



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:41 PM UTC

PDB ID : 5NFY / pdb_00005nfy
Title : SARS-CoV nsp10/nsp14 dynamic complex
Authors : Ferron, F.; Gluais, L.; Vonnrhein, C.; Bricogne, G.; Canard, B.; Imbert, I.
Deposited on : 2017-03-16
Resolution : 3.38 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:

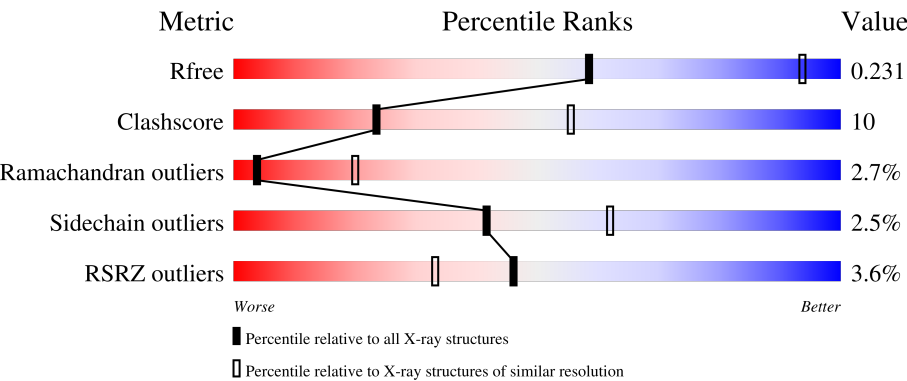
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.38 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	1047 (3.42-3.34)
Clashscore	190562	1067 (3.42-3.34)
Ramachandran outliers	187476	1056 (3.42-3.34)
Sidechain outliers	187428	1056 (3.42-3.34)
RSRZ outliers	180081	1047 (3.42-3.34)

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	534	2% 79% 13% ...
1	B	534	4% 76% 16% ...
1	C	534	2% 80% 12% ...
1	D	534	6% 78% 14% ...
2	M	138	% 80% 15% ..

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Mol	Chain	Length	Quality of chain
2	N	138	% 79% 16% ..
2	O	138	6% 80% 13% ..
2	P	138	2% 83% 12% ..

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
3	ZN	P	201	-	-	X	-
4	PEG	A	604	-	-	X	-
4	PEG	C	604	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20625 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 Polyprotein 1ab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	512	Total	C	N	O	S	0	0	0
			4098	2626	702	734	36			
1	B	514	Total	C	N	O	S	0	0	0
			4112	2634	704	738	36			
1	C	514	Total	C	N	O	S	0	0	0
			4112	2634	704	738	36			
1	D	514	Total	C	N	O	S	0	0	0
			4112	2634	704	738	36			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP Q1T6X8
A	-5	HIS	-	expression tag	UNP Q1T6X8
A	-4	HIS	-	expression tag	UNP Q1T6X8
A	-3	HIS	-	expression tag	UNP Q1T6X8
A	-2	HIS	-	expression tag	UNP Q1T6X8
A	-1	HIS	-	expression tag	UNP Q1T6X8
A	0	HIS	-	expression tag	UNP Q1T6X8
B	-6	MET	-	initiating methionine	UNP Q1T6X8
B	-5	HIS	-	expression tag	UNP Q1T6X8
B	-4	HIS	-	expression tag	UNP Q1T6X8
B	-3	HIS	-	expression tag	UNP Q1T6X8
B	-2	HIS	-	expression tag	UNP Q1T6X8
B	-1	HIS	-	expression tag	UNP Q1T6X8
B	0	HIS	-	expression tag	UNP Q1T6X8
C	-6	MET	-	initiating methionine	UNP Q1T6X8
C	-5	HIS	-	expression tag	UNP Q1T6X8
C	-4	HIS	-	expression tag	UNP Q1T6X8
C	-3	HIS	-	expression tag	UNP Q1T6X8
C	-2	HIS	-	expression tag	UNP Q1T6X8
C	-1	HIS	-	expression tag	UNP Q1T6X8
C	0	HIS	-	expression tag	UNP Q1T6X8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	MET	-	initiating methionine	UNP Q1T6X8
D	-5	HIS	-	expression tag	UNP Q1T6X8
D	-4	HIS	-	expression tag	UNP Q1T6X8
D	-3	HIS	-	expression tag	UNP Q1T6X8
D	-2	HIS	-	expression tag	UNP Q1T6X8
D	-1	HIS	-	expression tag	UNP Q1T6X8
D	0	HIS	-	expression tag	UNP Q1T6X8

- Molecule 2 is a protein called Polyprotein 1ab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	132	Total	C	N	O	S	0	0	0
			969	601	165	187	16			
2	N	133	Total	C	N	O	S	0	0	0
			979	607	168	188	16			
2	O	133	Total	C	N	O	S	0	0	0
			979	607	168	188	16			
2	P	133	Total	C	N	O	S	0	0	0
			979	607	168	188	16			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-6	MET	-	initiating methionine	UNP Q1T6X8
M	-5	HIS	-	expression tag	UNP Q1T6X8
M	-4	HIS	-	expression tag	UNP Q1T6X8
M	-3	HIS	-	expression tag	UNP Q1T6X8
M	-2	HIS	-	expression tag	UNP Q1T6X8
M	-1	HIS	-	expression tag	UNP Q1T6X8
M	0	HIS	-	expression tag	UNP Q1T6X8
N	-6	MET	-	initiating methionine	UNP Q1T6X8
N	-5	HIS	-	expression tag	UNP Q1T6X8
N	-4	HIS	-	expression tag	UNP Q1T6X8
N	-3	HIS	-	expression tag	UNP Q1T6X8
N	-2	HIS	-	expression tag	UNP Q1T6X8
N	-1	HIS	-	expression tag	UNP Q1T6X8
N	0	HIS	-	expression tag	UNP Q1T6X8
O	-6	MET	-	initiating methionine	UNP Q1T6X8
O	-5	HIS	-	expression tag	UNP Q1T6X8
O	-4	HIS	-	expression tag	UNP Q1T6X8
O	-3	HIS	-	expression tag	UNP Q1T6X8
O	-2	HIS	-	expression tag	UNP Q1T6X8

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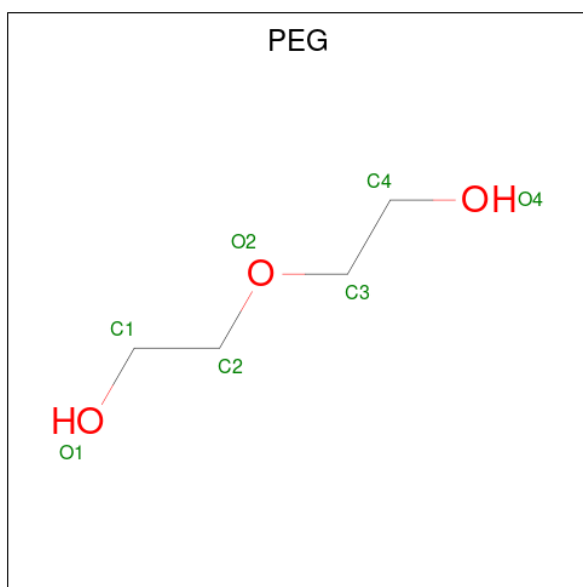
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Chain	Residue	Modelled	Actual	Comment	Reference
O	-1	HIS	-	expression tag	UNP Q1T6X8
O	0	HIS	-	expression tag	UNP Q1T6X8
P	-6	MET	-	initiating methionine	UNP Q1T6X8
P	-5	HIS	-	expression tag	UNP Q1T6X8
P	-4	HIS	-	expression tag	UNP Q1T6X8
P	-3	HIS	-	expression tag	UNP Q1T6X8
P	-2	HIS	-	expression tag	UNP Q1T6X8
P	-1	HIS	-	expression tag	UNP Q1T6X8
P	0	HIS	-	expression tag	UNP Q1T6X8

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total 3	Zn 3	0	0
3	B	3	Total 3	Zn 3	0	0
3	C	3	Total 3	Zn 3	0	0
3	D	3	Total 3	Zn 3	0	0
3	M	2	Total 2	Zn 2	0	0
3	N	2	Total 2	Zn 2	0	0
3	O	2	Total 2	Zn 2	0	0
3	P	2	Total 2	Zn 2	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		

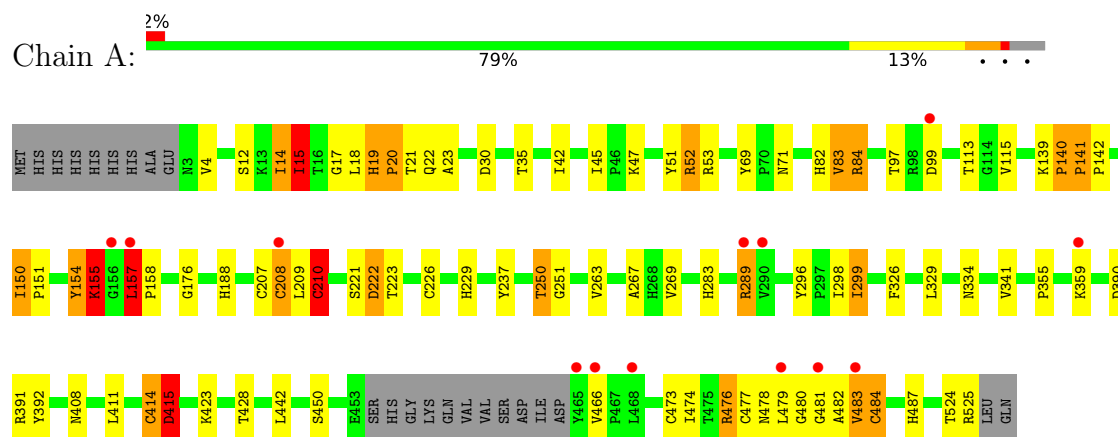
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	59	Total	O	0	0
			59	59		
5	B	56	Total	O	0	0
			56	56		
5	C	67	Total	O	0	0
			67	67		
5	D	34	Total	O	0	0
			34	34		
5	M	7	Total	O	0	0
			7	7		
5	N	6	Total	O	0	0
			6	6		
5	O	7	Total	O	0	0
			7	7		
5	P	8	Total	O	0	0
			8	8		

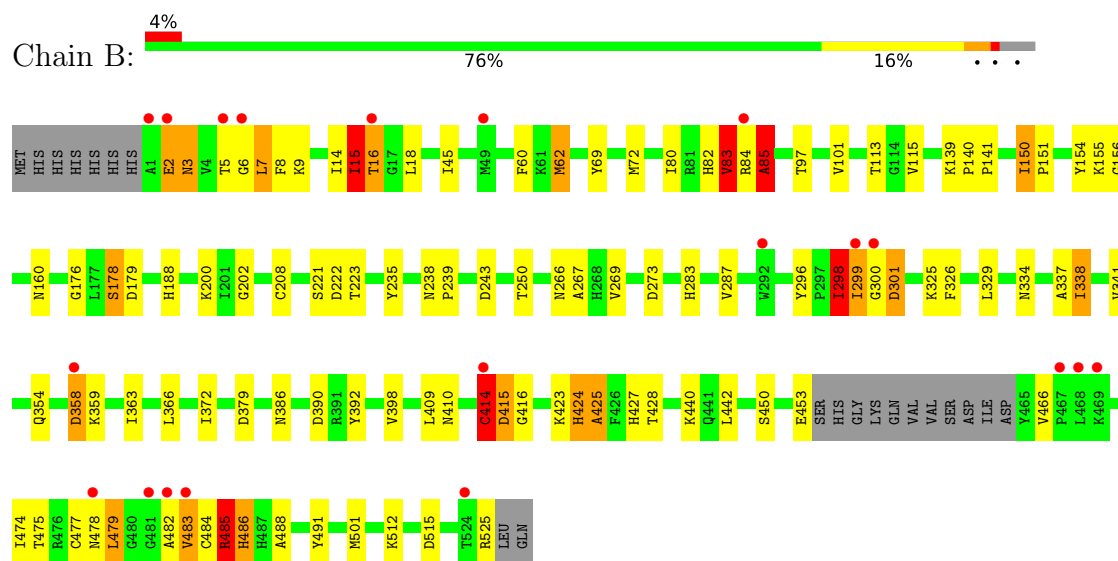
3 Residue-property plots [i](#)

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.

