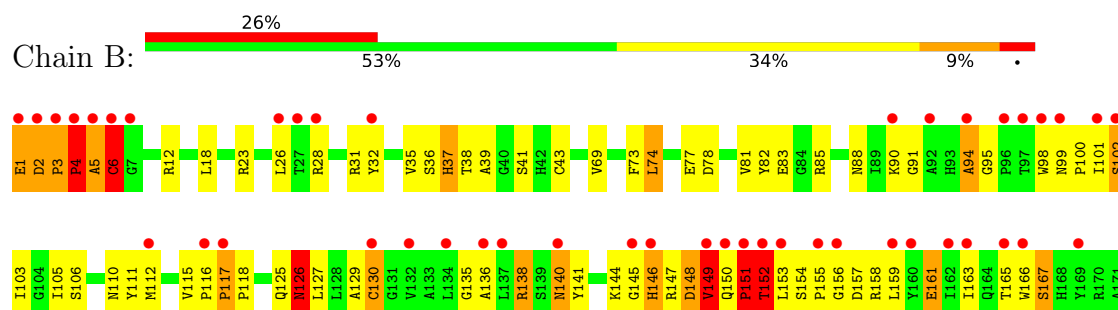
3 Residue-property plots [i](#)

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.

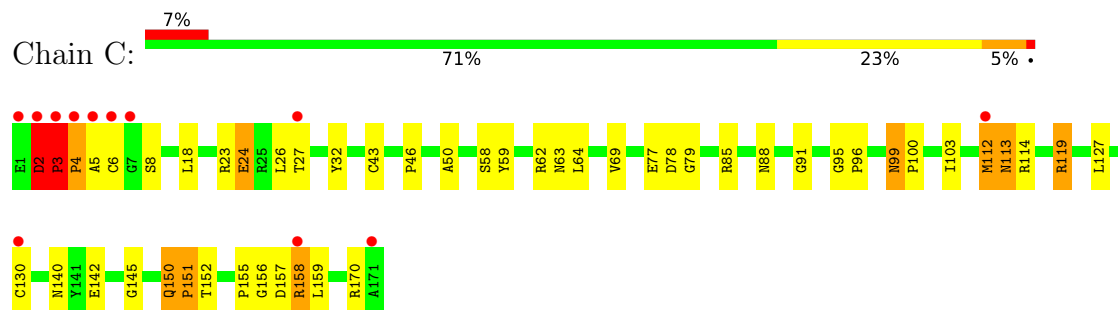
• Molecule 1: Peptidoglycan recognition protein



• Molecule 1: Peptidoglycan recognition protein

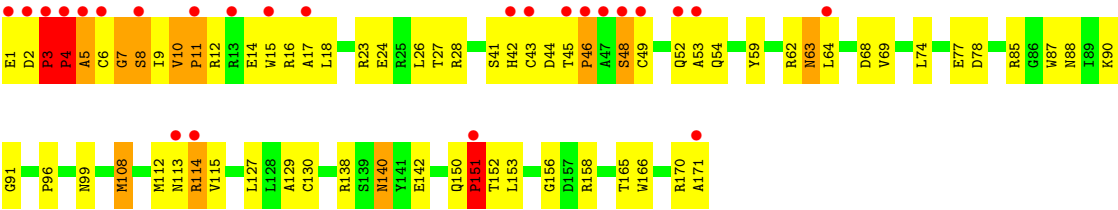


• Molecule 1: Peptidoglycan recognition protein



• Molecule 1: Peptidoglycan recognition protein





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	87.04Å 101.90Å 162.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.93 – 1.83 19.93 – 1.83	Depositor EDS
% Data completeness (in resolution range)	99.4 (19.93-1.83) 99.5 (19.93-1.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 1.82Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225 , 0.247 0.241 , 0.249	Depositor DCC
R_{free} test set	1289 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.798	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.7	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	0.94	EDS
Total number of atoms	6180	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% 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: TLA, SO4, 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	0.66	3/1374 (0.2%)	1.35	25/1871 (1.3%)
1	B	0.65	2/1374 (0.1%)	1.26	22/1871 (1.2%)
1	C	0.58	0/1374	1.28	26/1871 (1.4%)
1	D	0.70	2/1374 (0.1%)	1.41	25/1871 (1.3%)
All	All	0.65	7/5496 (0.1%)	1.33	98/7484 (1.3%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	PRO	CA-C	10.12	1.61	1.52
1	D	3	PRO	CA-C	8.35	1.59	1.52
1	A	6	CYS	N-CA	-6.84	1.38	1.46
1	D	108	MET	SD-CE	-6.65	1.62	1.79
1	A	4	PRO	N-CA	6.37	1.55	1.47
1	B	146	HIS	CB-CG	5.36	1.57	1.50
1	B	3	PRO	CA-C	5.05	1.56	1.52

