



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:21 PM UTC

PDB ID : 2W8B / pdb_00002w8b
Title : Crystal structure of processed TolB in complex with Pal
Authors : Sharma, A.; Bonsor, D.A.; Kleanthous, C.
Deposited on : 2009-01-15
Resolution : 1.86 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

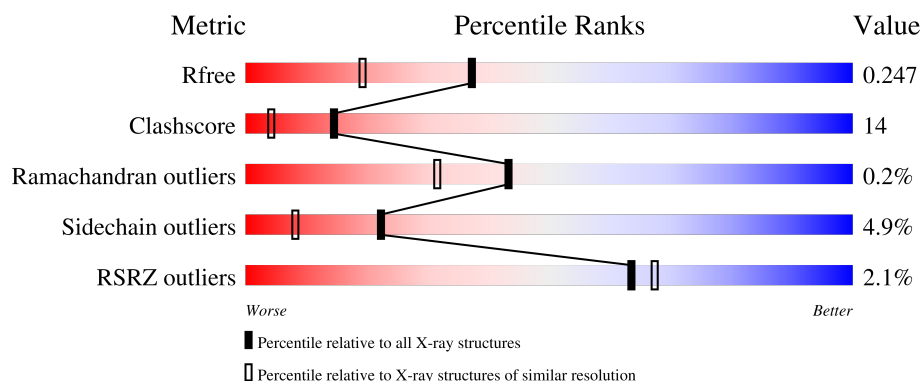
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	409	2% 85% 13% ..
2	B	409	% 84% 13% .
2	D	409	82% 16% .
2	F	409	80% 18% .
3	C	118	12% 50% 28% 8% . 12%

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Mol	Chain	Length	Quality of chain
3	E	118	
3	G	118	
3	H	118	

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
5	GOL	A	1434	-	-	X	-
5	GOL	B	1433	-	X	-	-
5	GOL	C	1174	-	-	X	-
5	GOL	D	1433	-	-	X	-
6	ACT	A	1435	-	-	X	-
6	ACT	B	1435	-	-	X	-
6	ACT	D	1434	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17488 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 PROTEIN TOLB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	6	0
			3110	1956	546	601	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	390	LEU	ILE	conflict	UNP P0A855

- Molecule 2 is a protein called PROTEIN TOLB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	409	Total	C	N	O	S	0	5	0
			3100	1947	544	603	6			
2	D	409	Total	C	N	O	S	0	3	0
			3091	1942	544	599	6			
2	F	409	Total	C	N	O	S	0	13	0
			3147	1978	553	609	7			

- Molecule 3 is a protein called PEPTIDOGLYCAN-ASSOCIATED LIPOPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	104	Total	C	N	O	S	0	2	0
			833	524	147	160	2			
3	E	107	Total	C	N	O	S	0	1	0
			857	539	152	164	2			
3	G	108	Total	C	N	O	S	0	3	0
			869	546	153	167	3			
3	H	108	Total	C	N	O	S	0	2	0
			864	542	153	167	2			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	H	1	Total	C	O	0	0
			4	2	2		

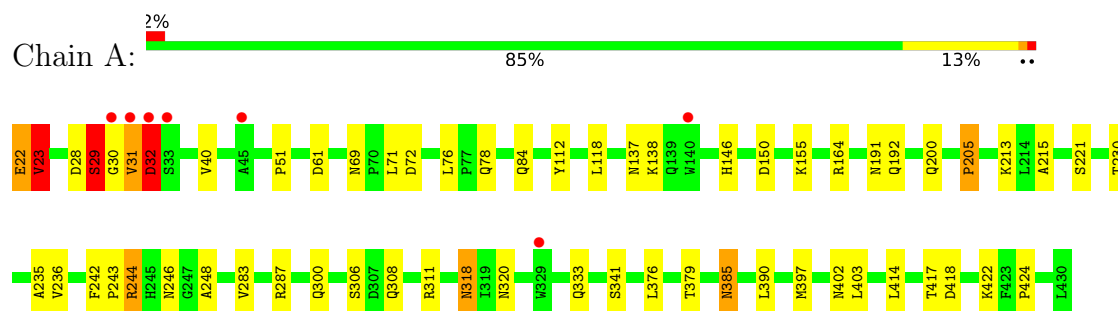
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	354	Total	O	0	0
			354	354		
7	B	314	Total	O	0	0
			314	314		
7	C	35	Total	O	0	0
			35	35		
7	D	316	Total	O	0	0
			316	316		
7	E	55	Total	O	0	0
			55	55		
7	F	329	Total	O	0	0
			329	329		
7	G	60	Total	O	0	0
			60	60		
7	H	56	Total	O	0	0
			56	56		

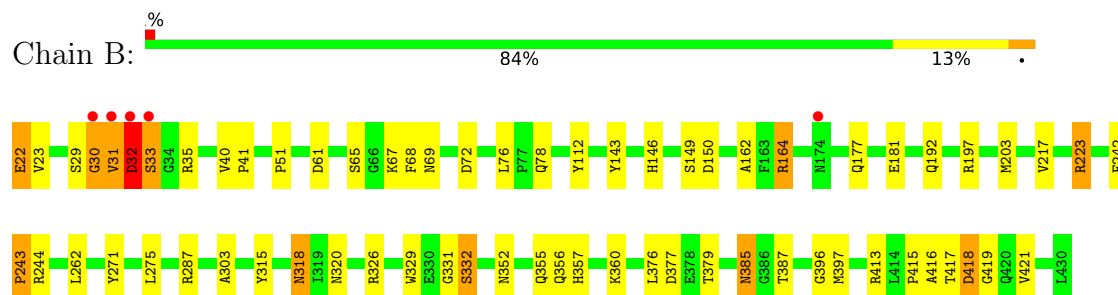
3 Residue-property plots [i](#)

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.