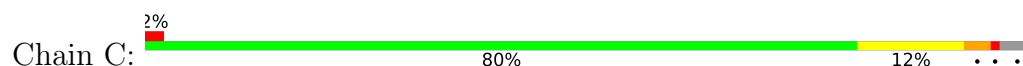
• Molecule 1: Polyprotein 1ab

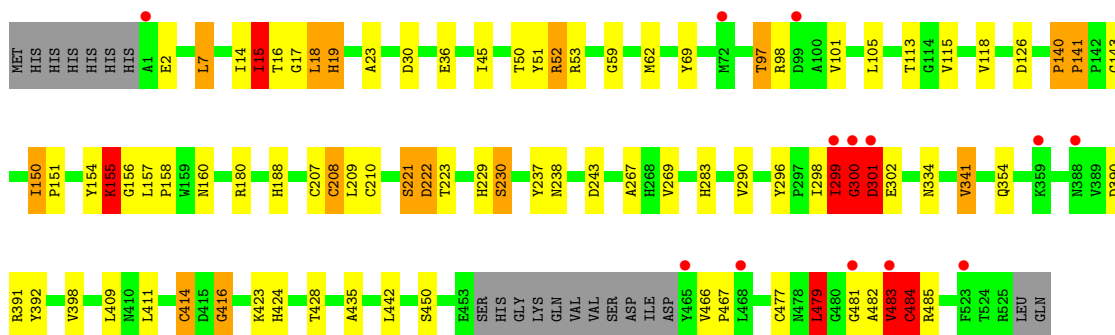


• Molecule 1: Polyprotein 1ab

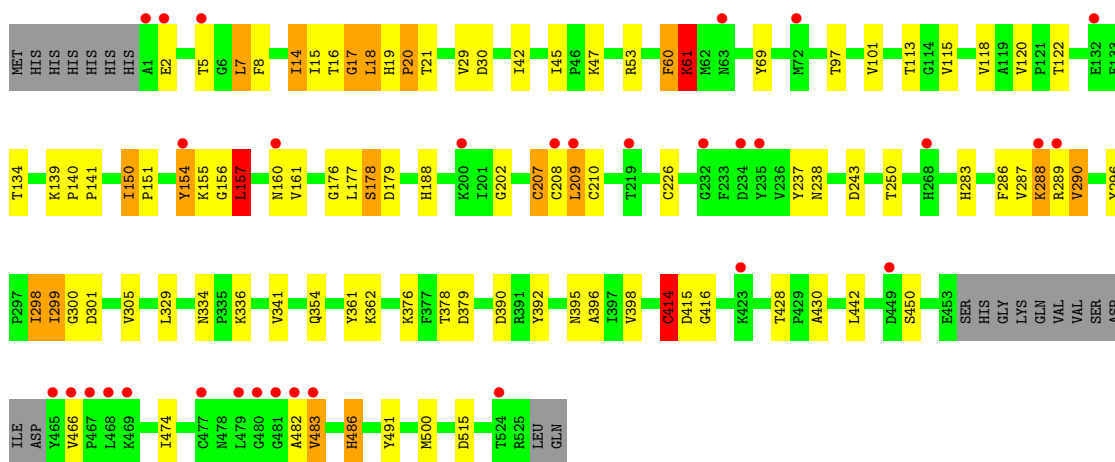
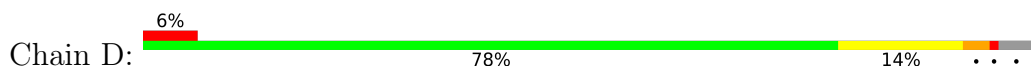


• Molecule 1: Polyprotein 1ab

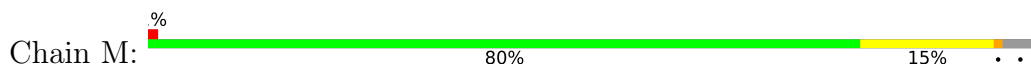




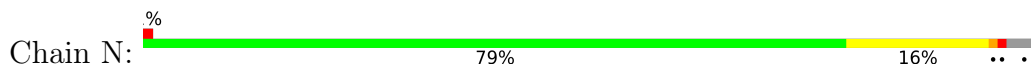
• Molecule 1: Polyprotein 1ab



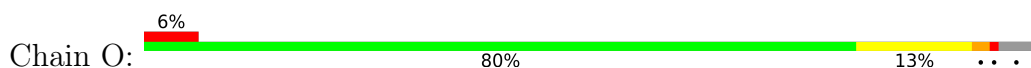
• Molecule 2: Polyprotein 1ab



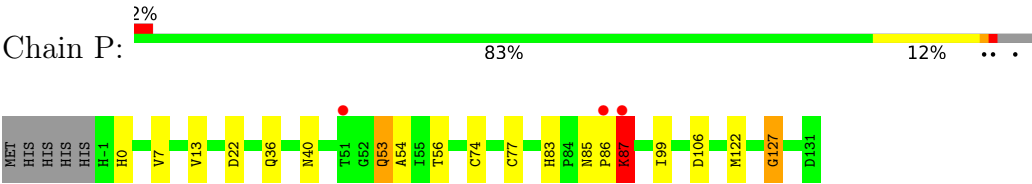
• Molecule 2: Polyprotein 1ab



• Molecule 2: Polyprotein 1ab



● Molecule 2: Polyprotein 1ab



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	185.88Å 189.79Å 196.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.40 – 3.38 66.40 – 3.38	Depositor EDS
% Data completeness (in resolution range)	99.5 (66.40-3.38) 99.5 (66.40-3.38)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 3.41Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.193 , 0.235 0.201 , 0.231	Depositor DCC
R_{free} test set	4907 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	100.4	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 76.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.004 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20625	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.85 % 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 6.4350e-03. 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: PEG, ZN

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	1.00	2/4215 (0.0%)	1.42	59/5727 (1.0%)
1	B	1.00	4/4229 (0.1%)	1.39	65/5746 (1.1%)
1	C	1.02	7/4229 (0.2%)	1.39	66/5746 (1.1%)
1	D	0.96	3/4229 (0.1%)	1.37	58/5746 (1.0%)
2	M	0.91	1/992 (0.1%)	1.44	16/1350 (1.2%)
2	N	0.92	0/1003	1.40	14/1365 (1.0%)
2	O	0.84	0/1003	1.40	17/1365 (1.2%)
2	P	0.90	0/1003	1.47	20/1365 (1.5%)
All	All	0.98	17/20903 (0.1%)	1.40	315/28410 (1.1%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	141	PRO	CA-C	8.56	1.56	1.51
1	C	98	ARG	CA-C	-8.09	1.47	1.52
1	A	474	ILE	CA-C	-6.21	1.46	1.53
1	B	424	HIS	CA-C	6.17	1.61	1.52
1	C	222	ASP	N-CA	5.88	1.53	1.46
1	B	141	PRO	CA-C	5.80	1.55	1.51
1	A	391	ARG	CA-C	5.62	1.59	1.52
1	C	423	LYS	CA-C	-5.57	1.45	1.52
1	C	180	ARG	CA-CB	-5.44	1.46	1.53
1	B	62	MET	CA-CB	-5.34	1.46	1.52
1	C	221	SER	CA-C	-5.28	1.46	1.53
1	D	61	LYS	CA-C	5.25	1.59	1.52
2	M	9	ALA	CA-C	-5.23	1.45	1.52
1	D	474	ILE	CA-C	-5.12	1.48	1.53
1	C	484	CYS	CA-CB	-5.11	1.44	1.53
1	D	430	ALA	CA-C	-5.05	1.46	1.52
1	B	474	ILE	CA-C	-5.03	1.48	1.53

