



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 4TLV / pdb_00004tlv
Title : CARDS TOXIN, NICKED
Authors : Taylor, A.B.; Pakhomova, O.N.; Hart, P.J.
Deposited on : 2014-05-30
Resolution : 1.90 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

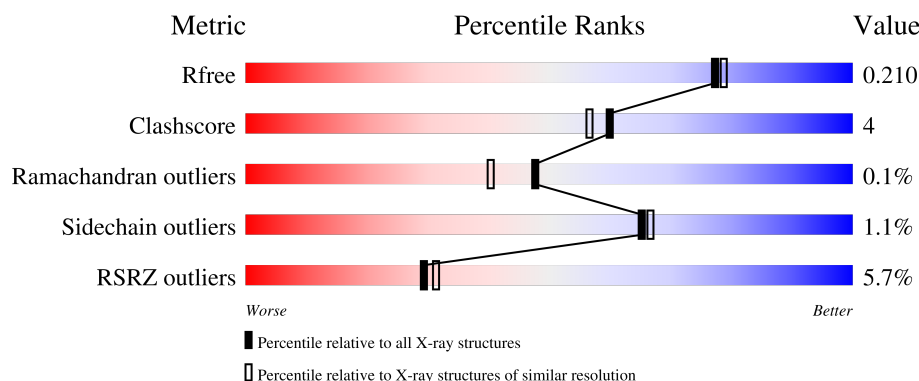
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	591	5% 89% 9%
1	B	591	8% 86% 11%
1	C	591	4% 90% 8%
1	D	591	5% 85% 12%
1	E	591	5% 88% 10%

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Mol	Chain	Length	Quality of chain
1	F	591	

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	GOL	D	603	-	-	X	-
3	GOL	E	603	-	-	X	-
3	GOL	E	604	-	-	X	-
3	GOL	F	603	-	-	X	-
4	ACT	D	608	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 30404 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 ADP-ribosylating toxin CARDS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	582	Total	C	N	O	S	0	1	0
			4752	3037	810	889	16			
1	B	580	Total	C	N	O	S	0	1	0
			4737	3027	808	887	15			
1	C	577	Total	C	N	O	S	0	0	0
			4718	3015	805	882	16			
1	D	577	Total	C	N	O	S	0	2	0
			4721	3018	805	883	15			
1	E	582	Total	C	N	O	S	0	4	0
			4769	3049	814	890	16			
1	F	573	Total	C	N	O	S	0	1	0
			4696	3000	803	878	15			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P75409
A	0	HIS	-	expression tag	UNP P75409
A	?	-	GLN	deletion	UNP P75409
A	?	-	LYS	deletion	UNP P75409
B	-1	GLY	-	expression tag	UNP P75409
B	0	HIS	-	expression tag	UNP P75409
B	?	-	GLN	deletion	UNP P75409
B	?	-	LYS	deletion	UNP P75409
C	-1	GLY	-	expression tag	UNP P75409
C	0	HIS	-	expression tag	UNP P75409
C	?	-	GLN	deletion	UNP P75409
C	?	-	LYS	deletion	UNP P75409
D	-1	GLY	-	expression tag	UNP P75409
D	0	HIS	-	expression tag	UNP P75409
D	?	-	GLN	deletion	UNP P75409
D	?	-	LYS	deletion	UNP P75409
E	-1	GLY	-	expression tag	UNP P75409

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Chain	Residue	Modelled	Actual	Comment	Reference
E	0	HIS	-	expression tag	UNP P75409
E	?	-	GLN	deletion	UNP P75409
E	?	-	LYS	deletion	UNP P75409
F	-1	GLY	-	expression tag	UNP P75409
F	0	HIS	-	expression tag	UNP P75409
F	?	-	GLN	deletion	UNP P75409
F	?	-	LYS	deletion	UNP P75409

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		

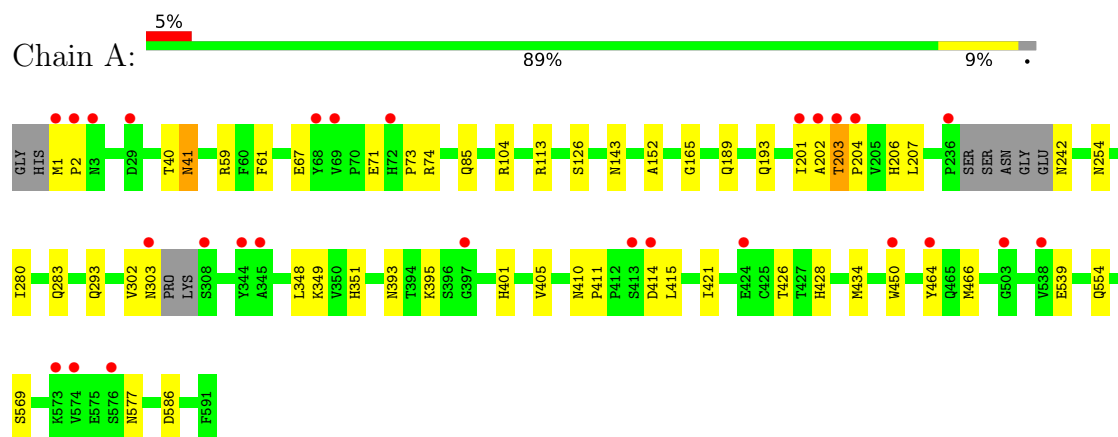
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	380	Total	O	0	0
			380	380		
5	B	296	Total	O	0	0
			296	296		
5	C	350	Total	O	0	0
			350	350		
5	D	305	Total	O	0	0
			305	305		
5	E	295	Total	O	0	0
			295	295		
5	F	182	Total	O	0	0
			182	182		