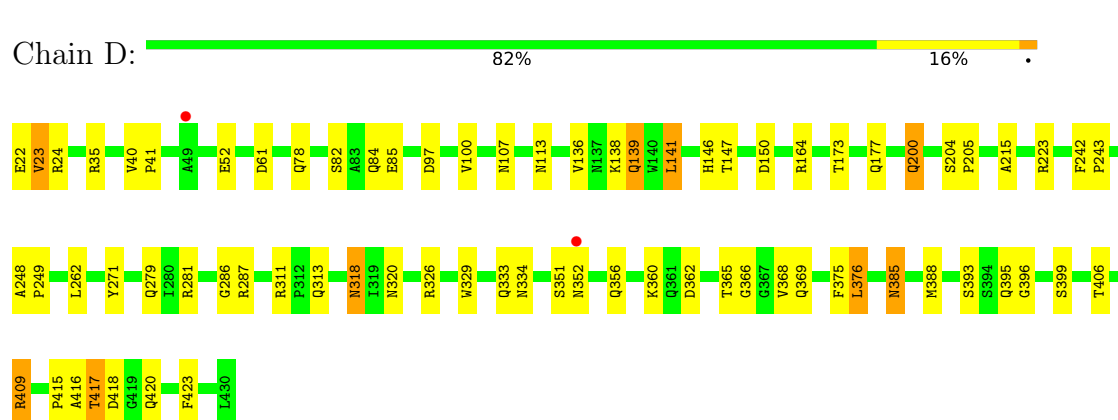
• Molecule 1: PROTEIN TOLB



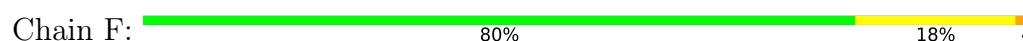
• Molecule 2: PROTEIN TOLB

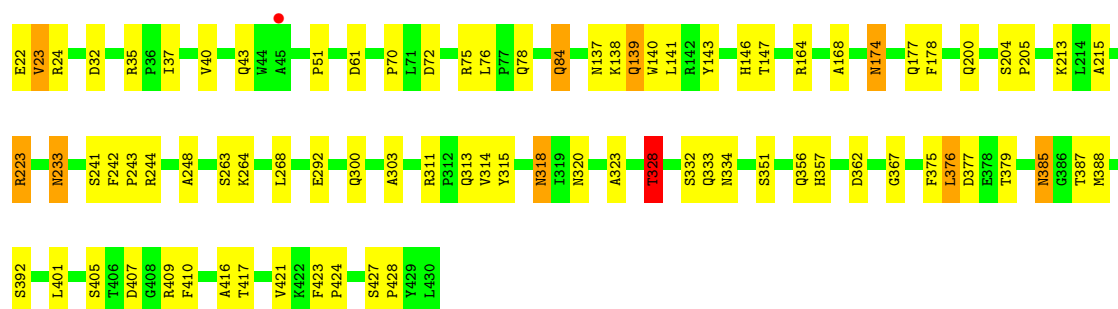


• Molecule 2: PROTEIN TOLB

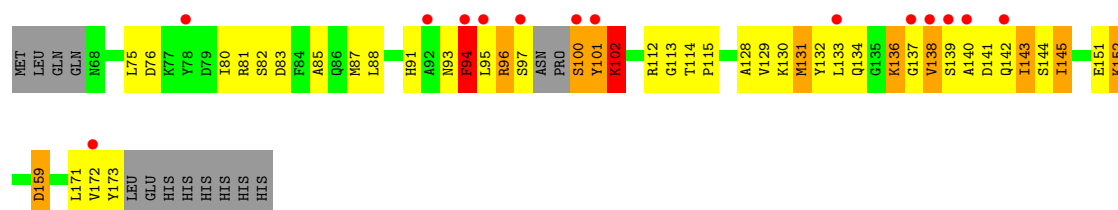


• Molecule 2: PROTEIN TOLB





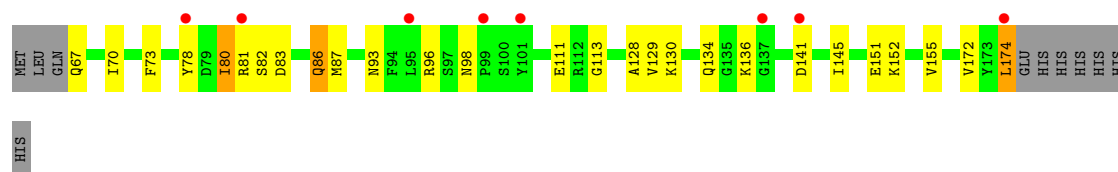
• Molecule 3: PEPTIDOGLYCAN-ASSOCIATED LIPOPROTEIN



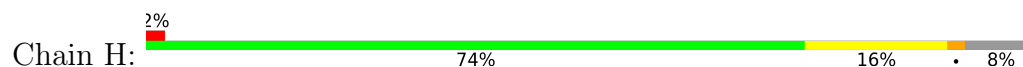
• Molecule 3: PEPTIDOGLYCAN-ASSOCIATED LIPOPROTEIN



• Molecule 3: PEPTIDOGLYCAN-ASSOCIATED LIPOPROTEIN



• Molecule 3: PEPTIDOGLYCAN-ASSOCIATED LIPOPROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	74.74Å 89.24Å 90.90Å 86.81° 89.81° 68.62°	Depositor
Resolution (Å)	45.36 – 1.86 45.36 – 1.86	Depositor EDS
% Data completeness (in resolution range)	96.2 (45.36-1.86) 86.4 (45.36-1.86)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 1.86Å)	Xtrriage
Refinement program	REFMAC 5.4.0077	Depositor
R, R_{free}	0.191 , 0.247 0.192 , 0.247	Depositor DCC
R_{free} test set	7981 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	17.3	Xtrriage
Anisotropy	0.121	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17488	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.20 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8264e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: ACT, 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	1.24	5/3196 (0.2%)	1.19	19/4354 (0.4%)
2	B	1.15	1/3189 (0.0%)	1.19	8/4345 (0.2%)
2	D	1.17	2/3174 (0.1%)	1.17	8/4326 (0.2%)
2	F	1.22	6/3251 (0.2%)	1.19	8/4427 (0.2%)
3	C	1.06	0/853	1.17	5/1148 (0.4%)
3	E	1.04	0/873	1.39	7/1178 (0.6%)
3	G	1.02	0/894	1.19	2/1205 (0.2%)
3	H	1.06	0/886	1.21	1/1195 (0.1%)
All	All	1.17	14/16316 (0.1%)	1.20	58/22178 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
2	F	1	0
3	E	0	1
All	All	1	3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	379	THR	CA-CB	8.17	1.58	1.52
1	A	248	ALA	C-O	7.47	1.27	1.23
2	F	292	GLU	C-O	-6.89	1.20	1.23
2	F	379	THR	CA-CB	6.71	1.58	1.52
2	F	204	SER	N-CA	6.15	1.50	1.46
2	D	204	SER	CA-C	-6.04	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	248	ALA	N-CA	5.61	1.50	1.46
1	A	205	PRO	CA-C	5.41	1.59	1.52
2	F	367	GLY	N-CA	5.36	1.51	1.45
1	A	235	ALA	CA-CB	5.29	1.62	1.53
1	A	23	VAL	CA-C	5.27	1.59	1.52
1	A	379	THR	CA-CB	5.22	1.57	1.52
2	F	204	SER	CA-CB	5.10	1.56	1.52
2	D	200	GLN	N-CA	5.05	1.49	1.46

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	75	LEU	N-CA-C	15.70	133.74	108.63
3	E	75	LEU	CB-CA-C	-12.77	90.44	110.88
3	E	75	LEU	CA-C-N	11.54	138.57	122.07
3	E	75	LEU	C-N-CA	11.54	138.57	122.07
2	B	30	GLY	N-CA-C	-10.89	102.12	115.08
2	F	178	PHE	CA-C-N	-9.37	110.05	120.45
2	F	178	PHE	C-N-CA	-9.37	110.05	120.45
2	F	323	ALA	N-CA-C	-7.94	98.65	110.24
1	A	31	VAL	CB-CA-C	-7.83	98.56	111.32
2	B	419	GLY	N-CA-C	7.47	122.36	112.65
3	C	100	SER	N-CA-C	7.16	126.05	110.80
2	D	23	VAL	N-CA-C	7.13	120.12	108.99
2	B	287	ARG	N-CA-C	-7.05	104.68	113.28
2	F	244	ARG	N-CA-C	6.90	118.21	108.00
1	A	69	ASN	CA-C-N	-6.87	112.89	119.76
1	A	69	ASN	C-N-CA	-6.87	112.89	119.76
2	B	32	ASP	N-CA-C	-6.85	91.82	111.00
2	F	328	THR	OG1-CB-CG2	6.74	122.78	109.30
3	E	152	LYS	CA-C-N	6.69	126.72	119.90
3	E	152	LYS	C-N-CA	6.69	126.72	119.90
2	D	366	GLY	N-CA-C	-6.21	107.11	115.36
1	A	71	LEU	CA-C-N	-6.20	111.21	120.94
1	A	71	LEU	C-N-CA	-6.20	111.21	120.94
2	D	368	VAL	N-CA-C	6.17	117.18	108.36
1	A	221	SER	CA-C-N	-6.14	116.14	123.44
1	A	221	SER	C-N-CA	-6.14	116.14	123.44
2	B	76	LEU	CA-C-N	-6.02	113.56	119.64
2	B	76	LEU	C-N-CA	-6.02	113.56	119.64
3	C	114	THR	CA-C-N	-6.02	112.37	119.05
3	C	114	THR	C-N-CA	-6.02	112.37	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	423	PHE	CA-C-N	-5.90	113.89	119.85
2	D	423	PHE	C-N-CA	-5.90	113.89	119.85
2	B	243	PRO	CB-CA-C	5.89	121.28	111.56
2	F	328	THR	CA-CB-CG2	5.75	120.27	110.50
2	D	100	VAL	CB-CA-C	-5.71	103.08	110.84
1	A	28	ASP	N-CA-C	-5.67	106.40	113.55
1	A	30	GLY	N-CA-C	-5.64	106.88	115.00
3	C	100	SER	N-CA-CB	-5.58	101.06	110.49
1	A	236	VAL	N-CA-C	5.53	115.91	108.17
2	D	136	VAL	CB-CA-C	-5.51	100.99	110.30
3	C	102	LYS	N-CA-C	5.50	117.59	108.13
2	B	164	ARG	CG-CD-NE	-5.50	99.90	112.00
1	A	84	GLN	N-CA-C	-5.46	105.88	112.54
1	A	29	SER	N-CA-C	5.43	117.33	109.07
2	F	40	VAL	CA-C-N	-5.33	114.27	119.76
2	F	40	VAL	C-N-CA	-5.33	114.27	119.76
1	A	76	LEU	CA-C-N	-5.33	114.26	119.64
1	A	76	LEU	C-N-CA	-5.33	114.26	119.64
1	A	23	VAL	N-CA-C	5.33	120.42	109.34
1	A	283	VAL	CB-CA-C	-5.30	106.21	111.30
1	A	244	ARG	N-CA-C	5.25	116.95	108.08
3	H	117	TYR	CA-CB-CG	-5.24	104.47	113.90
2	D	147	THR	N-CA-C	-5.13	105.38	111.69
3	E	119	ILE	N-CA-C	-5.06	105.46	110.62
1	A	40	VAL	CA-C-N	-5.05	114.75	119.90
1	A	40	VAL	C-N-CA	-5.05	114.75	119.90
3	G	98	ASN	CA-C-N	5.04	125.72	120.12
3	G	98	ASN	C-N-CA	5.04	125.72	120.12