All (315) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	LEU	CA-C-N	11.99	132.11	119.76
1	A	157	LEU	C-N-CA	11.99	132.11	119.76
1	D	140	PRO	CA-C-N	11.50	128.06	119.66
1	D	140	PRO	C-N-CA	11.50	128.06	119.66
1	A	466	VAL	CA-C-N	10.43	130.53	120.31
1	A	466	VAL	C-N-CA	10.43	130.53	120.31
1	D	141	PRO	CA-C-N	10.41	130.07	119.24
1	D	141	PRO	C-N-CA	10.41	130.07	119.24
1	B	392	TYR	CA-C-N	9.92	129.85	120.03
1	B	392	TYR	C-N-CA	9.92	129.85	120.03
1	A	141	PRO	CA-C-N	9.91	130.62	119.32
1	A	141	PRO	C-N-CA	9.91	130.62	119.32
1	C	113	THR	N-CA-C	-9.81	97.88	110.53
1	B	141	PRO	CA-C-N	9.78	129.42	119.24
1	B	141	PRO	C-N-CA	9.78	129.42	119.24
1	B	140	PRO	CA-C-N	9.69	126.73	119.66
1	B	140	PRO	C-N-CA	9.69	126.73	119.66
1	C	141	PRO	CA-C-N	9.58	131.82	119.84
1	C	141	PRO	C-N-CA	9.58	131.82	119.84
1	D	296	TYR	CA-C-N	9.40	129.34	120.03
1	D	296	TYR	C-N-CA	9.40	129.34	120.03
2	O	22	ASP	CA-C-N	9.40	129.01	119.24
2	O	22	ASP	C-N-CA	9.40	129.01	119.24
2	N	22	ASP	CA-C-N	9.34	128.96	119.24
2	N	22	ASP	C-N-CA	9.34	128.96	119.24
1	C	301	ASP	N-CA-C	-9.29	91.00	110.80
1	C	423	LYS	N-CA-C	-9.27	91.80	108.48
1	D	392	TYR	CA-C-N	9.15	129.09	119.85
1	D	392	TYR	C-N-CA	9.15	129.09	119.85
1	D	60	PHE	N-CA-C	9.05	125.85	113.37
1	B	7	LEU	N-CA-C	-9.03	97.71	110.35
1	C	296	TYR	CA-C-N	8.97	128.82	120.21
1	C	296	TYR	C-N-CA	8.97	128.82	120.21
1	A	140	PRO	CA-C-N	8.84	126.11	119.66
1	A	140	PRO	C-N-CA	8.84	126.11	119.66
2	M	106	ASP	CA-C-N	8.80	128.12	118.97
2	M	106	ASP	C-N-CA	8.80	128.12	118.97
2	P	106	ASP	CA-C-N	8.76	128.77	119.05
2	P	106	ASP	C-N-CA	8.76	128.77	119.05
2	O	7	VAL	CA-C-N	8.65	129.18	119.32
2	O	7	VAL	C-N-CA	8.65	129.18	119.32
1	A	296	TYR	CA-C-N	8.57	128.44	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	TYR	C-N-CA	8.57	128.44	120.21
1	C	140	PRO	CA-C-N	8.55	125.90	119.66
1	C	140	PRO	C-N-CA	8.55	125.90	119.66
1	B	341	VAL	CA-C-N	8.49	129.00	119.32
1	B	341	VAL	C-N-CA	8.49	129.00	119.32
1	B	334	ASN	CA-C-N	8.48	129.20	120.04
1	B	334	ASN	C-N-CA	8.48	129.20	120.04
1	A	423	LYS	N-CA-C	-8.47	95.43	109.24
1	C	334	ASN	CA-C-N	8.47	128.68	119.87
1	C	334	ASN	C-N-CA	8.47	128.68	119.87
2	O	36	GLN	CA-C-N	8.43	128.38	120.03
2	O	36	GLN	C-N-CA	8.43	128.38	120.03
2	N	7	VAL	CA-C-N	8.37	128.49	119.28
2	N	7	VAL	C-N-CA	8.37	128.49	119.28
1	C	237	TYR	CA-C-N	-8.25	114.00	122.74
1	C	237	TYR	C-N-CA	-8.25	114.00	122.74
1	C	466	VAL	CA-C-N	8.24	128.18	119.85
1	C	466	VAL	C-N-CA	8.24	128.18	119.85
1	A	139	LYS	CA-C-N	8.19	125.56	119.66
1	A	139	LYS	C-N-CA	8.19	125.56	119.66
1	C	392	TYR	CA-C-N	8.19	128.12	119.85
1	C	392	TYR	C-N-CA	8.19	128.12	119.85
2	M	36	GLN	CA-C-N	8.16	128.09	119.85
2	M	36	GLN	C-N-CA	8.16	128.09	119.85
2	P	7	VAL	CA-C-N	8.14	130.02	119.84
2	P	7	VAL	C-N-CA	8.14	130.02	119.84
1	B	442	LEU	CA-C-N	8.11	128.06	120.03
1	B	442	LEU	C-N-CA	8.11	128.06	120.03
2	P	36	GLN	CA-C-N	8.08	128.03	120.03
2	P	36	GLN	C-N-CA	8.08	128.03	120.03
2	N	83	HIS	CA-C-N	8.08	128.27	119.87
2	N	83	HIS	C-N-CA	8.08	128.27	119.87
1	A	450	SER	CA-C-N	8.00	128.01	119.78
1	A	450	SER	C-N-CA	8.00	128.01	119.78
2	P	83	HIS	CA-C-N	7.97	127.61	119.56
2	P	83	HIS	C-N-CA	7.97	127.61	119.56
1	B	115	VAL	N-CA-C	7.96	119.25	109.30
1	C	341	VAL	CA-C-N	7.96	128.40	119.32
1	C	341	VAL	C-N-CA	7.96	128.40	119.32
1	D	450	SER	CA-C-N	7.89	127.82	119.85
1	D	450	SER	C-N-CA	7.89	127.82	119.85
1	A	115	VAL	N-CA-C	7.89	119.16	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	392	TYR	CA-C-N	7.81	127.74	119.85
1	A	392	TYR	C-N-CA	7.81	127.74	119.85
1	B	178	SER	N-CA-C	7.73	118.19	108.45
1	D	341	VAL	CA-C-N	7.69	127.74	119.28
1	D	341	VAL	C-N-CA	7.69	127.74	119.28
1	B	296	TYR	CA-C-N	7.68	127.64	120.03
1	B	296	TYR	C-N-CA	7.68	127.64	120.03
1	A	334	ASN	CA-C-N	7.68	127.86	119.87
1	A	334	ASN	C-N-CA	7.68	127.86	119.87
1	B	85	ALA	N-CA-C	-7.64	94.52	110.80
1	D	69	TYR	CA-C-N	7.64	127.56	119.85
1	D	69	TYR	C-N-CA	7.64	127.56	119.85
1	D	334	ASN	CA-C-N	7.58	128.87	120.45
1	D	334	ASN	C-N-CA	7.58	128.87	120.45
2	M	22	ASP	CA-C-N	7.56	127.44	119.05
2	M	22	ASP	C-N-CA	7.56	127.44	119.05
2	N	36	GLN	CA-C-N	7.54	127.49	120.03
2	N	36	GLN	C-N-CA	7.54	127.49	120.03
1	B	428	THR	CA-C-N	7.53	127.49	120.03
1	B	428	THR	C-N-CA	7.53	127.49	120.03
2	P	22	ASP	CA-C-N	7.53	127.18	119.19
2	P	22	ASP	C-N-CA	7.53	127.18	119.19
1	D	160	ASN	CA-C-N	7.52	130.18	120.56
1	D	160	ASN	C-N-CA	7.52	130.18	120.56
1	C	115	VAL	N-CA-C	7.49	119.24	109.58
1	A	42	ILE	CA-C-N	7.47	127.18	119.56
1	A	42	ILE	C-N-CA	7.47	127.18	119.56
1	B	466	VAL	CA-C-N	7.43	129.12	119.84
1	B	466	VAL	C-N-CA	7.43	129.12	119.84
1	D	113	THR	N-CA-C	-7.30	98.40	109.79
1	D	442	LEU	CA-C-N	7.26	127.22	120.03
1	D	442	LEU	C-N-CA	7.26	127.22	120.03
1	B	97	THR	N-CA-C	7.24	126.21	110.80
1	A	442	LEU	CA-C-N	7.23	127.18	120.03
1	A	442	LEU	C-N-CA	7.23	127.18	120.03
2	M	13	VAL	CB-CA-C	-7.23	102.63	111.88
1	C	97	THR	N-CA-C	7.20	126.14	110.80
1	C	45	ILE	CA-C-N	7.15	127.07	119.85
1	C	45	ILE	C-N-CA	7.15	127.07	119.85
1	B	269	VAL	N-CA-C	7.13	119.71	109.51
1	B	354	GLN	CA-C-N	7.08	126.84	119.76
1	B	354	GLN	C-N-CA	7.08	126.84	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	VAL	CA-C-N	7.07	126.77	119.56
1	A	341	VAL	C-N-CA	7.07	126.77	119.56
1	B	45	ILE	CA-C-N	7.04	127.00	120.03
1	B	45	ILE	C-N-CA	7.04	127.00	120.03
1	A	487	HIS	CA-CB-CG	7.01	120.81	113.80
2	M	6	GLU	N-CA-C	7.00	120.52	109.81
1	A	222	ASP	CA-CB-CG	6.97	119.57	112.60
1	C	354	GLN	CA-C-N	6.96	126.93	119.76
1	C	354	GLN	C-N-CA	6.96	126.93	119.76
1	C	442	LEU	CA-C-N	6.91	127.09	120.31
1	C	442	LEU	C-N-CA	6.91	127.09	120.31
2	M	99	ILE	CA-C-N	6.89	128.45	119.84
2	M	99	ILE	C-N-CA	6.89	128.45	119.84
1	C	126	ASP	CA-CB-CG	6.87	119.47	112.60
1	A	99	ASP	CA-CB-CG	6.86	119.46	112.60
1	A	157	LEU	N-CA-C	6.85	114.17	108.07
1	B	150	ILE	CA-C-N	6.85	127.12	119.32
1	B	150	ILE	C-N-CA	6.85	127.12	119.32
1	A	69	TYR	CA-C-N	6.83	126.75	119.85
1	A	69	TYR	C-N-CA	6.83	126.75	119.85
1	A	411	LEU	CA-C-N	6.83	126.82	119.78
1	A	411	LEU	C-N-CA	6.83	126.82	119.78
1	C	188	HIS	N-CA-C	6.77	121.00	112.87
2	O	99	ILE	CA-C-N	6.77	128.31	119.84
2	O	99	ILE	C-N-CA	6.77	128.31	119.84
1	C	466	VAL	N-CA-C	6.77	113.72	107.56
1	D	115	VAL	N-CA-C	6.76	119.36	109.63
2	O	13	VAL	CB-CA-C	-6.75	103.34	111.97
1	A	45	ILE	CA-C-N	6.71	126.68	120.03
1	A	45	ILE	C-N-CA	6.71	126.68	120.03
2	P	13	VAL	CB-CA-C	-6.71	103.23	112.02
1	C	300	GLY	CA-C-N	-6.69	108.76	121.54
1	C	300	GLY	C-N-CA	-6.69	108.76	121.54
1	B	450	SER	CA-C-N	6.66	126.62	120.03
1	B	450	SER	C-N-CA	6.66	126.62	120.03
1	A	113	THR	N-CA-C	-6.64	99.42	109.79
1	A	237	TYR	CA-C-N	-6.63	110.55	122.28
1	A	237	TYR	C-N-CA	-6.63	110.55	122.28
1	D	237	TYR	CA-C-N	-6.62	114.53	123.46
1	D	237	TYR	C-N-CA	-6.62	114.53	123.46
1	B	16	THR	CB-CA-C	-6.61	107.93	115.79
1	A	154	TYR	N-CA-C	-6.60	96.75	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	CYS	N-CA-C	-6.59	101.39	110.35
2	O	106	ASP	CA-C-N	6.58	128.06	119.84
2	O	106	ASP	C-N-CA	6.58	128.06	119.84
1	D	45	ILE	CA-C-N	6.57	126.48	119.85
1	D	45	ILE	C-N-CA	6.57	126.48	119.85
1	B	266	ASN	N-CA-C	6.54	119.51	107.99
1	C	155	LYS	N-CA-C	-6.53	96.89	110.80
1	C	300	GLY	N-CA-C	6.53	128.65	113.18
2	M	58	THR	CA-C-N	6.53	126.92	119.93
2	M	58	THR	C-N-CA	6.53	126.92	119.93
2	O	85	ASN	CA-C-N	6.53	128.00	119.84
2	O	85	ASN	C-N-CA	6.53	128.00	119.84
1	B	358	ASP	N-CA-C	-6.52	100.63	110.28
1	C	97	THR	CA-C-N	-6.50	114.70	122.44
1	C	97	THR	C-N-CA	-6.50	114.70	122.44
1	B	113	THR	N-CA-C	-6.49	99.66	109.79
1	B	273	ASP	CA-CB-CG	6.44	119.04	112.60
1	C	69	TYR	CA-C-N	6.42	126.79	119.92
1	C	69	TYR	C-N-CA	6.42	126.79	119.92
2	P	99	ILE	CA-C-N	6.41	127.86	119.84
2	P	99	ILE	C-N-CA	6.41	127.86	119.84
1	B	69	TYR	CA-C-N	6.40	126.31	119.85
1	B	69	TYR	C-N-CA	6.40	126.31	119.85
1	B	60	PHE	N-CA-C	6.39	118.33	111.36
1	C	62	MET	CA-C-N	6.39	132.64	122.86
1	C	62	MET	C-N-CA	6.39	132.64	122.86
1	A	15	ILE	CB-CA-C	-6.38	103.14	111.88
1	A	188	HIS	N-CA-C	6.36	120.50	112.87
2	M	7	VAL	CA-C-N	6.33	127.75	119.84
2	M	7	VAL	C-N-CA	6.33	127.75	119.84
1	D	202	GLY	CA-C-N	6.32	126.29	120.03
1	D	202	GLY	C-N-CA	6.32	126.29	120.03
1	B	202	GLY	CA-C-N	6.27	126.18	119.85
1	B	202	GLY	C-N-CA	6.27	126.18	119.85
2	P	40	ASN	CA-CB-CG	6.25	118.85	112.60
1	D	150	ILE	CA-C-N	6.24	126.14	119.28
1	D	150	ILE	C-N-CA	6.24	126.14	119.28
1	D	238	ASN	CA-C-N	6.24	126.15	119.85
1	D	238	ASN	C-N-CA	6.24	126.15	119.85
2	N	99	ILE	CA-C-N	6.23	127.63	119.84
2	N	99	ILE	C-N-CA	6.23	127.63	119.84
1	C	150	ILE	CA-C-N	6.17	126.36	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	150	ILE	C-N-CA	6.17	126.36	119.32
2	M	83	HIS	CA-C-N	6.15	126.26	119.87
2	M	83	HIS	C-N-CA	6.15	126.26	119.87
1	C	237	TYR	N-CA-C	6.12	118.86	111.40
1	A	428	THR	CA-C-N	6.08	126.04	119.78
1	A	428	THR	C-N-CA	6.08	126.04	119.78
1	B	423	LYS	N-CA-C	-6.08	99.29	108.46
1	C	208	CYS	N-CA-C	-6.03	102.00	110.50
1	D	398	VAL	N-CA-C	6.02	116.79	108.12
1	D	396	ALA	N-CA-C	6.01	118.21	109.07
1	A	150	ILE	CA-C-N	6.01	125.89	119.28
1	A	150	ILE	C-N-CA	6.01	125.89	119.28
1	B	188	HIS	N-CA-C	5.95	120.08	112.34
2	P	87	LYS	N-CA-C	-5.94	104.50	110.97
1	D	139	LYS	CA-C-N	5.93	126.49	120.38
1	D	139	LYS	C-N-CA	5.93	126.49	120.38
1	D	188	HIS	N-CA-C	5.93	119.98	112.87
1	B	62	MET	CG-SD-CE	-5.92	87.88	100.90
1	A	267	ALA	N-CA-C	-5.91	102.91	110.53
1	D	354	GLN	CA-C-N	5.91	125.67	119.76
1	D	354	GLN	C-N-CA	5.91	125.67	119.76
1	C	19	HIS	CA-C-N	5.90	126.31	119.47
1	C	19	HIS	C-N-CA	5.90	126.31	119.47
1	C	269	VAL	N-CA-C	5.90	117.19	109.58
1	C	398	VAL	N-CA-C	5.86	116.55	108.12
1	C	428	THR	CA-C-N	5.86	125.76	119.85
1	C	428	THR	C-N-CA	5.86	125.76	119.85
1	B	160	ASN	CA-C-N	5.84	128.04	120.56
1	B	160	ASN	C-N-CA	5.84	128.04	120.56
1	C	238	ASN	CA-C-N	5.84	125.82	120.03
1	C	238	ASN	C-N-CA	5.84	125.82	120.03
1	B	287	VAL	N-CA-C	-5.84	107.22	112.12
1	D	378	THR	N-CA-C	5.82	117.62	111.28
1	A	269	VAL	N-CA-C	5.81	117.07	109.58
1	C	267	ALA	N-CA-C	-5.78	103.30	110.41
2	N	106	ASP	CA-C-N	5.76	125.61	119.28
2	N	106	ASP	C-N-CA	5.76	125.61	119.28
2	P	83	HIS	CA-CB-CG	-5.74	108.06	113.80
1	A	71	ASN	CA-CB-CG	5.73	118.33	112.60
1	D	428	THR	CA-C-N	5.73	125.70	120.03
1	D	428	THR	C-N-CA	5.73	125.70	120.03
1	A	97	THR	N-CA-C	5.73	123.00	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	51	THR	N-CA-C	-5.73	103.08	110.19
1	D	466	VAL	CA-C-N	5.69	126.58	119.98
1	D	466	VAL	C-N-CA	5.69	126.58	119.98
1	D	42	ILE	CA-C-N	5.68	126.94	119.84
1	D	42	ILE	C-N-CA	5.68	126.94	119.84
1	A	487	HIS	N-CA-CB	5.67	119.61	110.42
2	P	53	GLN	CB-CA-C	5.65	116.75	109.80
1	D	336	LYS	N-CA-C	-5.64	101.17	109.81
1	A	326	PHE	CA-C-N	5.64	126.89	119.84
1	A	326	PHE	C-N-CA	5.64	126.89	119.84
1	C	238	ASN	CA-CB-CG	5.64	118.24	112.60
1	C	484	CYS	N-CA-C	5.61	122.75	110.80
1	B	298	ILE	CB-CA-C	-5.58	105.88	111.80
1	B	366	LEU	N-CA-C	5.58	117.47	108.32
1	D	178	SER	N-CA-C	5.57	116.42	108.74
1	A	289	ARG	N-CA-C	5.56	122.64	110.80
1	D	289	ARG	N-CA-C	5.56	118.13	110.35
1	A	414	CYS	N-CA-C	5.55	117.71	110.43
1	B	409	LEU	CA-C-N	-5.53	113.77	122.73
1	B	409	LEU	C-N-CA	-5.53	113.77	122.73
1	C	450	SER	CA-C-N	5.50	125.40	119.85
1	C	450	SER	C-N-CA	5.50	125.40	119.85
1	B	84	ARG	N-CA-C	5.48	122.47	110.80
2	O	58	THR	CA-C-N	5.42	126.62	119.84
2	O	58	THR	C-N-CA	5.42	126.62	119.84
1	A	210	CYS	CA-CB-SG	5.42	126.86	114.40
1	C	238	ASN	N-CA-CB	5.40	117.79	111.09
1	B	424	HIS	CA-CB-CG	-5.40	108.40	113.80
1	C	160	ASN	CA-C-N	5.39	127.47	120.56
1	C	160	ASN	C-N-CA	5.39	127.47	120.56
1	B	326	PHE	CA-C-N	5.36	126.54	119.84
1	B	326	PHE	C-N-CA	5.36	126.54	119.84
1	C	105	LEU	CA-C-N	5.34	125.51	119.90
1	C	105	LEU	C-N-CA	5.34	125.51	119.90
1	B	208	CYS	N-CA-C	-5.31	102.66	110.52
1	D	17	GLY	N-CA-C	5.30	120.62	111.98
1	B	139	LYS	CA-C-N	5.25	125.79	120.38
1	B	139	LYS	C-N-CA	5.25	125.79	120.38
1	B	386	ASN	CA-CB-CG	-5.24	107.36	112.60
2	P	86	PRO	N-CA-C	-5.24	107.03	113.84
1	C	411	LEU	CA-C-N	5.23	125.48	119.83
1	C	411	LEU	C-N-CA	5.23	125.48	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	290	VAL	N-CA-C	5.23	120.22	109.34
2	P	54	ALA	N-CA-C	5.20	117.37	111.02
2	N	6	GLU	N-CA-C	5.18	117.75	110.14
1	D	305	VAL	N-CA-C	-5.16	107.37	111.81
1	C	230	SER	N-CA-C	5.14	121.76	110.80
1	C	416	GLY	N-CA-C	-5.14	108.23	115.32
1	D	336	LYS	CA-C-N	-5.14	116.11	123.20
1	D	336	LYS	C-N-CA	-5.14	116.11	123.20
2	O	116	VAL	N-CA-C	5.14	115.16	107.51
1	B	372	ILE	CB-CA-C	-5.13	105.47	111.94
1	B	363	ILE	N-CA-C	5.12	115.50	108.12
1	B	398	VAL	N-CA-C	5.10	115.46	108.12
1	B	325	LYS	N-CA-C	5.10	118.47	111.54
1	A	84	ARG	CA-C-N	5.08	127.80	120.38
1	A	84	ARG	C-N-CA	5.08	127.80	120.38
1	D	177	LEU	N-CA-C	5.08	116.82	111.28
1	D	97	THR	N-CA-C	5.06	121.58	110.80
2	O	40	ASN	CA-CB-CG	5.06	117.66	112.60
2	P	56	THR	N-CA-C	5.05	116.87	109.24
1	D	134	THR	N-CA-C	5.04	115.95	108.60
1	B	267	ALA	N-CA-C	-5.01	103.78	110.55