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	PRO	N-CA-C	13.90	127.66	110.70
1	D	3	PRO	N-CA-C	13.28	126.91	110.70
1	D	2	ASP	CA-C-N	11.28	132.00	120.38
1	D	2	ASP	C-N-CA	11.28	132.00	120.38
1	B	126	ASN	CA-CB-CG	11.18	123.78	112.60
1	B	3	PRO	CB-CA-C	10.71	123.99	110.92
1	A	6	CYS	CA-C-N	10.70	142.38	121.41
1	A	6	CYS	C-N-CA	10.70	142.38	121.41
1	C	6	CYS	N-CA-C	-10.39	92.51	109.96
1	C	150	GLN	OE1-CD-NE2	-9.72	112.88	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2	ASP	N-CA-C	-9.70	88.38	109.81
1	A	125	GLN	OE1-CD-NE2	-9.66	112.94	122.60
1	D	18	LEU	N-CA-C	-9.00	98.65	110.53
1	A	6	CYS	O-C-N	8.81	134.18	123.26
1	D	8	SER	N-CA-C	-8.73	94.17	108.41
1	C	3	PRO	CA-C-N	8.62	128.49	120.21
1	C	3	PRO	C-N-CA	8.62	128.49	120.21
1	D	48	SER	N-CA-C	-8.40	102.06	111.14
1	A	6	CYS	CA-C-O	8.31	130.12	119.98
1	C	2	ASP	N-CA-C	8.04	120.84	110.39
1	B	2	ASP	CA-CB-CG	7.86	120.46	112.60
1	D	151	PRO	CA-N-CD	-7.78	101.11	112.00
1	A	1	GLU	CA-C-N	-7.77	113.60	123.16
1	A	1	GLU	C-N-CA	-7.77	113.60	123.16
1	B	4	PRO	CB-CA-C	7.45	123.85	111.56
1	A	4	PRO	N-CA-C	7.42	127.76	112.47
1	A	126	ASN	CA-CB-CG	7.23	119.83	112.60
1	D	5	ALA	N-CA-C	7.21	121.58	111.92
1	D	6	CYS	CA-CB-SG	7.21	130.97	114.40
1	C	8	SER	N-CA-C	-7.08	91.27	107.48
1	D	7	GLY	N-CA-C	6.93	129.60	113.18
1	A	3	PRO	CA-N-CD	-6.87	102.38	112.00
1	A	125	GLN	CG-CD-NE2	6.72	126.48	116.40
1	B	32	TYR	N-CA-C	6.64	120.51	109.95
1	C	78	ASP	N-CA-C	-6.62	105.19	113.20
1	A	18	LEU	N-CA-C	-6.60	101.19	110.50
1	B	152	THR	N-CA-C	6.58	119.18	109.24
1	C	5	ALA	N-CA-C	-6.51	96.92	110.80
1	C	99	ASN	CA-C-N	6.47	126.16	119.56
1	C	99	ASN	C-N-CA	6.47	126.16	119.56
1	D	54	GLN	N-CA-C	-6.41	104.22	111.14
1	A	4	PRO	CA-N-CD	-6.37	103.09	112.00
1	B	18	LEU	N-CA-C	-6.35	101.54	110.50
1	D	16	ARG	N-CA-C	6.34	120.16	111.54
1	C	151	PRO	CA-C-N	-6.31	110.36	122.09
1	C	151	PRO	C-N-CA	-6.31	110.36	122.09
1	C	150	GLN	CG-CD-NE2	6.31	125.86	116.40
1	B	5	ALA	CA-C-N	6.24	133.46	121.54
1	B	5	ALA	C-N-CA	6.24	133.46	121.54
1	C	26	LEU	N-CA-C	-6.21	101.33	110.52
1	C	4	PRO	N-CA-C	6.18	119.88	111.22
1	A	96	PRO	N-CA-C	6.16	121.85	113.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	78	ASP	N-CA-C	-6.13	105.56	113.16
1	B	103	ILE	N-CA-C	-6.08	98.88	107.75
1	A	50	ALA	N-CA-C	-6.02	104.80	111.36
1	B	166	TRP	N-CA-C	6.02	119.33	109.76
1	B	149	VAL	N-CA-C	5.97	116.95	111.81
1	C	32	TYR	N-CA-C	5.87	119.11	109.72
1	D	88	ASN	N-CA-C	5.86	120.59	113.38
1	C	145	GLY	N-CA-C	-5.84	102.09	112.54
1	A	88	ASN	N-CA-C	5.74	120.40	113.17
1	A	78	ASP	N-CA-C	-5.70	106.09	113.16
1	B	78	ASP	N-CA-C	-5.68	106.33	113.20
1	C	95	GLY	CA-C-N	5.66	125.28	119.56
1	C	95	GLY	C-N-CA	5.66	125.28	119.56
1	D	26	LEU	CA-C-N	-5.65	115.13	123.05
1	D	26	LEU	C-N-CA	-5.65	115.13	123.05
1	C	69	VAL	N-CA-C	-5.59	101.51	109.51
1	C	18	LEU	N-CA-C	-5.57	102.23	110.48
1	C	88	ASN	N-CA-C	5.56	120.22	113.38
1	C	50	ALA	N-CA-C	-5.48	105.30	111.28
1	D	87	TRP	N-CA-C	5.48	118.18	111.82
1	A	32	TYR	N-CA-C	5.48	118.48	109.72
1	A	95	GLY	CA-C-N	5.47	125.14	119.56
1	A	95	GLY	C-N-CA	5.47	125.14	119.56
1	D	63	ASN	N-CA-C	5.46	117.32	111.36
1	B	6	CYS	N-CA-C	5.45	122.41	110.80
1	B	69	VAL	N-CA-C	-5.39	101.87	109.63
1	A	69	VAL	N-CA-C	-5.33	101.88	109.51
1	A	116	PRO	N-CA-C	-5.33	104.20	110.70
1	B	147	ARG	N-CA-C	-5.30	106.75	113.43
1	D	150	GLN	O-C-N	5.29	125.51	121.65
1	D	129	ALA	CA-C-N	5.24	127.25	120.44
1	D	129	ALA	C-N-CA	5.24	127.25	120.44
1	C	3	PRO	N-CA-C	-5.23	104.32	110.70
1	B	88	ASN	N-CA-C	5.22	119.61	112.88
1	D	166	TRP	N-CA-C	5.20	117.42	110.35
1	B	95	GLY	CA-C-N	5.20	124.86	119.56
1	B	95	GLY	C-N-CA	5.20	124.86	119.56
1	D	10	VAL	CA-C-N	5.20	125.19	119.89
1	D	10	VAL	C-N-CA	5.20	125.19	119.89
1	A	145	GLY	N-CA-C	-5.19	105.10	112.37
1	A	62	ARG	N-CA-C	5.09	116.91	111.36
1	B	94	ALA	N-CA-C	5.07	118.50	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	102	SER	N-CA-C	5.07	116.00	108.86
1	B	149	VAL	CB-CA-C	-5.06	105.73	111.55
1	C	103	ILE	N-CA-C	-5.06	101.09	108.17
1	C	158	ARG	CB-CG-CD	5.01	122.83	111.30