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	F	328	THR	CB

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	29	SER	Peptide
2	B	32	ASP	Peptide
3	E	75	LEU	Peptide

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	3110	0	3034	62	0
2	B	3100	0	3020	88	0
2	D	3091	0	3008	66	0
2	F	3147	0	3086	76	0
3	C	833	0	817	83	0
3	E	857	0	838	29	0
3	G	869	0	855	22	0
3	H	864	0	846	27	0
4	A	15	0	0	0	0
4	B	10	0	0	0	0
4	D	5	0	0	0	0
4	F	5	0	0	0	0
4	G	5	0	0	0	0
5	A	6	0	8	4	0
5	B	12	0	16	5	0
5	C	6	0	8	8	0
5	D	12	0	16	5	0
5	F	6	0	8	3	0
6	A	4	0	3	8	0
6	B	4	0	3	10	0
6	D	4	0	3	6	0
6	H	4	0	3	0	0
7	A	354	0	0	9	0
7	B	314	0	0	17	0
7	C	35	0	0	5	0
7	D	316	0	0	7	0
7	E	55	0	0	6	0
7	F	329	0	0	2	0
7	G	60	0	0	6	0
7	H	56	0	0	2	0
All	All	17488	0	15572	443	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (443) 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)
3:C:95:LEU:C	3:C:96:ARG:HD3	1.55	1.30
3:C:95:LEU:O	3:C:96:ARG:HD3	1.26	1.29
3:C:75:LEU:HD12	3:C:76:ASP:N	1.46	1.26
3:C:101:TYR:HD1	3:C:102:LYS:N	1.31	1.26
3:E:75:LEU:HD11	3:E:112:ARG:NH2	1.55	1.19
3:C:95:LEU:O	3:C:96:ARG:CD	1.93	1.16
2:B:29:SER:HA	2:B:31:VAL:HG12	1.14	1.11
2:F:24:ARG:HH22	5:F:1432:GOL:H12	1.06	1.10
2:B:150:ASP:OD2	6:B:1435:ACT:H1	1.51	1.10
1:A:22:GLU:O	1:A:22:GLU:HG3	1.43	1.08
3:E:75:LEU:CD1	3:E:112:ARG:HH22	1.66	1.08
3:C:101:TYR:CD1	3:C:102:LYS:N	2.11	1.07
3:C:134:GLN:HE22	3:C:140:ALA:CB	1.67	1.07
3:C:134:GLN:HE22	3:C:140:ALA:HB2	0.96	1.07
3:C:134:GLN:NE2	3:C:140:ALA:CA	2.18	1.06
1:A:390[B]:LEU:HD12	1:A:402:ASN:O	1.56	1.06
2:B:417:THR:HA	7:B:2302:HOH:O	1.56	1.05
3:C:134:GLN:HE21	3:C:140:ALA:CA	1.69	1.04
2:B:244:ARG:HE	5:C:1174:GOL:H31	1.14	1.04
3:C:131:MET:HE2	3:C:131:MET:HA	1.36	1.03
2:B:29:SER:HA	2:B:31:VAL:CG1	1.88	1.02
2:F:223:ARG:HH11	2:F:223:ARG:HB2	1.21	1.02
3:C:134:GLN:HE21	3:C:140:ALA:HA	1.24	1.01
2:F:137[B]:ASN:ND2	2:F:140:TRP:HD1	1.59	1.00
3:C:134:GLN:NE2	3:C:140:ALA:HB2	1.75	0.99
3:C:75:LEU:HD12	3:C:76:ASP:H	0.87	0.99
1:A:29:SER:HA	7:A:2003:HOH:O	1.62	0.98
3:H:75:LEU:O	3:H:77:LYS:HE2	1.63	0.98
1:A:311:ARG:NH1	1:A:333:GLN:HB2	1.78	0.98
3:C:134:GLN:HB2	7:C:2021:HOH:O	1.62	0.97
2:B:318:ASN:ND2	2:B:320:ASN:H	1.64	0.96
3:C:133:LEU:C	3:C:138:VAL:HG23	1.89	0.96
2:D:164:ARG:H	6:D:1434:ACT:H1	1.29	0.95
2:B:29:SER:CA	2:B:31:VAL:HG12	1.95	0.95
7:D:2249:HOH:O	3:E:112:ARG:HD2	1.65	0.95
3:C:133:LEU:HB3	3:C:138:VAL:HG21	1.48	0.95
3:C:134:GLN:NE2	3:C:140:ALA:CB	2.30	0.94
3:C:129:VAL:HG12	3:C:133:LEU:HD11	1.48	0.93
2:D:352:ASN:HB3	7:D:2247:HOH:O	1.69	0.93
2:D:399:SER:H	2:D:420:GLN:HE21	1.15	0.93
2:D:318:ASN:HD22	2:D:320:ASN:H	0.98	0.91
1:A:311:ARG:HH12	1:A:333:GLN:HB2	1.30	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:133:LEU:O	3:C:138:VAL:HG23	1.70	0.91
2:F:137[B]:ASN:OD1	2:F:139:GLN:HG2	1.70	0.90
2:F:401:LEU:HG	2:F:421[A]:VAL:HG23	1.54	0.89
3:C:131:MET:HE1	3:C:134:GLN:OE1	1.71	0.89
2:F:356:GLN:HE22	3:G:113:GLY:H	1.15	0.89
3:H:93:ASN:HD22	3:H:96:ARG:NH2	1.69	0.89
2:D:356:GLN:HE22	3:E:113:GLY:H	1.21	0.89
2:B:318:ASN:HD22	2:B:320:ASN:H	0.91	0.88
3:C:96:ARG:CG	3:C:96:ARG:HH11	1.85	0.88
3:H:93:ASN:ND2	3:H:96:ARG:HH22	1.71	0.88
3:H:75:LEU:C	3:H:75:LEU:HD23	1.98	0.88
2:B:164:ARG:H	6:B:1435:ACT:H3	1.35	0.88
2:D:318:ASN:ND2	2:D:320:ASN:H	1.70	0.87
2:F:24:ARG:NH2	5:F:1432:GOL:H12	1.88	0.87
2:B:356:GLN:HE22	3:C:113:GLY:H	1.22	0.87
1:A:318:ASN:HD22	1:A:320:ASN:H	1.23	0.86
1:A:390[A]:LEU:CD2	1:A:424:PRO:HB2	2.05	0.86
2:B:244:ARG:NE	5:C:1174:GOL:H31	1.90	0.86
2:B:244:ARG:HE	5:C:1174:GOL:C3	1.89	0.86
2:F:137[B]:ASN:HD21	2:F:140:TRP:HD1	1.19	0.86
2:F:200:GLN:HE22	3:G:152:LYS:NZ	1.75	0.85
2:F:137[B]:ASN:HD21	2:F:140:TRP:CD1	1.95	0.85
1:A:390[A]:LEU:HD23	1:A:424:PRO:HB2	1.59	0.84
3:C:75:LEU:CD1	3:C:76:ASP:N	2.38	0.84
3:C:96:ARG:HH11	3:C:96:ARG:HG3	1.42	0.84
3:C:75:LEU:CD1	3:C:76:ASP:H	1.83	0.84
3:C:129:VAL:CG1	3:C:133:LEU:HD11	2.08	0.84
3:H:74:ASP:CB	3:H:77:LYS:HE3	2.08	0.83
1:A:23:VAL:CG1	1:A:414:LEU:HB3	2.07	0.83
2:F:223:ARG:HH11	2:F:223:ARG:CB	1.91	0.83
1:A:22:GLU:O	1:A:22:GLU:CG	2.24	0.83
2:F:318:ASN:HD22	2:F:320:ASN:H	1.22	0.83
3:C:134:GLN:HA	3:C:138:VAL:O	1.79	0.83
2:D:22:GLU:OE1	2:D:22:GLU:C	2.22	0.82
3:C:134:GLN:NE2	3:C:140:ALA:HA	1.86	0.82
1:A:23:VAL:HG13	1:A:414:LEU:HB3	1.60	0.82
3:H:74:ASP:HB3	3:H:77:LYS:HE3	1.60	0.82
2:F:200:GLN:HE22	3:G:152:LYS:HZ1	1.26	0.81
1:A:417:THR:HA	7:A:2340:HOH:O	1.81	0.81
3:G:174:LEU:HB3	7:G:2058:HOH:O	1.78	0.81
3:C:152:LYS:HE2	7:C:2008:HOH:O	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:22:GLU:OE1	2:D:22:GLU:O	1.97	0.81
3:C:131:MET:HA	3:C:131:MET:CE	2.09	0.81
1:A:164:ARG:H	6:A:1435:ACT:H1	1.45	0.81
2:B:332[A]:SER:H	2:B:352:ASN:HD21	1.26	0.81
2:B:332[B]:SER:H	2:B:352:ASN:HD21	1.27	0.81
3:C:75:LEU:HD22	3:C:112:ARG:HH22	1.45	0.81
3:H:93:ASN:HD22	3:H:96:ARG:HH22	1.21	0.80
2:B:22:GLU:N	5:B:1434:GOL:HO1	1.80	0.80
2:B:61:ASP:OD2	2:B:146:HIS:HD2	1.65	0.80
2:D:360[A]:LYS:HE2	2:D:369:GLN:NE2	1.97	0.79
1:A:112:TYR:HE1	1:A:138:LYS:HG2	1.48	0.78
3:C:93:ASN:C	3:C:95:LEU:H	1.89	0.78
3:C:134:GLN:HE21	3:C:140:ALA:N	1.81	0.78
2:D:150:ASP:OD2	6:D:1434:ACT:H2	1.82	0.78
2:D:150:ASP:OD2	6:D:1434:ACT:CH3	2.32	0.77
3:E:81:ARG:NH1	3:E:82:SER:H	1.83	0.76
2:F:137[B]:ASN:ND2	2:F:140:TRP:CD1	2.49	0.76
2:B:65:SER:HA	5:B:1433:GOL:H32	1.68	0.76