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	4098	0	3972	96	1
1	B	4112	0	3986	75	1
1	C	4112	0	3987	73	1
1	D	4112	0	3985	88	1
2	M	969	0	921	6	0
2	N	979	0	929	14	0
2	O	979	0	928	33	0
2	P	979	0	931	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	3	0	0	1	0
3	B	3	0	0	0	0
3	C	3	0	0	1	0
3	D	3	0	0	0	0
3	M	2	0	0	0	0
3	N	2	0	0	0	0
3	O	2	0	0	0	0
3	P	2	0	0	2	0
4	A	14	0	20	9	0
4	C	7	0	10	3	0
5	A	59	0	0	1	0
5	B	56	0	0	2	0
5	C	67	0	0	4	0
5	D	34	0	0	0	0
5	M	7	0	0	2	0
5	N	6	0	0	0	0
5	O	7	0	0	0	0
5	P	8	0	0	0	0
All	All	20625	0	19669	406	2

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 10.

All (406) 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:O:117:CYS:CB	2:O:124:LYS:HD2	1.45	1.46
1:A:477:CYS:SG	3:A:603:ZN:ZN	1.10	1.38
2:O:110:PHE:HE2	2:O:123:TRP:NE1	1.24	1.29
1:D:18:LEU:HD21	1:D:53:ARG:NE	1.45	1.29
2:O:117:CYS:CA	2:O:124:LYS:HD2	1.61	1.28
1:D:19:HIS:ND1	1:D:20:PRO:HD2	1.50	1.26
2:O:117:CYS:CA	2:O:124:LYS:CD	2.13	1.26
1:C:209:LEU:O	4:C:604:PEG:H41	1.28	1.26
1:D:157:LEU:CD2	1:D:161:VAL:HG11	1.65	1.24
1:C:210:CYS:SG	3:C:601:ZN:ZN	1.29	1.21
1:A:19:HIS:CD2	1:A:47:LYS:HB3	1.75	1.20
1:C:7:LEU:CD1	1:C:59:GLY:O	1.90	1.18
2:O:110:PHE:CE2	2:O:123:TRP:NE1	2.12	1.17
1:C:300:GLY:O	1:C:301:ASP:HB3	1.42	1.16
1:A:157:LEU:HG	1:A:158:PRO:HD2	1.18	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:467:PRO:CB	1:C:483:VAL:HG11	1.76	1.14
1:B:484:CYS:SG	5:B:717:HOH:O	2.07	1.12
1:C:209:LEU:O	4:C:604:PEG:C4	1.98	1.12
1:A:157:LEU:HD12	1:A:158:PRO:HD3	1.27	1.12
2:O:117:CYS:HB2	2:O:124:LYS:HD2	1.12	1.11
1:D:157:LEU:CD2	1:D:161:VAL:CG1	2.29	1.10
1:A:482:ALA:O	1:A:484:CYS:N	1.84	1.10
2:O:117:CYS:HA	2:O:124:LYS:CD	1.76	1.10
1:A:209:LEU:HA	4:A:604:PEG:H32	1.22	1.08
2:P:85:ASN:OD1	2:P:87:LYS:CB	2.02	1.07
1:C:7:LEU:CD1	1:C:59:GLY:C	2.28	1.07
1:D:157:LEU:HD21	1:D:161:VAL:HG11	1.11	1.06
1:A:18:LEU:HD21	1:A:53:ARG:HE	1.19	1.06
1:C:300:GLY:O	1:C:301:ASP:CB	1.99	1.06
1:B:176:GLY:O	1:B:299:ILE:CD1	2.04	1.05
2:O:117:CYS:HA	2:O:124:LYS:HD3	1.33	1.05
2:O:110:PHE:HE2	2:O:123:TRP:CD1	1.75	1.05
1:A:18:LEU:HD21	1:A:53:ARG:NE	1.72	1.05
1:B:15:ILE:HD13	1:B:15:ILE:H	1.20	1.04
1:C:7:LEU:HD13	1:C:59:GLY:O	1.51	1.04
2:O:110:PHE:CE2	2:O:123:TRP:CD1	2.46	1.03
2:O:117:CYS:H	2:O:124:LYS:HG2	1.22	1.02
1:A:19:HIS:HD2	1:A:47:LYS:CB	1.71	1.02
1:A:157:LEU:CG	1:A:158:PRO:HD2	1.90	1.01
1:C:467:PRO:HB2	1:C:483:VAL:HG11	1.43	1.01
1:A:263:VAL:HG21	1:A:415:ASP:O	1.61	1.00
2:P:85:ASN:OD1	2:P:87:LYS:N	1.92	1.00
1:C:482:ALA:C	1:C:484:CYS:H	1.65	0.99
1:A:19:HIS:HD2	1:A:47:LYS:HB3	1.09	0.99
1:C:482:ALA:O	1:C:484:CYS:N	1.95	0.99
1:C:483:VAL:O	1:C:485:ARG:N	1.96	0.98
1:B:414:CYS:O	1:B:416:GLY:N	1.95	0.98
1:D:7:LEU:CD1	1:D:8:PHE:CD1	2.47	0.98
1:D:18:LEU:CD2	1:D:53:ARG:NE	2.26	0.98
2:N:85:ASN:OD1	2:N:89:PHE:O	1.79	0.98
2:O:117:CYS:N	2:O:124:LYS:CG	2.26	0.98
1:D:18:LEU:CD2	1:D:53:ARG:CZ	2.42	0.97
2:O:117:CYS:HB2	2:O:124:LYS:CD	1.93	0.97
1:A:19:HIS:ND1	1:A:20:PRO:HD2	1.79	0.97
2:O:117:CYS:CB	2:O:124:LYS:CD	2.39	0.97
1:A:209:LEU:CA	4:A:604:PEG:H32	1.94	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:479:LEU:HD12	5:C:746:HOH:O	1.63	0.96
1:A:263:VAL:CG2	1:A:415:ASP:O	2.13	0.96
1:B:176:GLY:O	1:B:299:ILE:HD13	1.64	0.96
1:D:7:LEU:HD12	1:D:8:PHE:N	1.82	0.95
2:P:77:CYS:HG	3:P:201:ZN:ZN	0.81	0.94
1:D:7:LEU:HD11	1:D:8:PHE:CE1	2.03	0.94
2:O:117:CYS:N	2:O:124:LYS:CD	2.28	0.94
1:D:414:CYS:O	1:D:416:GLY:N	2.01	0.93
1:C:52:ARG:HD2	5:C:734:HOH:O	1.66	0.93
1:D:19:HIS:ND1	1:D:20:PRO:CD	2.32	0.92
1:D:18:LEU:HD21	1:D:53:ARG:HE	1.32	0.91
2:P:85:ASN:OD1	2:P:87:LYS:HB3	1.71	0.90
1:D:7:LEU:HD12	1:D:8:PHE:CG	2.07	0.90
1:A:12:SER:OG	1:A:14:ILE:HG13	1.71	0.90
2:P:85:ASN:CG	2:P:87:LYS:HB3	1.97	0.90
2:O:110:PHE:HE2	2:O:123:TRP:HE1	0.90	0.90
1:A:209:LEU:HA	4:A:604:PEG:C3	2.03	0.89
1:B:2:GLU:O	1:B:3:ASN:C	2.15	0.88
2:O:123:TRP:HA	2:O:123:TRP:CE3	2.07	0.88
1:D:157:LEU:HD21	1:D:161:VAL:CG1	1.96	0.88
1:B:176:GLY:O	1:B:299:ILE:HD11	1.72	0.87
1:C:7:LEU:HD11	1:C:59:GLY:C	2.01	0.85
1:C:477:CYS:O	1:C:482:ALA:CB	2.25	0.84
1:D:18:LEU:HD21	1:D:53:ARG:CZ	2.05	0.84
1:C:15:ILE:HG23	1:C:16:THR:HG23	1.60	0.84
1:D:7:LEU:HD12	1:D:8:PHE:CD1	2.12	0.83
1:A:157:LEU:CD1	1:A:158:PRO:HD3	2.06	0.83
1:B:300:GLY:O	1:B:301:ASP:HB2	1.78	0.83
1:C:482:ALA:C	1:C:484:CYS:N	2.28	0.83
2:O:123:TRP:HA	2:O:123:TRP:HE3	1.44	0.82
1:A:157:LEU:CG	1:A:158:PRO:CD	2.57	0.82
1:C:283:HIS:HB2	1:C:414:CYS:SG	2.20	0.82
1:B:6:GLY:O	1:B:9:LYS:N	2.10	0.82
1:A:157:LEU:HG	1:A:158:PRO:CD	2.07	0.82
2:O:117:CYS:N	2:O:124:LYS:HG2	1.89	0.82
2:O:117:CYS:CA	2:O:124:LYS:HD3	1.96	0.82
1:A:19:HIS:HD2	1:A:47:LYS:CA	1.93	0.81
1:A:154:TYR:O	1:A:155:LYS:O	1.99	0.81
1:C:414:CYS:O	1:C:416:GLY:N	2.14	0.81
1:B:6:GLY:O	1:B:7:LEU:C	2.23	0.80
1:D:7:LEU:HD11	1:D:8:PHE:CD1	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:CYS:HB2	1:A:482:ALA:HB1	1.64	0.80
1:A:210:CYS:SG	1:A:229:HIS:CE1	2.73	0.79
2:P:87:LYS:O	2:P:87:LYS:NZ	2.13	0.79
1:A:482:ALA:C	1:A:484:CYS:H	1.90	0.79
1:A:157:LEU:HD12	1:A:158:PRO:CD	2.11	0.78
1:A:19:HIS:CD2	1:A:47:LYS:CB	2.54	0.78
2:O:117:CYS:H	2:O:124:LYS:CG	1.89	0.78
1:D:156:GLY:O	1:D:157:LEU:HB2	1.81	0.78
1:B:453:GLU:O	1:B:485:ARG:HD2	1.85	0.77
1:D:18:LEU:HD22	1:D:53:ARG:CZ	2.14	0.77
2:P:87:LYS:HZ2	2:P:87:LYS:HA	1.50	0.77
1:B:154:TYR:C	1:B:156:GLY:H	1.92	0.77
2:P:77:CYS:SG	3:P:201:ZN:ZN	1.73	0.77
1:B:300:GLY:O	1:B:301:ASP:CB	2.33	0.77
1:A:299:ILE:HD12	1:A:299:ILE:O	1.84	0.76
1:B:475:THR:HG22	1:B:478:ASN:HB2	1.67	0.76
1:B:453:GLU:C	1:B:485:ARG:HD2	2.10	0.75
1:C:7:LEU:HD12	1:C:59:GLY:C	2.09	0.74
2:M:4:ALA:N	5:M:301:HOH:O	2.21	0.73
1:D:19:HIS:CE1	1:D:20:PRO:HD2	2.23	0.72
1:C:477:CYS:O	1:C:482:ALA:HB1	1.87	0.72
1:D:157:LEU:HD23	1:D:161:VAL:CG1	2.18	0.72
1:A:299:ILE:HD11	1:A:408:ASN:CB	2.20	0.72
1:D:7:LEU:CD1	1:D:8:PHE:N	2.54	0.71
2:P:85:ASN:OD1	2:P:87:LYS:HB2	1.88	0.70
1:C:300:GLY:N	1:C:302:GLU:OE1	2.24	0.70
4:A:604:PEG:H21	1:C:221:SER:HB3	1.72	0.70
1:D:18:LEU:HD22	1:D:53:ARG:NH2	2.06	0.70