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	1337	0	1288	48	0
1	B	1337	0	1288	109	0
1	C	1337	0	1288	43	0
1	D	1337	0	1288	71	0
2	A	24	0	32	15	0
2	B	6	0	8	3	0
2	C	18	0	24	3	0
2	D	30	0	40	15	0
3	C	10	0	4	0	0
4	D	5	0	0	0	0
5	A	172	0	0	8	0
5	B	162	0	0	25	0
5	C	235	0	0	8	0
5	D	170	0	0	11	0
All	All	6180	0	5260	255	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 24.

All (255) 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:5:ALA:CB	1:B:129:ALA:HB1	1.59	1.32
1:D:96:PRO:HA	2:D:504:GOL:H32	1.30	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ALA:HB1	1:B:129:ALA:HB1	1.34	1.09
1:D:114:ARG:HG3	1:D:114:ARG:HH11	1.19	1.04
1:A:5:ALA:HB2	1:B:129:ALA:HB1	1.38	1.03
1:C:112:MET:HE2	1:C:157:ASP:H	1.18	1.03
1:B:90:LYS:HD2	5:B:365:HOH:O	1.64	0.97
1:C:150:GLN:HG2	5:C:6869:HOH:O	1.63	0.97
1:D:171:ALA:HB1	5:D:643:HOH:O	1.65	0.96
1:D:112:MET:HE2	1:D:156:GLY:HA2	1.50	0.92
1:B:157:ASP:HB2	5:B:298:HOH:O	1.70	0.92
1:C:64:LEU:CD1	1:D:151:PRO:HD3	2.01	0.90
1:C:113:ASN:HA	1:C:158:ARG:HE	1.36	0.90
1:A:126:ASN:HD21	1:B:5:ALA:C	1.80	0.90
1:A:96:PRO:HD3	2:A:175:GOL:H11	1.55	0.88
1:B:101:ILE:HG13	5:B:370:HOH:O	1.73	0.88
1:C:2:ASP:HB3	1:C:4:PRO:HD3	1.54	0.87
1:D:114:ARG:HH11	1:D:114:ARG:CG	1.88	0.85
1:A:5:ALA:HB1	1:B:129:ALA:CB	2.05	0.85
1:B:102:SER:HB3	5:B:370:HOH:O	1.76	0.83
1:B:2:ASP:N	1:B:3:PRO:CD	2.41	0.83
1:B:140:ASN:HD22	1:B:140:ASN:H	1.25	0.83
1:B:31:ARG:HA	1:B:138:ARG:HD2	1.60	0.82
1:B:145:GLY:HA3	5:B:331:HOH:O	1.78	0.82
1:C:158:ARG:HD2	5:C:6979:HOH:O	1.80	0.81
1:B:138:ARG:HG3	1:B:140:ASN:ND2	1.95	0.81
1:B:4:PRO:HA	5:B:403:HOH:O	1.80	0.81
1:B:146:HIS:HA	1:B:149:VAL:CG1	2.12	0.80
1:B:130:CYS:HB2	5:B:270:HOH:O	1.81	0.79
1:B:94:ALA:HB1	1:B:149:VAL:HG21	1.65	0.77
1:B:2:ASP:N	1:B:3:PRO:HD3	2.00	0.77
1:D:28:ARG:HD2	5:D:549:HOH:O	1.85	0.77
1:A:96:PRO:CD	2:A:175:GOL:H11	2.15	0.75
1:D:112:MET:CE	1:D:156:GLY:HA2	2.15	0.75
1:D:45:THR:HG22	5:D:590:HOH:O	1.85	0.75
1:A:126:ASN:HD21	1:B:5:ALA:HA	1.51	0.75
1:D:43:CYS:CB	1:D:49:CYS:HA	2.17	0.74
1:A:5:ALA:CB	1:B:129:ALA:CB	2.53	0.74
1:C:64:LEU:HD13	1:D:151:PRO:HD3	1.67	0.74
1:C:142:GLU:OE1	1:C:170:ARG:HD3	1.88	0.74
1:C:112:MET:HE2	1:C:157:ASP:N	1.99	0.74
1:D:43:CYS:O	1:D:77:GLU:HB2	1.87	0.74
1:B:111:TYR:CD2	1:B:116:PRO:HD3	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ASN:HD22	2:A:174:GOL:H11	1.52	0.73
1:B:85:ARG:HD2	1:B:91:GLY:HA2	1.69	0.72
1:B:36:SER:HA	1:B:155:PRO:HB3	1.71	0.72
1:B:154:SER:HA	1:B:156:GLY:H	1.53	0.72
1:B:37:HIS:ND1	1:B:154:SER:HB2	2.04	0.72
1:D:112:MET:HE1	1:D:153:LEU:HB3	1.71	0.72
1:A:52:GLN:HE22	2:A:172:GOL:H32	1.55	0.71
1:D:140:ASN:HD22	1:D:140:ASN:H	1.38	0.71
1:D:42:HIS:CE1	2:D:507:GOL:O2	2.43	0.70
1:D:85:ARG:HD2	1:D:91:GLY:HA2	1.72	0.70
1:D:138:ARG:HG2	1:D:138:ARG:HH11	1.56	0.70
1:A:126:ASN:HD21	1:B:5:ALA:CA	2.04	0.70
1:D:114:ARG:HG3	1:D:114:ARG:NH1	1.95	0.69