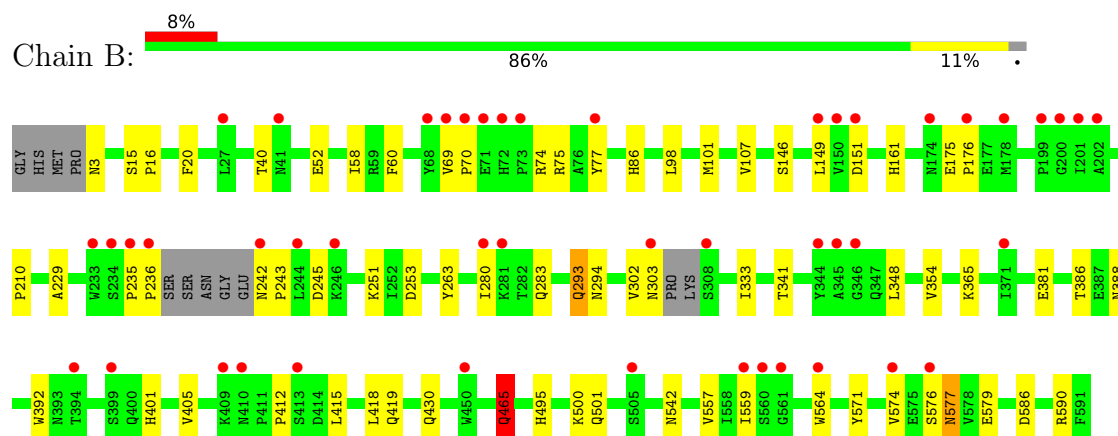
3 Residue-property plots [i](#)

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.

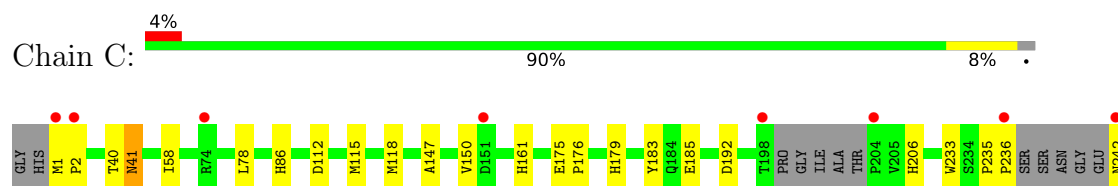
• Molecule 1: ADP-ribosylating toxin CARDS



• Molecule 1: ADP-ribosylating toxin CARDS

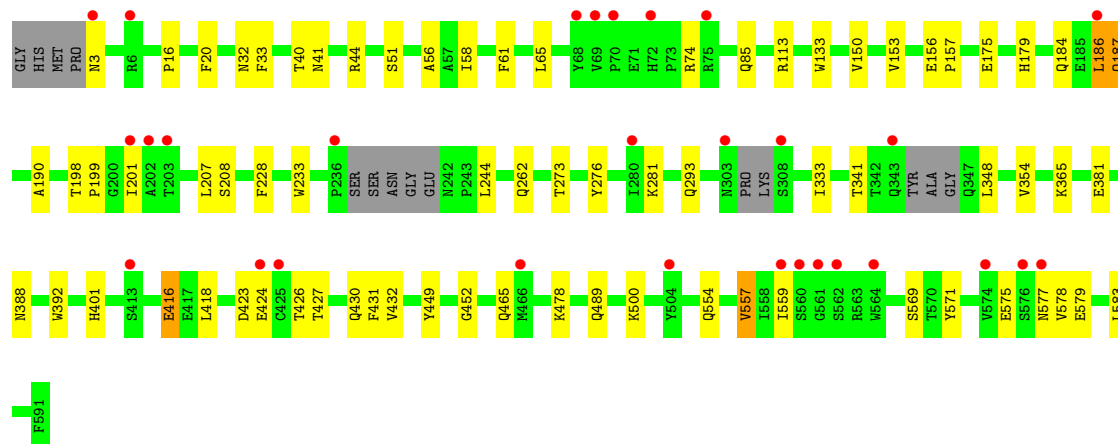
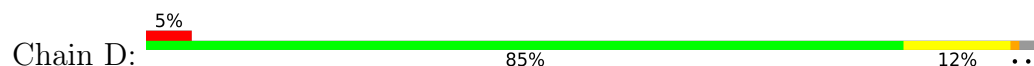