1:D:157:LEU:HD23	1:D:161:VAL:HG11	1.70	0.70
1:C:467:PRO:CA	1:C:483:VAL:HG11	2.21	0.69
1:C:300:GLY:HA3	1:C:302:GLU:HG3	1.73	0.69
2:O:110:PHE:CZ	2:O:123:TRP:CD1	2.80	0.69
2:P:85:ASN:OD1	2:P:87:LYS:CA	2.41	0.69
1:C:7:LEU:HD11	1:C:59:GLY:O	1.89	0.69
1:C:118:VAL:HG12	1:C:156:GLY:HA2	1.75	0.69
1:A:157:LEU:CD1	1:A:158:PRO:CD	2.68	0.68
1:D:486:HIS:C	1:D:486:HIS:HD1	2.01	0.68
2:P:87:LYS:NZ	2:P:87:LYS:HA	2.09	0.68
1:C:154:TYR:O	1:C:155:LYS:O	2.10	0.68
1:C:14:ILE:HG22	1:C:15:ILE:O	1.94	0.68
1:C:7:LEU:HD12	1:C:59:GLY:CA	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:LEU:HD12	1:C:59:GLY:HA3	1.75	0.67
1:D:7:LEU:CD1	1:D:8:PHE:CG	2.74	0.67
2:N:128:CYS:O	2:N:130:CYS:N	2.28	0.67
1:D:298:ILE:HD12	1:D:298:ILE:N	2.09	0.66
1:A:154:TYR:O	1:A:155:LYS:C	2.37	0.66
1:D:19:HIS:CD2	1:D:47:LYS:HB3	2.30	0.66
1:C:18:LEU:HB3	1:C:23:ALA:HB2	1.76	0.66
1:A:207:CYS:SG	1:A:208:CYS:O	2.55	0.65
1:B:283:HIS:HB2	1:B:414:CYS:SG	2.37	0.65
1:C:467:PRO:HB3	1:C:483:VAL:HG11	1.76	0.65
1:A:477:CYS:O	1:A:482:ALA:HB3	1.97	0.64
1:A:209:LEU:C	4:A:604:PEG:H32	2.23	0.64
1:C:154:TYR:C	1:C:155:LYS:O	2.41	0.64
1:C:479:LEU:CD1	5:C:746:HOH:O	2.32	0.64
1:A:18:LEU:O	1:A:19:HIS:C	2.40	0.63
1:D:482:ALA:O	1:D:483:VAL:C	2.41	0.63
1:B:482:ALA:C	1:B:483:VAL:HG22	2.22	0.63
1:D:14:ILE:HG21	1:D:53:ARG:NH2	2.14	0.63
1:A:19:HIS:CD2	1:A:47:LYS:CA	2.80	0.63
1:A:19:HIS:O	1:A:21:THR:N	2.32	0.63
1:A:299:ILE:HD12	1:A:299:ILE:C	2.23	0.63
1:B:154:TYR:C	1:B:156:GLY:N	2.57	0.63
1:A:478:ASN:C	1:A:480:GLY:H	2.06	0.62
1:C:208:CYS:O	1:C:209:LEU:HB2	1.99	0.62
1:D:17:GLY:N	1:D:30:ASP:OD2	2.29	0.62
1:D:299:ILE:HD12	1:D:299:ILE:O	2.00	0.62
1:B:3:ASN:O	2:N:8:PRO:HD3	1.99	0.62
2:N:124:LYS:HG2	2:N:128:CYS:SG	2.39	0.61
1:A:524:THR:HG22	1:A:524:THR:O	2.02	0.60
1:C:299:ILE:HG23	1:C:299:ILE:O	2.02	0.60
2:O:123:TRP:HB3	2:O:126:TYR:HB2	1.83	0.60
1:D:157:LEU:CD2	1:D:161:VAL:HG12	2.26	0.60
2:N:127:GLY:O	2:N:128:CYS:C	2.44	0.60
1:B:154:TYR:O	1:B:156:GLY:N	2.35	0.60
1:C:14:ILE:C	1:C:15:ILE:O	2.45	0.60
1:C:467:PRO:HB2	1:C:483:VAL:CG1	2.26	0.60
1:A:299:ILE:HD11	1:A:408:ASN:HB2	1.83	0.60
1:B:482:ALA:O	1:B:483:VAL:CG2	2.49	0.60
1:A:263:VAL:CB	1:A:415:ASP:O	2.50	0.59
1:B:453:GLU:C	1:B:485:ARG:HH21	2.09	0.59
1:D:7:LEU:HD12	1:D:7:LEU:C	2.26	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:115:THR:O	2:O:124:LYS:HG3	2.02	0.59
1:A:477:CYS:SG	1:A:484:CYS:CB	2.91	0.59
1:D:118:VAL:HG12	1:D:156:GLY:HA2	1.82	0.59
2:O:117:CYS:HA	2:O:124:LYS:HD2	1.51	0.59
1:C:483:VAL:C	1:C:485:ARG:H	2.07	0.59
1:C:17:GLY:HA3	1:C:30:ASP:HA	1.84	0.59
1:D:376:LYS:N	1:D:376:LYS:HD2	2.18	0.58
2:O:123:TRP:CE3	2:O:123:TRP:CA	2.85	0.58
1:C:479:LEU:HD13	1:C:479:LEU:N	2.18	0.58
1:A:51:TYR:C	1:A:52:ARG:HG2	2.27	0.58
1:A:209:LEU:O	4:A:604:PEG:H32	2.03	0.58
1:C:477:CYS:O	1:C:482:ALA:HB3	2.04	0.58
1:D:299:ILE:HD12	1:D:299:ILE:C	2.28	0.58
1:A:18:LEU:O	1:A:23:ALA:HB2	2.04	0.57
1:B:414:CYS:HB2	1:B:427:HIS:CE1	2.39	0.57
1:C:482:ALA:O	1:C:484:CYS:SG	2.62	0.57
1:A:83:VAL:O	1:A:84:ARG:HB2	2.04	0.57
1:A:19:HIS:O	1:A:20:PRO:C	2.47	0.57
1:D:283:HIS:HB2	1:D:414:CYS:SG	2.45	0.57
1:B:525:ARG:O	1:B:525:ARG:HG2	2.03	0.57
1:D:486:HIS:C	1:D:486:HIS:ND1	2.59	0.57
1:A:299:ILE:CD1	1:A:408:ASN:HD22	2.17	0.57
1:C:17:GLY:HA3	1:C:30:ASP:CA	2.35	0.57
1:C:7:LEU:O	5:C:701:HOH:O	2.18	0.57
1:A:19:HIS:O	1:A:22:GLN:N	2.37	0.56
1:D:154:TYR:CD1	1:D:154:TYR:C	2.84	0.56
1:B:82:HIS:C	1:B:83:VAL:O	2.47	0.56
1:B:15:ILE:HD13	1:B:15:ILE:N	2.04	0.56
1:A:154:TYR:C	1:A:155:LYS:O	2.48	0.56
1:B:482:ALA:C	1:B:483:VAL:CG2	2.79	0.55
1:D:286:PHE:N	1:D:286:PHE:CD2	2.73	0.55
1:A:209:LEU:O	4:A:604:PEG:C3	2.54	0.55
1:B:414:CYS:HB2	1:B:427:HIS:HE1	1.71	0.55
1:D:288:LYS:HD3	1:D:288:LYS:N	2.21	0.55
1:B:453:GLU:O	1:B:485:ARG:CD	2.53	0.55
1:D:154:TYR:C	1:D:154:TYR:HD1	2.15	0.55
2:P:122:MET:HB2	2:P:127:GLY:O	2.06	0.55
1:B:6:GLY:C	1:B:7:LEU:O	2.44	0.55
1:C:300:GLY:HA3	1:C:409:LEU:HD21	1.89	0.54
1:D:299:ILE:O	1:D:299:ILE:HG23	2.06	0.54
2:O:117:CYS:N	2:O:124:LYS:HD3	2.10	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ARG:NH1	1:A:299:ILE:CG2	2.71	0.54
1:D:157:LEU:HD23	1:D:161:VAL:HB	1.90	0.54
1:D:157:LEU:HD23	1:D:161:VAL:CB	2.38	0.53
1:B:15:ILE:H	1:B:15:ILE:CD1	1.97	0.53
1:B:486:HIS:HB3	5:B:717:HOH:O	2.08	0.53
1:A:263:VAL:HB	1:A:415:ASP:O	2.08	0.53
1:B:14:ILE:C	1:B:15:ILE:O	2.51	0.53
1:D:18:LEU:CD2	1:D:53:ARG:NH2	2.69	0.52
1:A:476:ARG:HB3	1:A:476:ARG:NH1	2.24	0.52
1:A:477:CYS:C	1:A:482:ALA:HB3	2.34	0.52
1:A:176:GLY:O	1:A:299:ILE:HD13	2.10	0.52
1:B:482:ALA:O	1:B:483:VAL:C	2.52	0.52
2:P:0:HIS:HD2	2:P:0:HIS:O	1.92	0.52
1:A:477:CYS:SG	1:A:484:CYS:HB2	2.49	0.52
1:D:288:LYS:N	1:D:288:LYS:CD	2.73	0.51
1:D:60:PHE:O	1:D:61:LYS:C	2.54	0.51
2:P:87:LYS:NZ	2:P:87:LYS:CA	2.73	0.51
1:B:477:CYS:SG	1:B:484:CYS:HB3	2.15	0.51
1:C:221:SER:O	1:C:223:THR:N	2.43	0.51
1:D:7:LEU:HD11	1:D:8:PHE:CZ	2.44	0.51
1:B:15:ILE:HG12	1:B:16:THR:HG23	1.91	0.51
2:P:122:MET:CB	2:P:127:GLY:O	2.57	0.51
1:D:243:ASP:OD1	1:D:243:ASP:C	2.52	0.51
1:D:483:VAL:HG23	1:D:483:VAL:O	2.09	0.51
1:C:101:VAL:O	1:C:101:VAL:HG13	2.10	0.51
1:A:157:LEU:CB	1:A:158:PRO:CD	2.87	0.50
1:A:35:THR:HG23	1:A:35:THR:O	2.11	0.50
1:C:18:LEU:HD21	1:C:53:ARG:NE	2.26	0.50
1:B:3:ASN:O	2:N:8:PRO:CD	2.60	0.50
2:N:128:CYS:C	2:N:130:CYS:N	2.69	0.50
1:A:359:LYS:O	5:A:702:HOH:O	2.20	0.50
1:A:15:ILE:HD12	1:A:15:ILE:H	1.76	0.50
1:A:19:HIS:ND1	1:A:20:PRO:CD	2.64	0.49
1:A:299:ILE:HD11	1:A:408:ASN:HD22	1.75	0.49
1:A:473:CYS:O	1:A:478:ASN:ND2	2.36	0.49
1:D:18:LEU:HD21	1:D:53:ARG:CD	2.35	0.49
1:D:19:HIS:O	1:D:20:PRO:C	2.55	0.49
1:B:414:CYS:C	1:B:416:GLY:N	2.61	0.49
2:O:89:PHE:CD1	2:O:89:PHE:N	2.73	0.49
1:C:483:VAL:C	1:C:485:ARG:N	2.68	0.49
1:D:19:HIS:O	1:D:21:THR:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:CYS:HB2	1:D:226:CYS:N	2.27	0.49
2:M:3:ASN:N	5:M:301:HOH:O	2.45	0.49
2:P:87:LYS:HZ1	2:P:87:LYS:C	2.14	0.49
1:D:7:LEU:CD1	1:D:7:LEU:C	2.85	0.49
1:B:243:ASP:OD1	1:B:243:ASP:C	2.56	0.49
1:D:156:GLY:O	1:D:157:LEU:CB	2.56	0.48