1:C:2:ASP:HB3	1:C:4:PRO:CD	2.21	0.69
1:D:43:CYS:HB2	1:D:49:CYS:N	2.07	0.69
1:B:37:HIS:HD2	1:B:111:TYR:H	1.38	0.69
1:B:138:ARG:HG3	1:B:140:ASN:HD22	1.56	0.69
1:B:146:HIS:H	1:B:155:PRO:HD3	1.57	0.69
1:D:5:ALA:HB2	5:D:538:HOH:O	1.93	0.68
1:D:44:ASP:OD1	1:D:45:THR:HG23	1.92	0.68
1:B:146:HIS:HD2	1:B:149:VAL:CG1	2.07	0.68
1:B:138:ARG:HD3	1:B:141:TYR:HA	1.76	0.68
5:A:281:HOH:O	1:C:23:ARG:HD2	1.92	0.68
1:B:90:LYS:HE3	1:B:100:PRO:HB3	1.76	0.67
1:A:96:PRO:HB3	2:A:175:GOL:H31	1.76	0.67
1:B:125:GLN:HG2	5:B:357:HOH:O	1.93	0.67
1:B:157:ASP:O	1:B:161:GLU:HG2	1.95	0.67
1:C:79:GLY:HA3	1:C:119:ARG:HG3	1.75	0.67
1:B:98:TRP:HZ2	5:B:308:HOH:O	1.77	0.67
1:B:146:HIS:HA	1:B:149:VAL:HG12	1.77	0.67
1:B:1:GLU:C	1:B:3:PRO:CD	2.68	0.67
1:B:41:SER:OG	2:B:172:GOL:H2	1.95	0.67
1:B:98:TRP:N	1:B:98:TRP:CD1	2.62	0.67
1:A:126:ASN:ND2	1:B:5:ALA:HA	2.10	0.66
1:B:154:SER:HA	1:B:156:GLY:N	2.10	0.66
1:D:74:LEU:HD22	1:D:108:MET:HE3	1.76	0.66
1:D:9:ILE:O	1:D:11:PRO:HD3	1.95	0.66
1:D:96:PRO:CA	2:D:504:GOL:H32	2.19	0.65
1:D:99:ASN:HD22	2:D:504:GOL:H31	1.60	0.65
1:C:64:LEU:HD11	1:D:151:PRO:HD3	1.77	0.65
1:B:144:LYS:HD2	1:B:148:ASP:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:GLU:C	1:B:3:PRO:HD2	2.22	0.64
1:B:165:THR:HA	5:B:377:HOH:O	1.96	0.64
1:B:28:ARG:HG2	1:B:135:GLY:O	1.97	0.64
1:B:37:HIS:CD2	1:B:111:TYR:H	2.14	0.64
1:C:3:PRO:N	1:C:4:PRO:HD3	2.13	0.64
1:B:111:TYR:CZ	1:B:116:PRO:HG3	2.33	0.63
1:A:37:HIS:HD2	1:A:37:HIS:O	1.81	0.63
1:A:122:ARG:HG2	1:B:4:PRO:HB3	1.81	0.63
1:C:99:ASN:HB2	1:C:100:PRO:HD3	1.81	0.62
1:C:151:PRO:O	1:C:152:THR:HB	1.98	0.62
1:D:15:TRP:CZ2	1:D:17:ALA:HB2	2.34	0.62
1:D:112:MET:CE	1:D:153:LEU:HB3	2.29	0.62
1:C:3:PRO:N	1:C:4:PRO:CD	2.62	0.62
1:D:43:CYS:HB2	1:D:48:SER:C	2.24	0.62
1:A:96:PRO:CA	2:A:175:GOL:H31	2.30	0.61
1:B:112:MET:HE2	1:B:156:GLY:HA2	1.82	0.61
1:A:96:PRO:HA	2:A:175:GOL:H31	1.82	0.61
1:A:88:ASN:ND2	2:A:174:GOL:H11	2.16	0.61
1:D:43:CYS:HB2	1:D:49:CYS:CA	2.31	0.60
5:A:280:HOH:O	1:B:4:PRO:HG2	2.02	0.60
1:D:43:CYS:HB2	1:D:49:CYS:HA	1.82	0.60
1:D:44:ASP:HB2	5:D:640:HOH:O	2.00	0.59
1:C:112:MET:HE3	1:C:156:GLY:HA2	1.85	0.59
1:B:146:HIS:HD2	1:B:149:VAL:HG13	1.67	0.59
1:C:112:MET:O	1:C:158:ARG:HG2	2.03	0.59
1:A:153:LEU:HG	5:A:248:HOH:O	2.01	0.59
1:A:96:PRO:HD3	2:A:175:GOL:C1	2.30	0.59
2:C:6750:GOL:H2	5:C:6808:HOH:O	2.02	0.59
1:B:155:PRO:CD	5:B:331:HOH:O	2.52	0.58
1:D:127:LEU:O	1:D:130:CYS:HB3	2.03	0.58
1:D:99:ASN:ND2	2:D:504:GOL:H11	2.18	0.58
1:C:140:ASN:HB3	5:C:6853:HOH:O	2.03	0.58
1:C:85:ARG:HD2	1:C:91:GLY:HA2	1.86	0.58
1:D:45:THR:HG21	5:D:510:HOH:O	2.04	0.57
1:D:42:HIS:HE1	2:D:507:GOL:C2	2.17	0.57
1:C:96:PRO:HA	2:C:6750:GOL:O2	2.04	0.57
1:C:24:GLU:HG3	5:C:6878:HOH:O	2.04	0.57
1:A:96:PRO:CB	2:A:175:GOL:H31	2.34	0.56
1:C:2:ASP:C	1:C:4:PRO:CD	2.78	0.56
1:A:85:ARG:HD2	1:A:91:GLY:HA2	1.86	0.56
1:A:37:HIS:O	1:A:37:HIS:CD2	2.58	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:GLY:CA	1:C:119:ARG:HG3	2.35	0.56