3:C:145:ILE:H	5:C:1174:GOL:H11	1.50	0.76
2:F:313:GLN:OE1	2:F:328:THR:HG23	1.86	0.75
1:A:318:ASN:ND2	1:A:320:ASN:H	1.83	0.75
2:F:61:ASP:OD2	2:F:146:HIS:HD2	1.69	0.75
1:A:29:SER:OG	1:A:31:VAL:HG12	1.86	0.74
3:C:134:GLN:NE2	3:C:140:ALA:N	2.35	0.74
2:F:223:ARG:HB2	2:F:223:ARG:NH1	2.00	0.74
3:E:131:MET:HG2	7:E:2002:HOH:O	1.85	0.74
3:C:129:VAL:HG12	3:C:133:LEU:CD1	2.18	0.73
2:B:318:ASN:HD22	2:B:320:ASN:N	1.77	0.73
3:C:97:SER:O	3:C:100:SER:N	2.22	0.73
1:A:150:ASP:OD2	6:A:1435:ACT:CH3	2.37	0.73
2:D:287:ARG:HE	5:D:1433:GOL:H31	1.53	0.73
2:B:355:GLN:HG3	7:B:2258:HOH:O	1.87	0.72
2:F:300:GLN:OE1	2:F:320:ASN:ND2	2.22	0.72
3:C:134:GLN:CB	7:C:2021:HOH:O	2.30	0.72
2:F:223:ARG:NH2	2:F:241:SER:O	2.22	0.72
3:C:95:LEU:C	3:C:96:ARG:CD	2.47	0.72
1:A:31:VAL:HG22	1:A:32:ASP:HB2	1.71	0.71
2:B:164:ARG:HB2	6:B:1435:ACT:H3	1.71	0.71
2:B:22:GLU:C	7:B:2002:HOH:O	2.34	0.71
2:F:375:PHE:CE2	2:F:376:LEU:HD22	2.25	0.70
3:H:74:ASP:HB2	3:H:77:LYS:HD2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ASN:HB2	7:A:2094:HOH:O	1.91	0.70
3:G:152:LYS:CE	7:G:2041:HOH:O	2.38	0.70
2:F:137[B]:ASN:OD1	2:F:139:GLN:CG	2.39	0.69
2:B:22:GLU:HB2	2:B:417:THR:OG1	1.92	0.69
2:D:365:THR:HG23	7:D:2259:HOH:O	1.92	0.69
2:B:22:GLU:CB	2:B:417:THR:OG1	2.41	0.69
1:A:31:VAL:HB	7:A:2003:HOH:O	1.92	0.69
3:E:131:MET:CG	7:E:2002:HOH:O	2.39	0.68
2:B:332[A]:SER:H	2:B:352:ASN:ND2	1.90	0.68
2:B:332[B]:SER:H	2:B:352:ASN:ND2	1.90	0.68
1:A:150:ASP:OD2	6:A:1435:ACT:H3	1.94	0.68
3:C:93:ASN:C	3:C:95:LEU:N	2.50	0.67
2:B:72:ASP:HB2	7:B:2038:HOH:O	1.94	0.67
3:G:80:ILE:HD12	3:G:128:ALA:HB1	1.74	0.67
3:C:129:VAL:O	3:C:133:LEU:HD12	1.95	0.67
2:F:146:HIS:HE1	7:F:2135:HOH:O	1.77	0.67
3:G:80:ILE:HD11	3:G:128:ALA:C	2.19	0.67
3:C:133:LEU:O	3:C:136:LYS:N	2.28	0.66
1:A:300:GLN:OE1	1:A:320:ASN:ND2	2.25	0.66
2:F:143:TYR:OH	2:F:164[A]:ARG:NH1	2.27	0.66
3:E:76:ASP:HB3	3:E:78:TYR:OH	1.95	0.66
3:C:96:ARG:HD3	3:C:96:ARG:N	1.96	0.66
7:B:2267:HOH:O	2:F:35:ARG:HG3	1.96	0.66
1:A:191:ASN:H	5:A:1434:GOL:H32	1.61	0.65
3:C:133:LEU:C	3:C:138:VAL:CG2	2.68	0.65
2:F:318:ASN:HD21	2:F:320:ASN:HD22	1.44	0.65
2:F:314:VAL:H	2:F:328:THR:CG2	2.09	0.65
1:A:61:ASP:OD2	1:A:146:HIS:HD2	1.80	0.65
3:C:145:ILE:HG13	3:C:145:ILE:O	1.96	0.65
3:E:74:ASP:HB2	3:E:77:LYS:HG3	1.78	0.65
2:F:401:LEU:HG	2:F:421[A]:VAL:CG2	2.25	0.65
5:F:1432:GOL:O1	5:F:1432:GOL:O3	1.94	0.64
3:E:76:ASP:O	3:E:78:TYR:CZ	2.50	0.64
3:C:142:GLN:C	3:C:143:ILE:HG13	2.21	0.64
2:D:318:ASN:HD22	2:D:320:ASN:N	1.82	0.64
3:H:165:LYS:HE3	7:H:2055:HOH:O	1.96	0.63
2:D:23:VAL:HG12	2:D:416:ALA:HB2	1.81	0.63
2:D:164:ARG:H	6:D:1434:ACT:CH3	2.06	0.63
1:A:31:VAL:HG13	1:A:31:VAL:O	1.99	0.63
2:D:61:ASP:OD2	2:D:146:HIS:HD2	1.81	0.63
2:D:82:SER:OG	2:D:85:GLU:HG3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:311:ARG:HE	2:D:333:GLN:HE21	1.46	0.63
3:H:75:LEU:C	3:H:75:LEU:CD2	2.72	0.62
3:E:174:LEU:C	7:E:2055:HOH:O	2.42	0.62
2:D:375:PHE:CE2	2:D:376:LEU:HD22	2.34	0.62
3:H:74:ASP:HB2	3:H:77:LYS:HE3	1.79	0.62
2:D:287:ARG:HE	5:D:1433:GOL:C3	2.12	0.61
2:D:287:ARG:HG3	5:D:1433:GOL:H31	1.82	0.61
2:B:22:GLU:HB2	7:B:2002:HOH:O	1.99	0.61
2:F:314:VAL:H	2:F:328:THR:HG21	1.66	0.61
1:A:150:ASP:OD2	6:A:1435:ACT:H2	2.00	0.60
2:B:146:HIS:HE1	7:B:2137:HOH:O	1.84	0.60
1:A:242:PHE:C	1:A:243:PRO:O	2.42	0.60
2:D:164:ARG:HG3	6:D:1434:ACT:H2	1.82	0.60
2:B:318:ASN:HD21	2:B:320:ASN:ND2	2.00	0.59
2:F:242:PHE:CG	2:F:264[B]:LYS:HD3	2.37	0.59
2:B:360:LYS:HE3	7:B:2260:HOH:O	2.01	0.59
3:C:80:ILE:HG21	3:C:88:LEU:HD12	1.84	0.59
3:C:81:ARG:NH2	3:C:83:ASP:OD2	2.35	0.59
3:C:95:LEU:O	3:C:96:ARG:HD2	1.98	0.59
2:D:107:ASN:HD21	2:D:113:ASN:ND2	1.99	0.59
2:D:318:ASN:HD21	2:D:320:ASN:HD22	1.49	0.59
2:B:318:ASN:HD21	2:B:320:ASN:HD22	1.49	0.59
1:A:390[B]:LEU:HD13	1:A:403:LEU:CD2	2.33	0.59
1:A:244:ARG:HH22	3:H:127:ASN:ND2	2.01	0.58
2:B:242:PHE:C	2:B:243:PRO:O	2.41	0.58
2:B:385:ASN:C	2:B:385:ASN:HD22	2.11	0.58
2:D:24:ARG:O	2:D:415:PRO:HD2	2.03	0.58
2:F:242:PHE:HB3	2:F:243:PRO:CD	2.33	0.58
2:B:418:ASP:O	2:B:418:ASP:OD2	2.20	0.58
2:F:375:PHE:CZ	2:F:376:LEU:HD22	2.38	0.58
2:B:22:GLU:OE1	2:B:418:ASP:OD2	2.21	0.58
3:C:75:LEU:HD12	3:C:75:LEU:C	2.16	0.58
1:A:287:ARG:HD2	7:A:2238:HOH:O	2.04	0.58
3:C:139:SER:H	3:C:142:GLN:HE21	1.50	0.58
3:E:75:LEU:HD11	3:E:112:ARG:HH22	0.70	0.58
3:C:172[A]:VAL:HG12	3:C:173:TYR:N	2.19	0.57
2:D:360[A]:LYS:CE	2:D:369:GLN:NE2	2.67	0.57
1:A:191:ASN:H	5:A:1434:GOL:C3	2.16	0.57
2:B:35:ARG:HD3	2:B:68:PHE:CE2	2.40	0.57
2:B:31:VAL:HG23	2:B:32:ASP:CG	2.30	0.57
3:H:74:ASP:HB2	3:H:77:LYS:CE	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390[B]:LEU:CD1	1:A:402:ASN:O	2.42	0.57
2:D:150:ASP:OD2	6:D:1434:ACT:H3	2.05	0.56
2:B:33:SER:HB2	2:B:69:ASN:CG	2.30	0.56
2:B:162:ALA:HA	6:B:1435:ACT:H2	1.87	0.56
2:D:313:GLN:HE22	2:D:334:ASN:HD22	1.52	0.56
2:D:376:LEU:HD21	3:E:111:GLU:CD	2.31	0.56
3:G:172:VAL:HG12	3:G:174:LEU:HD23	1.88	0.56
1:A:341:SER:HB3	7:A:2122:HOH:O	2.05	0.56
3:C:96:ARG:HG3	3:C:96:ARG:NH1	2.16	0.56
2:D:318:ASN:HD21	2:D:320:ASN:ND2	2.03	0.56
3:E:81:ARG:HH11	3:E:82:SER:H	1.53	0.56
2:B:164:ARG:H	6:B:1435:ACT:CH3	2.16	0.56
2:F:263:SER:HB3	2:F:268:LEU:HD23	1.87	0.56
2:D:40:VAL:HG13	2:D:41:PRO:HD2	1.87	0.56
1:A:164:ARG:H	6:A:1435:ACT:CH3	2.16	0.56
3:C:93:ASN:O	3:C:95:LEU:N	2.39	0.55