1:D:176:GLY:O	1:D:299:ILE:HG12	2.13	0.48
2:O:110:PHE:CZ	2:O:123:TRP:HD1	2.31	0.48
2:P:85:ASN:CG	2:P:87:LYS:CB	2.68	0.48
1:B:358:ASP:O	1:B:359:LYS:HB2	2.13	0.48
1:A:478:ASN:O	1:A:480:GLY:N	2.46	0.48
1:D:298:ILE:N	1:D:298:ILE:CD1	2.73	0.48
1:D:379:ASP:OD1	1:D:379:ASP:C	2.57	0.48
1:B:178:SER:OG	1:B:179:ASP:N	2.47	0.48
1:D:157:LEU:HD22	1:D:161:VAL:HG12	1.94	0.47
1:D:482:ALA:C	1:D:483:VAL:HG22	2.39	0.47
1:B:14:ILE:HG22	1:B:15:ILE:O	2.13	0.47
2:P:87:LYS:NZ	2:P:87:LYS:C	2.72	0.47
1:D:16:THR:HB	1:D:30:ASP:OD2	2.14	0.47
1:B:440:LYS:HD2	1:B:512:LYS:HA	1.97	0.47
1:D:150:ILE:HB	1:D:151:PRO:HD3	1.97	0.47
1:A:299:ILE:HD11	1:A:408:ASN:HB3	1.96	0.47
1:A:483:VAL:O	1:A:484:CYS:C	2.58	0.47
1:B:475:THR:HG23	1:B:477:CYS:H	1.78	0.47
1:B:484:CYS:O	1:B:488:ALA:N	2.42	0.47
1:C:300:GLY:CA	1:C:302:GLU:HG3	2.42	0.47
1:D:19:HIS:ND1	1:D:19:HIS:C	2.72	0.47
1:B:101:VAL:HG13	1:B:101:VAL:O	2.14	0.47
1:B:329:LEU:C	1:B:329:LEU:HD23	2.40	0.47
1:B:482:ALA:O	1:B:483:VAL:HG23	2.13	0.46
1:B:479:LEU:HD12	1:B:479:LEU:HA	1.64	0.46
1:A:17:GLY:O	1:A:53:ARG:NH2	2.48	0.46
1:B:62:MET:HE1	2:N:19:PHE:CD1	2.50	0.46
1:C:18:LEU:HD21	1:C:53:ARG:CD	2.45	0.46
1:C:50:THR:O	1:C:51:TYR:HB3	2.15	0.46
2:N:128:CYS:C	2:N:130:CYS:H	2.23	0.46
1:A:476:ARG:CZ	1:A:476:ARG:CB	2.94	0.46
1:B:379:ASP:OD1	1:B:379:ASP:C	2.56	0.46
1:C:300:GLY:HA3	1:C:302:GLU:OE1	2.14	0.46
1:B:150:ILE:N	1:B:151:PRO:CD	2.78	0.46
1:D:329:LEU:C	1:D:329:LEU:HD23	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:GLY:HA3	1:A:30:ASP:HB2	1.97	0.46
1:D:491:TYR:CD1	1:D:491:TYR:C	2.93	0.46
2:O:117:CYS:HB2	2:O:124:LYS:CG	2.44	0.46
1:A:12:SER:HG	1:A:14:ILE:HG13	1.76	0.45
1:A:207:CYS:HB2	1:A:226:CYS:N	2.31	0.45
2:N:123:TRP:HB2	2:N:126:TYR:HB2	1.99	0.45
2:P:85:ASN:ND2	2:P:87:LYS:HB3	2.30	0.45
1:D:482:ALA:O	1:D:483:VAL:CG2	2.65	0.45
2:P:74:CYS:CB	2:P:77:CYS:HG	2.29	0.45
1:B:491:TYR:C	1:B:491:TYR:CD1	2.94	0.45
1:D:14:ILE:O	1:D:14:ILE:HG22	2.16	0.45
1:D:18:LEU:HD13	1:D:18:LEU:HA	1.56	0.45
1:D:120:VAL:HG13	1:D:157:LEU:H	1.82	0.45
1:D:178:SER:OG	1:D:179:ASP:N	2.50	0.45
1:D:208:CYS:O	1:D:209:LEU:HB2	2.17	0.45
2:P:0:HIS:O	2:P:0:HIS:CD2	2.70	0.45
1:C:391:ARG:HA	1:C:435:ALA:HA	1.99	0.44
2:P:74:CYS:SG	2:P:77:CYS:SG	3.06	0.44
1:B:80:ILE:O	1:B:83:VAL:CG2	2.66	0.44
2:N:110:PHE:CD1	2:N:110:PHE:C	2.95	0.44
2:N:128:CYS:O	2:N:129:SER:C	2.61	0.44
1:B:221:SER:O	1:B:223:THR:N	2.50	0.44
1:B:414:CYS:HB3	1:B:415:ASP:H	1.44	0.44
2:M:100:PRO:HG2	2:M:126:TYR:HD2	1.82	0.44
1:A:250:THR:OG1	1:A:251:GLY:N	2.49	0.44
1:B:200:LYS:HG2	1:B:235:TYR:CD2	2.53	0.44
1:A:209:LEU:O	4:A:604:PEG:C4	2.66	0.44
1:B:298:ILE:H	1:B:298:ILE:HG12	1.55	0.44
1:C:150:ILE:N	1:C:151:PRO:CD	2.80	0.44
1:D:395:ASN:CG	1:D:395:ASN:O	2.60	0.44
1:C:467:PRO:HB2	1:C:483:VAL:HG21	2.00	0.44
1:A:140:PRO:HA	1:A:141:PRO:HD3	1.88	0.44
1:A:478:ASN:C	1:A:480:GLY:N	2.73	0.44
1:D:18:LEU:O	1:D:29:VAL:HA	2.18	0.44
1:A:19:HIS:C	1:A:21:THR:N	2.76	0.44
1:A:298:ILE:N	1:A:298:ILE:HD12	2.33	0.44
1:D:101:VAL:O	1:D:101:VAL:HG13	2.18	0.44
1:D:176:GLY:O	1:D:299:ILE:CG1	2.66	0.44
2:M:122:MET:HE2	2:M:127:GLY:O	2.17	0.44
2:P:122:MET:HE2	2:P:127:GLY:HA3	2.00	0.44
1:B:2:GLU:O	1:B:3:ASN:O	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:GLY:C	1:B:299:ILE:CD1	2.86	0.43
1:A:18:LEU:CD2	1:A:53:ARG:NE	2.62	0.43
1:C:210:CYS:SG	1:C:229:HIS:CE1	3.11	0.43
1:C:300:GLY:HA3	1:C:302:GLU:CG	2.45	0.43
1:A:82:HIS:C	1:A:83:VAL:O	2.60	0.43
2:N:13:VAL:HG22	2:N:30:TYR:CE2	2.54	0.43
2:O:13:VAL:HG22	2:O:30:TYR:CE1	2.53	0.43
1:B:14:ILE:O	1:B:15:ILE:O	2.36	0.43
1:B:85:ALA:HB2	1:B:178:SER:CB	2.48	0.43
1:B:337:ALA:O	1:B:338:ILE:C	2.61	0.43
1:A:482:ALA:C	1:A:484:CYS:N	2.55	0.43
1:B:62:MET:HG2	1:B:72:MET:HE2	2.01	0.43
1:B:80:ILE:O	1:B:83:VAL:HG22	2.19	0.43
1:B:85:ALA:HB2	1:B:178:SER:HB2	1.99	0.43
1:B:150:ILE:HB	1:B:151:PRO:HD3	2.00	0.43
1:C:300:GLY:CA	1:C:302:GLU:OE1	2.66	0.43
1:C:157:LEU:HA	1:C:158:PRO:HD3	1.85	0.43
1:D:7:LEU:CD1	1:D:8:PHE:H	2.28	0.43
1:D:120:VAL:HG23	1:D:122:THR:HG23	2.01	0.43
1:D:482:ALA:O	1:D:483:VAL:O	2.36	0.43
1:C:243:ASP:C	1:C:243:ASP:OD1	2.62	0.43
1:D:19:HIS:HD2	1:D:47:LYS:CA	2.31	0.43
1:A:18:LEU:CD2	1:A:53:ARG:HE	2.09	0.42
1:A:150:ILE:HB	1:A:151:PRO:HD3	2.02	0.42
1:C:97:THR:O	1:C:97:THR:OG1	2.32	0.42
1:C:207:CYS:SG	1:C:208:CYS:O	2.77	0.42
1:C:341:VAL:O	1:C:341:VAL:HG12	2.19	0.42
1:C:18:LEU:HD22	1:C:53:ARG:CZ	2.49	0.42
2:M:100:PRO:HG2	2:M:126:TYR:CD2	2.54	0.42
1:A:298:ILE:HD12	1:A:298:ILE:H	1.85	0.42
1:B:501:MET:HE3	1:B:501:MET:HB2	1.94	0.42
1:C:18:LEU:O	1:C:19:HIS:C	2.62	0.42
1:B:424:HIS:O	1:B:425:ALA:HB3	2.19	0.42
1:A:209:LEU:O	4:A:604:PEG:O4	2.33	0.41
1:A:482:ALA:O	1:A:483:VAL:C	2.48	0.41
1:A:19:HIS:CD2	1:A:47:LYS:HA	2.55	0.41
1:A:221:SER:O	1:A:223:THR:N	2.53	0.41
1:B:18:LEU:HD23	1:B:18:LEU:HA	1.80	0.41
1:C:208:CYS:O	1:C:209:LEU:CB	2.63	0.41
1:D:361:TYR:CE2	1:D:362:LYS:HG3	2.54	0.41
1:C:140:PRO:HA	1:C:141:PRO:HD3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:PRO:HA	1:A:142:PRO:HD3	1.73	0.41
1:B:482:ALA:O	1:B:483:VAL:HG22	2.18	0.41
2:O:30:TYR:CE1	2:O:35:GLY:HA3	2.56	0.41
1:A:283:HIS:HB2	1:A:414:CYS:SG	2.61	0.41
1:B:485:ARG:O	1:B:486:HIS:C	2.61	0.41
2:M:125:GLY:C	2:M:126:TYR:CD1	2.99	0.41
1:C:209:LEU:O	4:C:604:PEG:C3	2.65	0.41
2:O:78:ARG:HA	2:O:78:ARG:HD2	1.87	0.41
2:P:53:GLN:HA	2:P:122:MET:HG2	2.02	0.41
1:A:4:VAL:O	1:A:4:VAL:HG13	2.21	0.41
1:B:475:THR:HG23	1:B:477:CYS:N	2.36	0.41
1:D:19:HIS:ND1	1:D:20:PRO:N	2.67	0.41
1:A:299:ILE:CD1	1:A:408:ASN:HB3	2.51	0.40
1:A:329:LEU:HD23	1:A:329:LEU:C	2.46	0.40
1:B:15:ILE:HB	1:B:16:THR:H	1.58	0.40
2:N:127:GLY:O	2:N:129:SER:N	2.53	0.40
1:A:299:ILE:CD1	1:A:408:ASN:ND2	2.83	0.40
1:D:300:GLY:O	1:D:301:ASP:HB2	2.22	0.40
1:D:500:MET:HE2	1:D:500:MET:HB2	1.96	0.40
1:A:477:CYS:SG	1:A:484:CYS:HB3	2.61	0.40
1:B:7:LEU:O	1:B:8:PHE:HB2	2.22	0.40
1:D:17:GLY:HA3	1:D:30:ASP:HA	2.02	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ARG:NH1	1:D:515:ASP:OD2[4_557]	1.35	0.85
1:B:515:ASP:OD2	1:C:52:ARG:NH2[4_456]	1.81	0.39