1:C:151:PRO:HD3	1:D:64:LEU:HD11	1.88	0.55
1:A:88:ASN:HD22	2:A:174:GOL:C1	2.19	0.55
1:C:151:PRO:HD3	1:D:64:LEU:CD1	2.36	0.55
1:B:1:GLU:C	1:B:3:PRO:HD3	2.31	0.55
5:A:243:HOH:O	1:B:6:CYS:HB2	2.06	0.55
1:B:144:LYS:HD2	1:B:148:ASP:CB	2.37	0.54
1:B:26:LEU:HD21	1:B:102:SER:O	2.08	0.54
1:A:97:THR:HG23	5:A:342:HOH:O	2.08	0.53
1:B:126:ASN:HB3	5:B:295:HOH:O	2.09	0.53
1:B:28:ARG:HG3	5:B:284:HOH:O	2.09	0.53
1:D:24:GLU:OE1	1:D:90:LYS:HE2	2.09	0.53
1:C:113:ASN:HA	1:C:158:ARG:NE	2.15	0.53
1:D:24:GLU:HB2	5:D:539:HOH:O	2.09	0.52
1:D:52:GLN:HG2	1:D:108:MET:HE2	1.90	0.52
1:C:2:ASP:C	1:C:4:PRO:HD3	2.34	0.52
1:D:15:TRP:CH2	1:D:17:ALA:HB2	2.44	0.52
1:D:99:ASN:HD22	2:D:504:GOL:H11	1.75	0.52
1:B:98:TRP:C	1:B:100:PRO:HD2	2.34	0.52
1:B:28:ARG:HG3	1:B:136:ALA:HA	1.91	0.52
1:B:111:TYR:CE2	1:B:116:PRO:HG3	2.43	0.52
1:B:12:ARG:HD2	5:B:329:HOH:O	2.08	0.52
1:B:146:HIS:HD2	1:B:149:VAL:HG11	1.73	0.52
1:B:73:PHE:HB2	1:B:105:ILE:HG22	1.91	0.51
1:B:43:CYS:O	1:B:77:GLU:HB2	2.11	0.51
1:B:98:TRP:CD1	1:B:98:TRP:H	2.28	0.51
1:D:53:ALA:CA	1:D:108:MET:HE1	2.40	0.51
1:B:140:ASN:HD22	1:B:140:ASN:N	1.98	0.51
1:B:41:SER:CB	2:B:172:GOL:H2	2.41	0.51
1:A:139:SER:HA	2:A:173:GOL:O1	2.11	0.50
1:B:99:ASN:N	1:B:100:PRO:HD2	2.26	0.50
1:D:138:ARG:HG2	1:D:138:ARG:NH1	2.22	0.50
1:A:43:CYS:O	1:A:77:GLU:HB2	2.11	0.50
1:B:37:HIS:CD2	1:B:110:ASN:HA	2.46	0.50
1:B:74:LEU:HB2	1:B:82:TYR:HB2	1.93	0.50
1:C:96:PRO:HG3	1:D:96:PRO:HG3	1.94	0.50
1:B:117:PRO:HG2	5:B:375:HOH:O	2.11	0.50
1:B:154:SER:CA	1:B:156:GLY:H	2.22	0.49
1:D:12:ARG:HA	1:D:15:TRP:NE1	2.27	0.49
1:A:168:HIS:NE2	2:A:173:GOL:H2	2.26	0.49
1:B:98:TRP:CD1	5:B:286:HOH:O	2.65	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:HIS:HE1	2:D:507:GOL:O2	1.95	0.49
1:D:170:ARG:HH22	2:D:506:GOL:H11	1.77	0.49
1:A:37:HIS:CD2	1:A:37:HIS:C	2.91	0.49
1:D:138:ARG:NE	5:D:627:HOH:O	2.44	0.49
1:D:59:TYR:O	1:D:63:ASN:HB2	2.12	0.49
1:D:4:PRO:O	1:D:5:ALA:HB3	2.13	0.49
1:A:126:ASN:ND2	1:B:5:ALA:C	2.62	0.49
1:A:99:ASN:N	1:A:100:PRO:HD2	2.28	0.49
1:B:150:GLN:HG2	1:B:151:PRO:N	2.28	0.48
1:C:158:ARG:CD	5:C:6979:HOH:O	2.49	0.48
1:C:2:ASP:C	1:C:4:PRO:HD2	2.39	0.48
1:B:138:ARG:O	1:B:138:ARG:HG2	2.13	0.48
1:D:42:HIS:CE1	2:D:507:GOL:C2	2.97	0.48
1:B:138:ARG:HG2	1:B:141:TYR:N	2.28	0.48
1:B:138:ARG:CD	1:B:141:TYR:HA	2.42	0.48
1:C:127:LEU:O	1:C:130:CYS:HB3	2.14	0.48
1:A:105:ILE:O	1:A:105:ILE:HG13	2.13	0.48
1:B:159:LEU:O	1:B:163:ILE:HG12	2.13	0.48
1:A:52:GLN:OE1	2:A:172:GOL:H12	2.13	0.47
1:A:71:TYR:CD2	1:A:106:SER:HB2	2.50	0.47
1:D:151:PRO:O	1:D:152:THR:HB	2.13	0.47
1:A:58:SER:O	1:A:62:ARG:HB2	2.15	0.47
1:B:90:LYS:HE3	1:B:100:PRO:CB	2.42	0.47
1:B:153:LEU:HD12	5:B:307:HOH:O	2.14	0.47
1:A:9:ILE:O	1:A:11:PRO:HD3	2.14	0.47
1:B:12:ARG:HG3	1:B:83:GLU:OE1	2.15	0.47
1:B:145:GLY:O	1:B:149:VAL:HG12	2.14	0.47
1:B:35:VAL:HG22	1:B:105:ILE:HD11	1.96	0.47