2:D:22:GLU:HB3	2:D:417[B]:THR:OG1	2.06	0.55
2:B:65:SER:HA	5:B:1433:GOL:C3	2.35	0.55
3:E:77:LYS:C	3:E:78:TYR:CD2	2.85	0.55
3:H:74:ASP:HB2	3:H:77:LYS:CD	2.36	0.55
2:B:33:SER:HB3	2:B:69:ASN:HB2	1.89	0.55
2:B:23:VAL:HG22	7:B:2141:HOH:O	2.06	0.55
1:A:23:VAL:CG1	1:A:414:LEU:HD23	2.36	0.55
2:D:365:THR:CG2	7:D:2259:HOH:O	2.54	0.55
3:C:142:GLN:C	3:C:143:ILE:CG1	2.80	0.55
2:F:51:PRO:HG2	2:F:141:LEU:HD11	1.90	0.54
2:F:139:GLN:HE21	2:F:139:GLN:HA	1.72	0.54
3:G:152:LYS:HE2	7:G:2041:HOH:O	2.03	0.54
2:B:29:SER:C	2:B:31:VAL:H	2.15	0.54
2:D:385:ASN:HD22	2:D:385:ASN:C	2.14	0.54
1:A:112:TYR:CE1	1:A:138:LYS:HG2	2.37	0.54
1:A:385:ASN:C	1:A:385:ASN:HD22	2.15	0.53
2:B:396:GLY:C	2:B:397:MET:HE2	2.33	0.53
2:D:107:ASN:HD21	2:D:113:ASN:HD21	1.56	0.53
1:A:242:PHE:O	1:A:243:PRO:O	2.25	0.53
2:B:22:GLU:N	5:B:1434:GOL:O1	2.40	0.53
2:F:311:ARG:HD2	2:F:333:GLN:HE21	1.74	0.53
1:A:242:PHE:O	1:A:243:PRO:C	2.49	0.53
3:H:75:LEU:O	3:H:75:LEU:HD23	2.08	0.53
2:B:162:ALA:CA	6:B:1435:ACT:H2	2.39	0.53
2:F:147:THR:OG1	2:F:164[B]:ARG:NH1	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:85:ALA:HB1	3:C:132:TYR:OH	2.09	0.52
3:C:134:GLN:O	3:C:137:GLY:N	2.42	0.52
2:B:164:ARG:N	6:B:1435:ACT:H3	2.15	0.52
1:A:146:HIS:HE1	7:A:2159:HOH:O	1.91	0.52
2:D:409:ARG:HD2	7:D:2006:HOH:O	2.08	0.52
1:A:191:ASN:N	5:A:1434:GOL:H32	2.24	0.52
2:F:318:ASN:ND2	2:F:320:ASN:H	2.01	0.51
3:C:133:LEU:O	3:C:134:GLN:C	2.51	0.51
2:B:51:PRO:HG3	2:B:112:TYR:CE2	2.45	0.51
3:H:75:LEU:O	3:H:77:LYS:CE	2.50	0.51
2:B:262:LEU:HB2	2:B:271:TYR:CE1	2.46	0.51
2:F:205:PRO:HA	2:F:215:ALA:O	2.11	0.51
3:G:80:ILE:CD1	3:G:128:ALA:C	2.84	0.51
3:E:77:LYS:HE3	3:E:77:LYS:HA	1.92	0.51
3:C:131:MET:CE	3:C:131:MET:CA	2.88	0.51
1:A:311:ARG:HH12	1:A:333:GLN:CB	2.13	0.50
2:D:362:ASP:OD1	2:D:365:THR:N	2.30	0.50
2:F:311:ARG:HH11	2:F:333:GLN:HE21	1.60	0.50
2:D:409:ARG:NH1	2:D:409:ARG:HG3	2.26	0.50
2:D:40:VAL:CG1	2:D:41:PRO:HD2	2.41	0.50
2:D:205:PRO:HA	2:D:215:ALA:O	2.12	0.50
1:A:23:VAL:HG12	1:A:414:LEU:HD23	1.92	0.50
2:B:203:MET:HB2	2:B:217:VAL:HB	1.94	0.50
3:E:124:ARG:CZ	7:E:2035:HOH:O	2.59	0.50
1:A:306:SER:OG	1:A:308[A]:GLN:HG2	2.10	0.50
2:F:385:ASN:C	2:F:385:ASN:HD22	2.18	0.49
3:C:132:TYR:C	3:C:132:TYR:CD2	2.91	0.49
3:C:172[B]:VAL:HG23	3:C:173:TYR:N	2.27	0.49
2:D:139:GLN:H	2:D:139:GLN:NE2	2.10	0.49
3:H:115:PRO:HB3	3:H:151:GLU:OE2	2.12	0.49
2:D:242:PHE:HB3	2:D:243:PRO:CD	2.42	0.49
3:C:96:ARG:HH11	3:C:96:ARG:HG2	1.75	0.49
3:E:77:LYS:HE3	3:E:77:LYS:CA	2.42	0.49
2:F:357:HIS:HD2	2:F:377:ASP:OD2	1.95	0.49
3:C:102:LYS:HD2	3:C:144[B]:SER:OG	2.13	0.49
2:F:174:ASN:H	2:F:174:ASN:ND2	2.10	0.49
3:G:93:ASN:HB3	3:G:96:ARG:NH2	2.27	0.49
2:F:22:GLU:N	2:F:417:THR:HG1	2.11	0.49
2:D:279:GLN:HE21	3:G:83:ASP:CG	2.21	0.49
1:A:164:ARG:HB2	6:A:1435:ACT:H2	1.94	0.48
2:B:22:GLU:HA	7:B:2001:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:242:PHE:HB3	2:D:243:PRO:HD2	1.95	0.48
2:D:286:GLY:HA2	5:D:1433:GOL:H2	1.95	0.48
3:C:138:VAL:HA	7:C:2022:HOH:O	2.13	0.48
2:B:30:GLY:O	2:B:33:SER:HA	2.14	0.48
3:C:133:LEU:CB	3:C:138:VAL:HG21	2.33	0.48
3:G:136:LYS:HA	3:G:136:LYS:HD3	1.66	0.48
2:B:31:VAL:HG23	2:B:32:ASP:OD2	2.14	0.48
2:F:376:LEU:HD21	3:G:111:GLU:CD	2.37	0.48
2:B:32:ASP:HA	2:B:33:SER:OG	2.14	0.48
3:G:81:ARG:HD2	7:G:2010:HOH:O	2.12	0.48
2:B:162:ALA:C	6:B:1435:ACT:H2	2.38	0.48
2:F:328:THR:HG21	2:F:334:ASN:HB2	1.96	0.48
1:A:422:LYS:NZ	7:A:2344:HOH:O	2.31	0.48
3:C:87:MET:HE3	3:C:87:MET:HB3	1.76	0.47
2:F:223:ARG:HH11	2:F:223:ARG:CG	2.27	0.47
1:A:192:GLN:H	5:A:1434:GOL:H12	1.79	0.47
2:B:40:VAL:HG13	2:B:41:PRO:HD2	1.96	0.47
3:C:133:LEU:HB3	3:C:138:VAL:CG2	2.33	0.47
2:F:407:ASP:OD1	2:F:409:ARG:HB2	2.14	0.47
2:B:223:ARG:NH1	2:B:242:PHE:O	2.47	0.47
2:F:242:PHE:CB	2:F:264[B]:LYS:HD3	2.45	0.47
2:B:223:ARG:HD3	2:B:242:PHE:O	2.15	0.47
2:F:233:ASN:HD22	2:F:233:ASN:H	1.63	0.47
3:G:130:LYS:O	3:G:134:GLN:HG3	2.15	0.47
1:A:418:ASP:OD1	1:A:418:ASP:N	2.39	0.47
1:A:164:ARG:HG3	6:A:1435:ACT:H2	1.97	0.47
3:C:171:LEU:HD12	3:C:171:LEU:N	2.30	0.47
3:E:79:ASP:OD1	3:E:79:ASP:N	2.41	0.47
3:E:81:ARG:NH2	7:E:2014:HOH:O	2.47	0.47
3:H:93:ASN:ND2	3:H:96:ARG:NH2	2.40	0.47
2:B:244:ARG:HH21	5:C:1174:GOL:H31	1.79	0.46
2:D:146:HIS:HE1	7:D:2122:HOH:O	1.98	0.46
2:F:168:ALA:O	2:F:424:PRO:HA	2.15	0.46
2:F:242:PHE:HB3	2:F:243:PRO:HD2	1.95	0.46
3:G:151:GLU:CD	7:G:2039:HOH:O	2.58	0.46
1:A:164:ARG:HB2	6:A:1435:ACT:CH3	2.46	0.46
2:D:375:PHE:O	2:D:393:SER:HB2	2.15	0.46
3:C:96:ARG:CG	3:C:96:ARG:NH1	2.58	0.46
3:E:77:LYS:O	3:E:78:TYR:CD2	2.68	0.46
2:D:173:THR:HG22	2:D:418:ASP:O	2.16	0.46
2:D:409:ARG:HG3	2:D:409:ARG:HH11	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:242:PHE:O	2:F:243:PRO:C	2.58	0.46
7:B:2269:HOH:O	2:F:32:ASP:HB3	2.15	0.45
3:G:67:GLN:CD	3:G:70:ILE:HD12	2.41	0.45
2:B:244:ARG:CZ	5:C:1174:GOL:H31	2.45	0.45
2:B:318:ASN:ND2	2:B:320:ASN:N	2.47	0.45
3:H:86:GLN:HG3	7:H:2016:HOH:O	2.15	0.45
2:D:22:GLU:C	2:D:22:GLU:CD	2.85	0.45
3:C:159:ASP:HB2	7:C:2029:HOH:O	2.15	0.45
3:H:68:ASN:C	3:H:68:ASN:OD1	2.59	0.45
1:A:200:GLN:HE22	3:H:152:LYS:NZ	2.15	0.45
1:A:390[A]:LEU:CD2	1:A:424:PRO:CB	2.86	0.45
2:B:242:PHE:HB3	2:B:243:PRO:HD2	1.99	0.45
2:F:427:SER:HB2	2:F:428:PRO:HD2	1.99	0.45
2:F:313:GLN:OE1	2:F:328:THR:CG2	2.62	0.45
3:C:81:ARG:HH21	3:C:83:ASP:CG	2.24	0.45