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	508/534 (95%)	450 (89%)	44 (9%)	14 (3%)	4	19
1	B	510/534 (96%)	456 (89%)	37 (7%)	17 (3%)	3	17
1	C	510/534 (96%)	449 (88%)	44 (9%)	17 (3%)	3	17
1	D	510/534 (96%)	461 (90%)	38 (8%)	11 (2%)	5	23
2	M	130/138 (94%)	116 (89%)	11 (8%)	3 (2%)	5	23
2	N	131/138 (95%)	119 (91%)	9 (7%)	3 (2%)	5	23
2	O	131/138 (95%)	115 (88%)	13 (10%)	3 (2%)	5	23
2	P	131/138 (95%)	122 (93%)	8 (6%)	1 (1%)	16	44
All	All	2561/2688 (95%)	2288 (89%)	204 (8%)	69 (3%)	4	20

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	LYS
1	A	222	ASP
1	A	250	THR
1	A	483	VAL
1	B	15	ILE
1	B	83	VAL
1	B	85	ALA
1	B	222	ASP
1	B	238	ASN
1	B	239	PRO
1	B	301	ASP
1	B	415	ASP
1	C	155	LYS
1	C	222	ASP
1	C	230	SER
1	C	483	VAL
1	C	484	CYS
1	D	157	LEU
1	D	290	VAL
1	D	415	ASP
2	N	129	SER
1	A	289	ARG
1	A	415	ASP
1	A	479	LEU
1	A	484	CYS
1	B	390	ASP
1	C	15	ILE