1:B:146:HIS:CD2	1:B:149:VAL:HG13	2.49	0.47
1:C:3:PRO:HD2	5:C:6910:HOH:O	2.14	0.47
1:B:152:THR:HA	5:B:292:HOH:O	2.15	0.46
1:A:132:VAL:HG11	2:A:173:GOL:O1	2.15	0.46
2:C:6750:GOL:H32	1:D:96:PRO:HG3	1.97	0.46
1:D:74:LEU:CD2	1:D:108:MET:HE3	2.42	0.46
1:A:157:ASP:O	1:A:161:GLU:HG2	2.16	0.46
1:A:114:ARG:HD2	5:A:262:HOH:O	2.16	0.46
1:D:99:ASN:HB2	2:D:504:GOL:H31	1.97	0.46
1:A:46:PRO:HD2	5:A:181:HOH:O	2.16	0.46
1:B:31:ARG:HG3	1:B:138:ARG:CZ	2.46	0.46
1:C:43:CYS:O	1:C:77:GLU:HB2	2.16	0.46
1:C:155:PRO:HB2	1:C:159:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:GLU:OE1	1:D:170:ARG:HD3	2.17	0.45
1:B:155:PRO:HD2	5:B:331:HOH:O	2.16	0.45
1:C:158:ARG:HG2	1:C:158:ARG:H	1.65	0.45
1:B:38:THR:O	1:B:39:ALA:HB3	2.16	0.45
1:B:167:SER:HB3	5:B:382:HOH:O	2.17	0.45
1:D:115:VAL:HG12	1:D:158:ARG:HB3	1.98	0.45
1:B:146:HIS:CD2	1:B:149:VAL:CG1	2.96	0.45
1:C:2:ASP:HA	1:C:3:PRO:HD3	1.73	0.44
1:D:68:ASP:OD1	1:D:69:VAL:N	2.47	0.44
1:D:41:SER:HB2	5:D:531:HOH:O	2.15	0.44
1:B:158:ARG:O	1:B:161:GLU:HG3	2.18	0.44
1:D:170:ARG:HH22	2:D:506:GOL:C1	2.31	0.44
1:D:114:ARG:CG	1:D:114:ARG:NH1	2.61	0.43
1:B:99:ASN:N	1:B:100:PRO:CD	2.81	0.43
1:B:23:ARG:HG2	5:B:390:HOH:O	2.17	0.43
1:B:94:ALA:C	5:B:404:HOH:O	2.61	0.43
1:B:140:ASN:H	1:B:140:ASN:ND2	2.04	0.43
1:C:59:TYR:O	1:C:63:ASN:HB2	2.18	0.43
1:A:59:TYR:O	1:A:63:ASN:HB2	2.19	0.43
1:C:112:MET:CE	1:C:156:GLY:HA2	2.48	0.43
1:B:4:PRO:CA	5:B:403:HOH:O	2.54	0.43
1:A:95:GLY:HA3	1:A:150:GLN:NE2	2.34	0.42
1:B:81:VAL:HG11	1:B:127:LEU:HD13	2.00	0.42
1:A:150:GLN:O	1:A:152:THR:HG22	2.18	0.42
1:B:117:PRO:CG	5:B:375:HOH:O	2.67	0.42
1:D:170:ARG:HH22	2:D:506:GOL:C2	2.32	0.42
1:C:99:ASN:CB	1:C:100:PRO:HD3	2.48	0.42
1:D:23:ARG:HD3	5:D:595:HOH:O	2.20	0.42
1:B:94:ALA:O	1:B:98:TRP:CD1	2.73	0.42
1:D:53:ALA:HA	1:D:108:MET:CE	2.51	0.41
1:B:37:HIS:HD2	1:B:110:ASN:HA	1.83	0.41
1:D:42:HIS:HE1	2:D:507:GOL:H2	1.83	0.41
1:A:23:ARG:NE	5:A:300:HOH:O	2.53	0.41
1:B:41:SER:HB2	2:B:172:GOL:H2	2.03	0.41
1:D:53:ALA:HB2	1:D:108:MET:HE1	2.01	0.41
1:B:112:MET:HE2	1:B:157:ASP:H	1.85	0.41
1:C:58:SER:OG	1:C:62:ARG:HD2	2.21	0.41
1:B:146:HIS:N	5:B:331:HOH:O	2.53	0.41
1:D:62:ARG:HA	5:D:666:HOH:O	2.20	0.41
1:A:153:LEU:N	1:A:153:LEU:CD1	2.83	0.41
1:B:112:MET:CE	1:B:156:GLY:HA2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:PRO:HD2	5:C:6838:HOH:O	2.20	0.40
1:B:36:SER:O	1:B:106:SER:HA	2.21	0.40
1:D:10:VAL:HG13	1:D:14:GLU:HB3	2.03	0.40
1:D:96:PRO:HA	2:D:504:GOL:C3	2.22	0.40
1:A:68:ASP:O	1:A:69:VAL:C	2.64	0.40
1:A:99:ASN:N	1:A:100:PRO:CD	2.85	0.40
1:B:112:MET:HE3	1:B:153:LEU:HG	2.02	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	169/171 (99%)	161 (95%)	5 (3%)	3 (2%)	6	1
1	B	169/171 (99%)	158 (94%)	8 (5%)	3 (2%)	6	1
1	C	169/171 (99%)	162 (96%)	6 (4%)	1 (1%)	21	9
1	D	169/171 (99%)	157 (93%)	8 (5%)	4 (2%)	4	0
All	All	676/684 (99%)	638 (94%)	27 (4%)	11 (2%)	7	1