1:A:31:VAL:O	1:A:32:ASP:C	2.59	0.44
1:A:112:TYR:HE1	1:A:138:LYS:CG	2.25	0.44
2:F:311:ARG:HH11	2:F:333:GLN:NE2	2.15	0.44
2:B:23:VAL:N	7:B:2002:HOH:O	2.51	0.44
2:B:318:ASN:ND2	2:B:320:ASN:HB2	2.32	0.44
2:F:314:VAL:H	2:F:328:THR:HG22	1.82	0.44
3:H:98:ASN:O	3:H:100:SER:N	2.50	0.44
3:C:75:LEU:CD2	3:C:112:ARG:HH22	2.25	0.44
3:C:128:ALA:O	3:C:129:VAL:C	2.56	0.44
3:C:130:LYS:HA	3:C:133:LEU:HD13	1.99	0.44
2:F:318:ASN:HD21	2:F:320:ASN:ND2	2.13	0.44
2:D:326:ARG:HB3	2:D:329:TRP:CZ2	2.53	0.44
2:F:223:ARG:NH1	2:F:223:ARG:CG	2.79	0.44
3:G:80:ILE:HD11	3:G:129:VAL:N	2.32	0.44
2:B:223:ARG:HG2	7:B:2176:HOH:O	2.17	0.43
3:C:136:LYS:HD2	3:C:136:LYS:HA	1.71	0.43
2:B:51:PRO:HG3	2:B:112:TYR:CZ	2.53	0.43
2:D:139:GLN:H	2:D:139:GLN:CD	2.26	0.43
2:B:413:ARG:C	2:B:415:PRO:HD3	2.43	0.43
2:D:311:ARG:HE	2:D:333:GLN:NE2	2.14	0.43
1:A:213[A]:LYS:HG2	1:A:230:THR:HA	2.00	0.43
2:D:35:ARG:NH2	2:D:97:ASP:OD2	2.46	0.43
2:D:200:GLN:HE22	3:E:152:LYS:NZ	2.17	0.43
2:F:388:MET:HE2	2:F:388:MET:HB2	1.86	0.43
3:H:79:ASP:OD1	3:H:79:ASP:N	2.50	0.43
2:B:33:SER:CB	2:B:69:ASN:HB2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181:GLU:HG2	2:B:197:ARG:HG2	2.00	0.43
2:D:360[A]:LYS:NZ	2:D:406:THR:O	2.35	0.43
3:C:102:LYS:HE3	3:C:144[B]:SER:OG	2.18	0.43
2:B:164:ARG:CB	6:B:1435:ACT:H3	2.44	0.43
3:E:130:LYS:NZ	3:E:134:GLN:HE22	2.16	0.43
2:F:37:ILE:O	2:F:70:PRO:HA	2.19	0.43
2:F:242:PHE:C	2:F:243:PRO:O	2.57	0.43
1:A:205:PRO:HA	1:A:215:ALA:O	2.19	0.43
2:F:409:ARG:HD2	2:F:409:ARG:HA	1.82	0.43
2:B:192:GLN:H	5:B:1434:GOL:H12	1.84	0.43
2:B:275:LEU:HD23	2:B:275:LEU:HA	1.84	0.43
2:F:139:GLN:HE21	2:F:139:GLN:CA	2.30	0.43
2:D:318:ASN:ND2	2:D:320:ASN:HB2	2.34	0.42
3:E:112:ARG:HE	3:E:112:ARG:HB2	1.61	0.42
2:F:84:GLN:HE21	2:F:84:GLN:HB3	1.50	0.42
2:F:23:VAL:HG12	2:F:416:ALA:HB2	2.01	0.42
3:H:102:LYS:HE2	3:H:102:LYS:HB3	1.94	0.42
3:E:103:VAL:HG21	3:E:171[B]:LEU:HD22	2.01	0.42
3:C:145:ILE:H	5:C:1174:GOL:C1	2.27	0.42
2:B:67:LYS:NZ	7:B:2034:HOH:O	2.44	0.42
3:G:73:PHE:CD2	3:G:78:TYR:HA	2.55	0.42
3:C:80:ILE:HG21	3:C:88:LEU:CD1	2.49	0.42
2:D:287:ARG:HH21	5:D:1433:GOL:C1	2.33	0.42
3:E:105:VAL:HG22	3:E:171[B]:LEU:CD2	2.50	0.42
2:D:351:SER:C	2:D:352:ASN:ND2	2.78	0.42
2:B:150:ASP:CG	6:B:1435:ACT:H1	2.36	0.42
3:E:112:ARG:HD3	3:E:163:TYR:CE1	2.54	0.42
2:F:138:LYS:HB2	2:F:138:LYS:HE2	1.83	0.42
3:C:82:SER:O	3:C:85:ALA:HB3	2.20	0.42
2:F:303:ALA:HA	2:F:315:TYR:O	2.19	0.42
3:C:115:PRO:HB3	3:C:151:GLU:OE2	2.20	0.41
2:B:244:ARG:NH2	5:C:1174:GOL:H31	2.34	0.41
1:A:51:PRO:HG3	1:A:112:TYR:CZ	2.55	0.41
2:B:357:HIS:HD2	2:B:377:ASP:OD2	2.03	0.41
2:B:385:ASN:ND2	2:B:387:THR:H	2.18	0.41
2:D:262:LEU:HB2	2:D:271:TYR:CE1	2.56	0.41
1:A:390[B]:LEU:HD13	1:A:403:LEU:HD23	2.03	0.41
1:A:403:LEU:HD11	1:A:414:LEU:HD11	2.03	0.41
2:F:213[B]:LYS:HD2	7:F:2075:HOH:O	2.21	0.41
2:F:405:SER:HB3	2:F:410:PHE:HB3	2.03	0.41
1:A:31:VAL:HG22	1:A:32:ASP:N	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:75:ARG:O	2:F:76:LEU:C	2.64	0.41
2:F:333:GLN:HB3	2:F:351[A]:SER:HB2	2.01	0.41
2:B:303:ALA:HA	2:B:315:TYR:O	2.21	0.41
2:B:326:ARG:HD3	2:B:329:TRP:CH2	2.56	0.41
2:D:395:GLN:O	2:D:396:GLY:C	2.62	0.41
3:E:131:MET:HG3	7:E:2002:HOH:O	2.11	0.41
1:A:308[A]:GLN:NE2	7:A:2252:HOH:O	2.53	0.41
3:C:91:HIS:HA	3:C:94:PHE:HB2	2.03	0.41
3:E:145:ILE:O	3:E:145:ILE:HG13	2.18	0.41
2:F:147:THR:HG23	2:F:164[B]:ARG:NH1	2.36	0.41
2:F:263:SER:O	2:F:264[A]:LYS:C	2.64	0.41
2:F:385:ASN:ND2	2:F:387:THR:H	2.18	0.41
2:F:423:PHE:N	2:F:424:PRO:CD	2.84	0.41
3:H:165:LYS:HA	3:H:165:LYS:HD2	1.94	0.41
1:A:155:LYS:HA	1:A:155:LYS:HD2	1.95	0.41
2:B:331:GLY:CA	2:B:352:ASN:HD21	2.34	0.41
2:D:356:GLN:NE2	7:D:2253:HOH:O	2.53	0.41
2:B:223:ARG:HH11	2:B:243:PRO:HA	1.86	0.40
3:G:152:LYS:HE3	7:G:2041:HOH:O	2.13	0.40
3:H:139:SER:HB2	3:H:142:GLN:HE21	1.86	0.40
2:B:416:ALA:HA	7:B:2002:HOH:O	2.21	0.40
2:B:331:GLY:HA3	7:B:2253:HOH:O	2.21	0.40
2:B:360:LYS:CE	7:B:2260:HOH:O	2.66	0.40
2:D:248:ALA:N	2:D:249:PRO:CD	2.83	0.40
3:H:74:ASP:CB	3:H:77:LYS:CE	2.88	0.40
3:C:75:LEU:HD22	3:C:112:ARG:NH2	2.24	0.40
2:D:138:LYS:HA	2:D:141:LEU:HD22	2.03	0.40
2:D:388:MET:HE2	2:D:388:MET:HB2	1.93	0.40
2:B:143:TYR:CE1	2:B:164:ARG:HD2	2.57	0.40
2:B:242:PHE:HB3	2:B:243:PRO:CD	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	413/409 (101%)	402 (97%)	9 (2%)	2 (0%)	24	13
2	B	412/409 (101%)	399 (97%)	13 (3%)	0	100	100
2	D	410/409 (100%)	402 (98%)	8 (2%)	0	100	100
2	F	420/409 (103%)	414 (99%)	6 (1%)	0	100	100
3	C	102/118 (86%)	91 (89%)	9 (9%)	2 (2%)	6	1
3	E	106/118 (90%)	104 (98%)	2 (2%)	0	100	100
3	G	109/118 (92%)	107 (98%)	2 (2%)	0	100	100
3	H	108/118 (92%)	106 (98%)	2 (2%)	0	100	100
All	All	2080/2108 (99%)	2025 (97%)	51 (2%)	4 (0%)	43	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	94	PHE
1	A	32	ASP
1	A	23	VAL
3	C	143	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	332/327 (102%)	321 (97%)	11 (3%)	33	18
2	B	332/327 (102%)	318 (96%)	14 (4%)	26	12
2	D	329/327 (101%)	315 (96%)	14 (4%)	26	11
2	F	340/327 (104%)	321 (94%)	19 (6%)	19	6
3	C	88/100 (88%)	77 (88%)	11 (12%)	4	0
3	E	90/100 (90%)	85 (94%)	5 (6%)	19	6
3	G	93/100 (93%)	84 (90%)	9 (10%)	8	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	H	92/100 (92%)	88 (96%)	4 (4%)	26	11
All	All	1696/1708 (99%)	1609 (95%)	87 (5%)	22	7