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Mol	Chain	Res	Type
1	C	390	ASP
1	C	424	HIS
1	C	481	GLY
1	D	61	LYS
1	D	390	ASP
1	D	483	VAL
2	M	8	PRO
2	N	128	CYS
2	O	89	PHE
1	A	20	PRO
1	A	83	VAL
1	A	390	ASP
1	B	3	ASN
1	B	155	LYS
1	B	250	THR
1	B	338	ILE
1	B	414	CYS
1	C	301	ASP
1	C	414	CYS
1	C	479	LEU
1	D	250	THR
2	M	9	ALA
1	A	355	PRO
1	B	425	ALA
1	B	485	ARG
1	C	290	VAL
1	D	20	PRO
1	D	209	LEU
1	D	414	CYS
1	A	19	HIS
1	C	143	GLY
1	C	299	ILE
2	O	124	LYS
1	A	481	GLY
1	B	483	VAL
1	C	36	GLU
1	C	300	GLY
1	D	210	CYS
2	P	127	GLY
2	M	70	GLY
2	N	70	GLY
2	O	70	GLY

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	450/470 (96%)	440 (98%)	10 (2%)	45	63
1	B	451/470 (96%)	440 (98%)	11 (2%)	43	62
1	C	451/470 (96%)	442 (98%)	9 (2%)	48	66
1	D	451/470 (96%)	435 (96%)	16 (4%)	32	56
2	M	107/113 (95%)	104 (97%)	3 (3%)	38	60
2	N	108/113 (96%)	106 (98%)	2 (2%)	50	66
2	O	108/113 (96%)	105 (97%)	3 (3%)	38	60
2	P	108/113 (96%)	107 (99%)	1 (1%)	70	76
All	All	2234/2332 (96%)	2179 (98%)	55 (2%)	42	62

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ILE
1	A	15	ILE
1	A	52	ARG
1	A	155	LYS
1	A	157	LEU
1	A	210	CYS
1	A	299	ILE
1	A	415	ASP
1	A	476	ARG
1	A	525	ARG
1	B	2	GLU
1	B	5	THR
1	B	15	ILE
1	B	83	VAL
1	B	298	ILE
1	B	299	ILE
1	B	410	ASN
1	B	414	CYS
1	B	479	LEU

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Mol	Chain	Res	Type
1	B	485	ARG
1	B	486	HIS
1	C	2	GLU
1	C	7	LEU
1	C	15	ILE
1	C	18	LEU
1	C	52	ARG
1	C	298	ILE
1	C	299	ILE
1	C	479	LEU
1	C	483	VAL
1	D	2	GLU
1	D	5	THR
1	D	7	LEU
1	D	14	ILE
1	D	15	ILE
1	D	18	LEU
1	D	154	TYR
1	D	155	LYS
1	D	157	LEU
1	D	207	CYS
1	D	287	VAL
1	D	288	LYS
1	D	298	ILE
1	D	299	ILE
1	D	414	CYS
1	D	486	HIS
2	M	0	HIS
2	M	87	LYS
2	M	128	CYS
2	N	87	LYS
2	N	128	CYS
2	O	87	LYS
2	O	123	TRP
2	O	124	LYS
2	P	87	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	HIS
1	A	26	HIS

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Mol	Chain	Res	Type
1	A	408	ASN
1	B	26	HIS
1	B	108	GLN
1	B	410	ASN
1	C	82	HIS
1	C	108	GLN
1	C	374	HIS
1	C	521	ASN
1	D	108	GLN
1	D	256	ASN
2	N	48	HIS
2	N	85	ASN
2	P	0	HIS

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](#)

Of 23 ligands modelled in this entry, 20 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	PEG	A	604	-	6,6,6	0.34	0	5,5,5	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PEG	C	604	-	6,6,6	0.42	0	5,5,5	0.28	0
4	PEG	A	605	-	6,6,6	0.34	0	5,5,5	0.32	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	A	604	-	-	3/4/4/4	-
4	PEG	C	604	-	-	2/4/4/4	-
4	PEG	A	605	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	604	PEG	C4-C3-O2-C2
4	C	604	PEG	O1-C1-C2-O2
4	A	604	PEG	C1-C2-O2-C3
4	A	604	PEG	O1-C1-C2-O2
4	A	605	PEG	C4-C3-O2-C2
4	A	604	PEG	O2-C3-C4-O4
4	A	605	PEG	O1-C1-C2-O2
4	A	605	PEG	C1-C2-O2-C3
4	A	605	PEG	O2-C3-C4-O4

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	604	PEG	9	0
4	C	604	PEG	3	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	512/534 (95%)	0.11	13 (2%) 58 43	61, 89, 127, 156	0
1	B	514/534 (96%)	0.09	20 (3%) 43 30	61, 87, 128, 192	0
1	C	514/534 (96%)	0.07	13 (2%) 58 43	55, 93, 147, 171	0
1	D	514/534 (96%)	0.35	32 (6%) 26 20	66, 99, 142, 193	0
2	M	132/138 (95%)	0.09	2 (1%) 72 57	69, 103, 129, 165	0
2	N	133/138 (96%)	0.23	2 (1%) 72 57	70, 92, 123, 162	0
2	O	133/138 (96%)	0.69	8 (6%) 27 21	83, 121, 159, 181	0
2	P	133/138 (96%)	0.01	3 (2%) 61 45	66, 88, 124, 151	0
All	All	2585/2688 (96%)	0.18	93 (3%) 46 33	55, 94, 141, 193	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	482	ALA	6.8
1	D	468	LEU	6.4
1	B	481	GLY	6.0
1	D	481	GLY	6.0
1	D	483	VAL	5.6
1	A	483	VAL	5.1
1	C	523	PHE	4.8
1	D	467	PRO	4.6
1	B	299	ILE	4.5
1	A	479	LEU	4.5
1	B	468	LEU	4.3
1	B	483	VAL	4.2
1	A	465	TYR	4.2
1	A	468	LEU	4.2
1	C	468	LEU	4.1
1	B	300	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	1	ALA	3.9
2	O	120	CYS	3.8
1	C	300	GLY	3.8
1	B	482	ALA	3.7
1	A	466	VAL	3.6
1	C	388	ASN	3.5
1	C	1	ALA	3.5
1	B	84	ARG	3.5
1	A	156	GLY	3.4
1	B	524	THR	3.4
1	C	299	ILE	3.4
1	C	481	GLY	3.2
2	O	122	MET	3.2
1	D	72	MET	3.1
1	D	232	GLY	3.1
2	N	-1	HIS	3.0
1	D	5	THR	3.0
1	C	465	TYR	2.9
1	D	234	ASP	2.9
1	B	358	ASP	2.9
1	B	467	PRO	2.9
1	B	6	GLY	2.9
1	B	292	TRP	2.8
1	D	479	LEU	2.8
2	O	-1	HIS	2.8
1	A	290	VAL	2.7
1	A	481	GLY	2.7
1	D	200	LYS	2.7
1	D	219	THR	2.6
1	A	157	LEU	2.6
1	D	480	GLY	2.6
1	B	5	THR	2.6
1	C	99	ASP	2.5
1	C	359	LYS	2.5
1	B	469	LYS	2.5
1	D	160	ASN	2.5
1	D	477	CYS	2.5
2	N	128	CYS	2.4
1	D	2	GLU	2.4
1	D	209	LEU	2.4
2	O	126	TYR	2.4
1	C	483	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	154	TYR	2.4
1	B	2	GLU	2.4
1	A	208	CYS	2.4
2	P	86	PRO	2.4
2	O	128	CYS	2.3
2	O	19	PHE	2.3
1	D	524	THR	2.3
1	D	466	VAL	2.3
1	B	49	MET	2.3
1	D	469	LYS	2.3
2	P	51	THR	2.2
1	B	478	ASN	2.2
1	D	63	ASN	2.2
1	B	16	THR	2.2
2	M	0	HIS	2.2
1	D	268	HIS	2.2
1	D	132	GLU	2.1
1	C	301	ASP	2.1
2	O	28	LYS	2.1
1	A	359	LYS	2.1
1	D	423	LYS	2.1
1	D	465	TYR	2.1
1	D	449	ASP	2.1
2	M	87	LYS	2.1
2	O	113	ARG	2.1
1	C	72	MET	2.1
1	B	1	ALA	2.1
1	D	289	ARG	2.1
1	A	99	ASP	2.1
1	D	235	TYR	2.1
1	D	288	LYS	2.0
1	B	414	CYS	2.0
1	D	208	CYS	2.0
2	P	87	LYS	2.0
1	A	289	ARG	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 ⓘ

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
4	PEG	C	604	7/7	0.51	0.47	92,105,127,133	0
3	ZN	O	202	1/1	0.63	0.30	175,175,175,175	0
4	PEG	A	604	7/7	0.82	0.25	83,87,103,115	0
3	ZN	N	202	1/1	0.86	0.25	148,148,148,148	0
4	PEG	A	605	7/7	0.88	0.29	99,103,118,128	0
3	ZN	A	601	1/1	0.89	0.10	161,161,161,161	0
3	ZN	D	603	1/1	0.90	0.20	115,115,115,115	0
3	ZN	D	601	1/1	0.90	0.09	144,144,144,144	0
3	ZN	B	603	1/1	0.92	0.13	119,119,119,119	0
3	ZN	O	201	1/1	0.93	0.14	196,196,196,196	0
3	ZN	C	603	1/1	0.93	0.17	168,168,168,168	0
3	ZN	P	202	1/1	0.93	0.23	142,142,142,142	0
3	ZN	B	601	1/1	0.96	0.16	123,123,123,123	0
3	ZN	P	201	1/1	0.96	0.11	161,161,161,161	0
3	ZN	M	202	1/1	0.96	0.20	155,155,155,155	0
3	ZN	C	601	1/1	0.97	0.06	155,155,155,155	0
3	ZN	C	602	1/1	0.97	0.18	107,107,107,107	0
3	ZN	B	602	1/1	0.99	0.17	111,111,111,111	0
3	ZN	M	201	1/1	0.99	0.14	112,112,112,112	0
3	ZN	A	603	1/1	0.99	0.06	92,92,92,92	0
3	ZN	N	201	1/1	0.99	0.16	88,88,88,88	0
3	ZN	A	602	1/1	0.99	0.14	102,102,102,102	0
3	ZN	D	602	1/1	0.99	0.14	107,107,107,107	0

6.5 Other polymers ⓘ

There are no such residues in this entry.