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	PRO
1	A	5	ALA
1	C	3	PRO
1	D	3	PRO
1	D	4	PRO
1	D	7	GLY
1	A	7	GLY
1	B	4	PRO

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Mol	Chain	Res	Type
1	B	6	CYS
1	B	151	PRO
1	D	46	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	139/139 (100%)	132 (95%)	7 (5%)	22	6
1	B	139/139 (100%)	123 (88%)	16 (12%)	5	0
1	C	139/139 (100%)	132 (95%)	7 (5%)	22	6
1	D	139/139 (100%)	127 (91%)	12 (9%)	10	1
All	All	556/556 (100%)	514 (92%)	42 (8%)	12	2

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	PRO
1	A	4	PRO
1	A	6	CYS
1	A	8	SER
1	A	97	THR
1	A	155	PRO
1	A	161	GLU
1	B	1	GLU
1	B	37	HIS
1	B	74	LEU
1	B	115	VAL
1	B	117	PRO
1	B	118	PRO
1	B	126	ASN
1	B	130	CYS
1	B	138	ARG
1	B	140	ASN
1	B	148	ASP

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Mol	Chain	Res	Type
1	B	149	VAL
1	B	151	PRO
1	B	152	THR
1	B	161	GLU
1	B	167	SER
1	C	2	ASP
1	C	24	GLU
1	C	27	THR
1	C	112	MET
1	C	113	ASN
1	C	114	ARG
1	C	119	ARG
1	D	1	GLU
1	D	3	PRO
1	D	4	PRO
1	D	8	SER
1	D	11	PRO
1	D	27	THR
1	D	46	PRO
1	D	113	ASN
1	D	114	ARG
1	D	140	ASN
1	D	151	PRO
1	D	165	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	HIS
1	A	88	ASN
1	A	93	HIS
1	A	126	ASN
1	A	150	GLN
1	B	37	HIS
1	B	113	ASN
1	B	126	ASN
1	B	140	ASN
1	B	146	HIS
1	C	164	GLN
1	D	42	HIS
1	D	140	ASN

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](#)

15 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	D	503	-	5,5,5	0.10	0	5,5,5	1.22	1 (20%)
2	GOL	C	6751	-	5,5,5	0.36	0	5,5,5	1.29	1 (20%)
2	GOL	B	172	-	5,5,5	0.22	0	5,5,5	1.43	1 (20%)
2	GOL	C	6749	-	5,5,5	0.38	0	5,5,5	0.54	0
2	GOL	D	504	-	5,5,5	0.37	0	5,5,5	1.43	1 (20%)
2	GOL	D	506	-	5,5,5	0.29	0	5,5,5	0.30	0
2	GOL	D	507	-	5,5,5	0.29	0	5,5,5	0.30	0
2	GOL	A	174	-	5,5,5	0.36	0	5,5,5	1.33	1 (20%)
3	TLA	C	6748	-	9,9,9	1.55	2 (22%)	12,12,12	1.35	3 (25%)
2	GOL	D	505	-	5,5,5	0.24	0	5,5,5	1.58	1 (20%)
4	SO4	D	502	-	4,4,4	0.20	0	6,6,6	0.09	0
2	GOL	C	6750	-	5,5,5	0.28	0	5,5,5	1.31	1 (20%)
2	GOL	A	172	-	5,5,5	0.34	0	5,5,5	1.41	1 (20%)
2	GOL	A	173	-	5,5,5	0.27	0	5,5,5	1.29	1 (20%)
2	GOL	A	175	-	5,5,5	0.39	0	5,5,5	1.52	1 (20%)

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	D	503	-	-	0/4/4/4	-
2	GOL	C	6751	-	-	0/4/4/4	-
2	GOL	B	172	-	-	0/4/4/4	-
2	GOL	C	6749	-	-	0/4/4/4	-
2	GOL	D	504	-	-	0/4/4/4	-
2	GOL	D	506	-	-	0/4/4/4	-
2	GOL	D	507	-	-	0/4/4/4	-
2	GOL	A	174	-	-	0/4/4/4	-
3	TLA	C	6748	-	-	0/12/12/12	-
2	GOL	D	505	-	-	0/4/4/4	-
2	GOL	C	6750	-	-	0/4/4/4	-
2	GOL	A	172	-	-	0/4/4/4	-
2	GOL	A	173	-	-	0/4/4/4	-
2	GOL	A	175	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	6748	TLA	C2-C1	2.91	1.56	1.52
3	C	6748	TLA	O11-C1	-2.88	1.21	1.30