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
1	A	29	SER
1	A	32	ASP
1	A	72	ASP
1	A	78	GLN
1	A	118	LEU
1	A	246	ASN
1	A	318	ASN
1	A	376	LEU
1	A	385	ASN
1	A	397	MET
2	B	22	GLU
2	B	31	VAL
2	B	33	SER
2	B	78	GLN
2	B	149	SER
2	B	177	GLN
2	B	223	ARG
2	B	318	ASN
2	B	332[A]	SER
2	B	332[B]	SER
2	B	376	LEU
2	B	385	ASN
2	B	418	ASP
2	B	421	VAL
3	C	94	PHE
3	C	96	ARG
3	C	101	TYR
3	C	102	LYS
3	C	131	MET
3	C	136	LYS
3	C	138	VAL
3	C	141	ASP
3	C	145	ILE
3	C	152	LYS
3	C	159	ASP

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Mol	Chain	Res	Type
2	D	52	GLU
2	D	78	GLN
2	D	84	GLN
2	D	139	GLN
2	D	141	LEU
2	D	177	GLN
2	D	223	ARG
2	D	281	ARG
2	D	318	ASN
2	D	376	LEU
2	D	385	ASN
2	D	409	ARG
2	D	417[A]	THR
2	D	417[B]	THR
3	E	75	LEU
3	E	77	LYS
3	E	102	LYS
3	E	136	LYS
3	E	145	ILE
2	F	23	VAL
2	F	43	GLN
2	F	72	ASP
2	F	78	GLN
2	F	84	GLN
2	F	139	GLN
2	F	174	ASN
2	F	177	GLN
2	F	223	ARG
2	F	233	ASN
2	F	318	ASN
2	F	328	THR
2	F	332[A]	SER
2	F	332[B]	SER
2	F	362	ASP
2	F	376	LEU
2	F	385	ASN
2	F	392[A]	SER
2	F	392[B]	SER
3	G	80	ILE
3	G	82	SER
3	G	86	GLN
3	G	87[A]	MET

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Mol	Chain	Res	Type
3	G	87[B]	MET
3	G	141	ASP
3	G	145	ILE
3	G	155	VAL
3	G	174	LEU
3	H	75	LEU
3	H	139	SER
3	H	145	ILE
3	H	174	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	107	ASN
1	A	113	ASN
1	A	137	ASN
1	A	146	HIS
1	A	192	GLN
1	A	200	GLN
1	A	229	GLN
1	A	318	ASN
1	A	385	ASN
2	B	146	HIS
2	B	279	GLN
2	B	300	GLN
2	B	318	ASN
2	B	320	ASN
2	B	325	GLN
2	B	335	GLN
2	B	352	ASN
2	B	356	GLN
2	B	357	HIS
2	B	385	ASN
2	B	395	GLN
3	C	134	GLN
3	C	142	GLN
2	D	113	ASN
2	D	139	GLN
2	D	146	HIS
2	D	200	GLN
2	D	229	GLN

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Mol	Chain	Res	Type
2	D	269	ASN
2	D	279	GLN
2	D	300	GLN
2	D	301	ASN
2	D	308	GLN
2	D	313	GLN
2	D	318	ASN
2	D	333	GLN
2	D	352	ASN
2	D	356	GLN
2	D	357	HIS
2	D	369	GLN
2	D	385	ASN
2	D	395	GLN
2	D	402	ASN
2	D	420	GLN
3	E	127	ASN
3	E	134	GLN
2	F	43	GLN
2	F	84	GLN
2	F	87	GLN
2	F	103	GLN
2	F	117	GLN
2	F	139	GLN
2	F	146	HIS
2	F	174	ASN
2	F	200	GLN
2	F	229	GLN
2	F	233	ASN
2	F	269	ASN
2	F	308	GLN
2	F	318	ASN
2	F	325	GLN
2	F	333	GLN
2	F	355	GLN
2	F	356	GLN
2	F	357	HIS
2	F	369	GLN
2	F	385	ASN
2	F	395	GLN
2	F	402	ASN
3	G	67	GLN

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Mol	Chain	Res	Type
3	G	98	ASN
3	G	127	ASN
3	G	142	GLN
3	H	93	ASN
3	H	98	ASN
3	H	118	ASN
3	H	127	ASN
3	H	142	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](#)

19 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	$\# Z > 2$
5	GOL	B	1433	-	5,5,5	0.97	0	5,5,5	2.51	3 (60%)
6	ACT	A	1435	-	3,3,3	1.66	0	3,3,3	0.36	0
5	GOL	D	1432	-	5,5,5	0.89	0	5,5,5	0.82	0
5	GOL	D	1433	-	5,5,5	0.91	0	5,5,5	1.19	0
4	SO4	A	1433	-	4,4,4	0.30	0	6,6,6	0.60	0
4	SO4	D	1431	-	4,4,4	0.32	0	6,6,6	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	G	1175	-	4,4,4	0.37	0	6,6,6	0.25	0
6	ACT	B	1435	-	3,3,3	0.47	0	3,3,3	1.73	1 (33%)
6	ACT	D	1434	-	3,3,3	1.34	1 (33%)	3,3,3	0.33	0
5	GOL	B	1434	-	5,5,5	0.69	0	5,5,5	1.16	0
4	SO4	A	1431	-	4,4,4	0.64	0	6,6,6	0.97	0
4	SO4	A	1432	-	4,4,4	0.21	0	6,6,6	0.35	0
5	GOL	F	1432	-	5,5,5	0.15	0	5,5,5	1.57	1 (20%)
4	SO4	B	1432	-	4,4,4	0.19	0	6,6,6	0.48	0
4	SO4	B	1431	-	4,4,4	0.33	0	6,6,6	0.40	0
4	SO4	F	1431	-	4,4,4	0.30	0	6,6,6	0.56	0
5	GOL	C	1174	-	5,5,5	0.37	0	5,5,5	0.81	0
5	GOL	A	1434	-	5,5,5	0.63	0	5,5,5	1.53	1 (20%)
6	ACT	H	1175	-	3,3,3	0.80	0	3,3,3	1.28	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
5	GOL	B	1433	-	-	3/4/4/4	-
5	GOL	D	1433	-	-	2/4/4/4	-
5	GOL	F	1432	-	-	2/4/4/4	-
5	GOL	D	1432	-	-	0/4/4/4	-
5	GOL	A	1434	-	-	2/4/4/4	-
5	GOL	B	1434	-	-	2/4/4/4	-
5	GOL	C	1174	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1434	ACT	O-C	2.03	1.31	1.22

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1433	GOL	O2-C2-C3	4.69	128.58	109.18
5	A	1434	GOL	O2-C2-C1	-2.87	97.30	109.18
5	F	1432	GOL	C3-C2-C1	-2.72	101.81	111.80
6	B	1435	ACT	OXT-C-CH3	2.27	124.56	115.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1433	GOL	O3-C3-C2	2.10	119.81	110.38
5	B	1433	GOL	O1-C1-C2	-2.09	100.98	110.38

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1434	GOL	C1-C2-C3-O3
5	B	1433	GOL	O1-C1-C2-C3
5	B	1434	GOL	C1-C2-C3-O3
5	C	1174	GOL	O1-C1-C2-C3
5	D	1433	GOL	O1-C1-C2-C3
5	F	1432	GOL	C1-C2-C3-O3
5	F	1432	GOL	O2-C2-C3-O3
5	A	1434	GOL	O2-C2-C3-O3
5	B	1433	GOL	O1-C1-C2-O2
5	C	1174	GOL	O1-C1-C2-O2
5	B	1434	GOL	O2-C2-C3-O3
5	B	1433	GOL	C1-C2-C3-O3
5	D	1433	GOL	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1433	GOL	2	0
6	A	1435	ACT	8	0
5	D	1433	GOL	5	0
6	B	1435	ACT	10	0
6	D	1434	ACT	6	0
5	B	1434	GOL	3	0
5	F	1432	GOL	3	0
5	C	1174	GOL	8	0
5	A	1434	GOL	4	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	409/409 (100%)	-0.41	7 (1%) 69 73	4, 14, 30, 48	6 (1%)
2	B	409/409 (100%)	-0.35	5 (1%) 76 80	6, 15, 31, 54	5 (1%)
2	D	409/409 (100%)	-0.42	2 (0%) 87 90	7, 15, 30, 39	3 (0%)
2	F	409/409 (100%)	-0.44	1 (0%) 91 93	5, 15, 29, 40	13 (3%)
3	C	104/118 (88%)	0.69	14 (13%) 7 6	11, 28, 55, 61	2 (1%)
3	E	107/118 (90%)	0.20	4 (3%) 45 49	10, 23, 42, 49	1 (0%)
3	G	108/118 (91%)	0.29	8 (7%) 20 22	10, 24, 46, 55	3 (2%)
3	H	108/118 (91%)	0.14	2 (1%) 66 70	7, 21, 43, 50	2 (1%)
All	All	2063/2108 (97%)	-0.25	43 (2%) 63 67	4, 16, 37, 61	35 (1%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	94	PHE	6.7
3	E	76	ASP	6.2
1	A	31	VAL	5.6
3	C	101	TYR	5.0
1	A	30	GLY	4.6
2	B	30	GLY	4.2
3	C	92	ALA	4.1
1	A	45	ALA	4.0
3	E	75	LEU	3.9
3	C	140	ALA	3.9
2	B	32	ASP	3.8
3	E	78	TYR	3.8
2	B	31	VAL	3.8
3	C	133	LEU	3.4
1	A	32	ASP	3.3
3	C	78	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
2	F	45	ALA	3.2
3	C	95	LEU	3.0
3	G	78	TYR	3.0
3	C	138	VAL	3.0
3	C	139	SER	2.9
3	G	101	TYR	2.9
3	H	174	LEU	2.9
2	B	33	SER	2.7
3	H	78	TYR	2.7
3	C	97	SER	2.7
3	C	142	GLN	2.6
2	D	49	ALA	2.6
3	C	100	SER	2.6
2	D	352	ASN	2.6
2	B	174	ASN	2.5
1	A	33	SER	2.5
3	G	141	ASP	2.4
3	G	174	LEU	2.4
3	E	77	LYS	2.4
3	G	95	LEU	2.3
3	G	99	PRO	2.3
3	C	137	GLY	2.3
3	G	137	GLY	2.3
3	C	172[A]	VAL	2.3
1	A	140	TRP	2.2
1	A	329	TRP	2.2
3	G	81	ARG	2.2

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
5	GOL	D	1433	6/6	0.72	0.18	35,36,37,41	0
4	SO4	G	1175	5/5	0.78	0.14	60,61,62,65	0
4	SO4	A	1433	5/5	0.78	0.14	57,58,60,61	0
6	ACT	A	1435	4/4	0.78	0.14	10,16,16,20	0
5	GOL	A	1434	6/6	0.84	0.13	33,34,36,39	0
4	SO4	F	1431	5/5	0.85	0.16	79,81,82,82	0
4	SO4	D	1431	5/5	0.87	0.12	48,48,49,50	0
5	GOL	B	1434	6/6	0.87	0.12	31,34,35,40	0
6	ACT	B	1435	4/4	0.87	0.12	12,17,17,19	0
4	SO4	B	1431	5/5	0.88	0.10	50,52,54,54	0
4	SO4	A	1431	5/5	0.88	0.22	21,28,40,43	0
5	GOL	C	1174	6/6	0.88	0.12	35,37,39,42	0
5	GOL	D	1432	6/6	0.89	0.12	27,32,35,38	0
5	GOL	F	1432	6/6	0.89	0.12	28,31,34,38	0
5	GOL	B	1433	6/6	0.90	0.14	16,22,25,30	0
4	SO4	A	1432	5/5	0.90	0.13	69,70,71,71	0
4	SO4	B	1432	5/5	0.91	0.09	54,56,57,58	0
6	ACT	D	1434	4/4	0.94	0.08	10,13,14,16	0
6	ACT	H	1175	4/4	0.96	0.07	16,18,18,18	0

6.5 Other polymers ⓘ

There are no such residues in this entry.