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	505	GOL	O1-C1-C2	3.26	125.06	110.38
2	A	175	GOL	O1-C1-C2	3.17	124.64	110.38
2	D	504	GOL	O1-C1-C2	3.10	124.35	110.38
2	B	172	GOL	O1-C1-C2	3.10	124.33	110.38
2	A	172	GOL	O1-C1-C2	3.01	123.91	110.38
2	C	6750	GOL	O1-C1-C2	2.90	123.42	110.38
2	A	174	GOL	O1-C1-C2	2.88	123.33	110.38
2	C	6751	GOL	O1-C1-C2	2.82	123.06	110.38
2	A	173	GOL	O1-C1-C2	2.77	122.85	110.38
2	D	503	GOL	O1-C1-C2	2.60	122.06	110.38
3	C	6748	TLA	O4-C4-C3	-2.56	114.79	121.62
3	C	6748	TLA	O41-C4-C3	2.56	120.42	113.31
3	C	6748	TLA	O1-C1-C2	-2.02	116.23	121.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	172	GOL	3	0
2	D	504	GOL	7	0
2	D	506	GOL	3	0
2	D	507	GOL	5	0
2	A	174	GOL	3	0
2	C	6750	GOL	3	0
2	A	172	GOL	2	0
2	A	173	GOL	3	0
2	A	175	GOL	7	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	171/171 (100%)	0.70	13 (7%)	20 20	21, 34, 49, 88	0
1	B	171/171 (100%)	1.34	45 (26%)	1 1	21, 39, 58, 85	0
1	C	171/171 (100%)	0.29	12 (7%)	22 23	15, 26, 40, 75	0
1	D	171/171 (100%)	1.01	25 (14%)	6 6	24, 34, 52, 89	0
All	All	684/684 (100%)	0.83	95 (13%)	6 6	15, 33, 53, 89	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	ALA	7.8
1	D	3	PRO	7.6
1	C	5	ALA	7.6
1	B	4	PRO	6.2
1	A	3	PRO	6.0
1	B	3	PRO	5.6
1	D	5	ALA	5.2
1	A	2	ASP	5.2
1	A	6	CYS	4.9
1	B	149	VAL	4.9
1	B	145	GLY	4.7
1	D	4	PRO	4.6
1	B	5	ALA	4.4
1	C	171	ALA	4.4
1	B	98	TRP	4.2
1	D	46	PRO	4.1
1	D	6	CYS	4.1
1	B	163	ILE	4.0
1	D	1	GLU	3.8
1	B	101	ILE	3.8
1	C	3	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	6	CYS	3.7
1	B	160	TYR	3.7
1	C	6	CYS	3.7
1	B	1	GLU	3.6
1	C	7	GLY	3.6
1	C	4	PRO	3.4
1	B	94	ALA	3.3
1	C	1	GLU	3.3
1	A	4	PRO	3.3
1	B	2	ASP	3.2
1	A	151	PRO	3.2
1	D	48	SER	3.2
1	B	156	GLY	3.2
1	B	140	ASN	3.2
1	B	159	LEU	3.1
1	D	47	ALA	3.1
1	C	2	ASP	3.1
1	D	2	ASP	3.1
1	B	146	HIS	3.1
1	B	102	SER	3.0
1	B	155	PRO	3.0
1	D	42	HIS	3.0
1	B	27	THR	3.0
1	B	112	MET	3.0
1	B	26	LEU	2.9
1	A	7	GLY	2.9
1	D	43	CYS	2.9
1	D	49	CYS	2.9
1	D	114	ARG	2.9
1	B	162	ILE	2.9
1	A	59	TYR	2.9
1	B	90	LYS	2.8
1	D	17	ALA	2.8
1	D	151	PRO	2.8
1	B	152	THR	2.8
1	A	156	GLY	2.6
1	B	166	TRP	2.6
1	B	136	ALA	2.6
1	B	153	LEU	2.6
1	B	32	TYR	2.6
1	B	137	LEU	2.6
1	B	116	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	130	CYS	2.5
1	B	151	PRO	2.5
1	B	99	ASN	2.4
1	B	96	PRO	2.4
1	B	28	ARG	2.4
1	C	27	THR	2.4
1	C	158	ARG	2.4
1	D	13	ARG	2.3
1	B	169	TYR	2.3
1	A	171	ALA	2.3
1	B	92	ALA	2.3
1	D	11	PRO	2.3
1	D	52	GLN	2.3
1	D	53	ALA	2.3
1	D	171	ALA	2.3
1	D	45	THR	2.3
1	B	7	GLY	2.2
1	B	165	THR	2.2
1	D	64	LEU	2.2
1	B	132	VAL	2.2
1	D	8	SER	2.2
1	D	15	TRP	2.2
1	C	130	CYS	2.2
1	A	153	LEU	2.2
1	A	97	THR	2.1
1	B	134	LEU	2.1
1	A	161	GLU	2.1
1	B	97	THR	2.1
1	B	117	PRO	2.1
1	B	150	GLN	2.1
1	D	113	ASN	2.0
1	C	112	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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	D	507	6/6	0.37	0.22	48,48,48,49	6
2	GOL	A	175	6/6	0.49	0.17	48,50,51,52	0
2	GOL	C	6749	6/6	0.55	0.18	43,43,43,44	6
2	GOL	D	506	6/6	0.56	0.13	58,58,59,59	0
2	GOL	A	174	6/6	0.58	0.15	51,52,52,52	0
2	GOL	B	172	6/6	0.59	0.22	51,54,55,55	0
2	GOL	A	172	6/6	0.60	0.23	57,57,57,59	0
2	GOL	D	505	6/6	0.60	0.16	49,50,51,52	0
2	GOL	A	173	6/6	0.70	0.16	44,45,45,46	0
2	GOL	C	6750	6/6	0.71	0.20	56,56,57,57	0
4	SO4	D	502	5/5	0.71	0.15	62,62,63,63	0
2	GOL	D	503	6/6	0.74	0.17	40,41,43,44	0
2	GOL	C	6751	6/6	0.78	0.10	50,51,51,52	0
2	GOL	D	504	6/6	0.79	0.14	45,45,46,47	0
3	TLA	C	6748	10/10	0.91	0.07	28,29,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.