• Molecule 1: ADP-ribosylating toxin CARDS

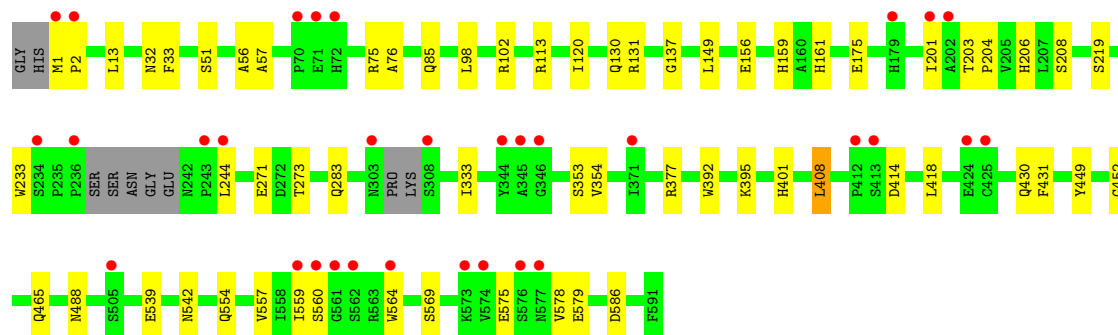
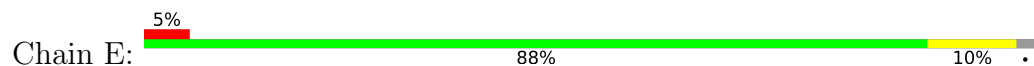




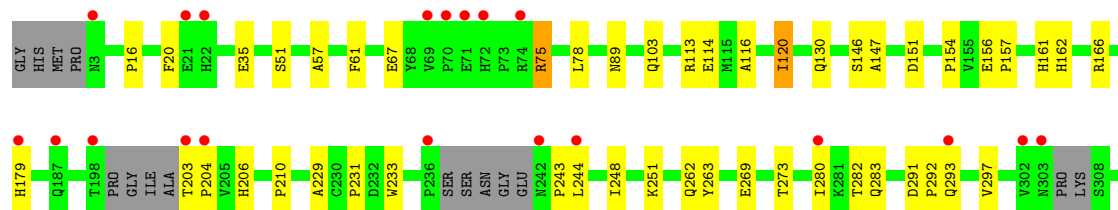
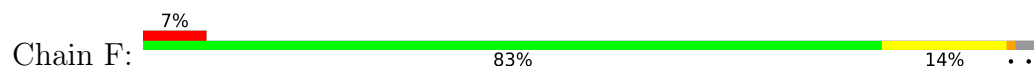
• Molecule 1: ADP-ribosylating toxin CARDS

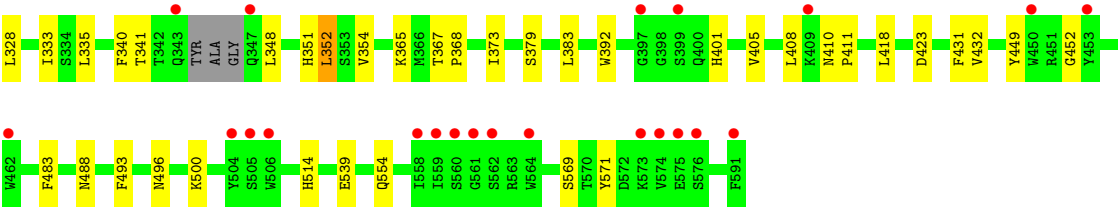


• Molecule 1: ADP-ribosylating toxin CARDS



• Molecule 1: ADP-ribosylating toxin CARDS





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	191.70Å 107.41Å 222.26Å 90.00° 90.64° 90.00°	Depositor
Resolution (Å)	38.87 – 1.90 38.87 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (38.87-1.90) 99.4 (38.87-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 1.91Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.3_928)	Depositor
R, R_{free}	0.186 , 0.215 0.182 , 0.210	Depositor DCC
R_{free} test set	17675 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.005 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.005 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.029 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.019 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.010 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	30404	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ACT, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.63	10/4894 (0.2%)	0.81	11/6661 (0.2%)
1	B	0.60	10/4878 (0.2%)	0.78	8/6639 (0.1%)
1	C	0.61	6/4855 (0.1%)	0.78	10/6604 (0.2%)
1	D	0.60	11/4863 (0.2%)	0.78	5/6617 (0.1%)
1	E	0.57	8/4922 (0.2%)	0.77	8/6699 (0.1%)
1	F	0.56	12/4834 (0.2%)	0.77	10/6575 (0.2%)
All	All	0.59	57/29246 (0.2%)	0.78	52/39795 (0.1%)

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	262	GLN	CD-OE1	5.85	1.34	1.23
1	A	351	HIS	ND1-CE1	5.64	1.38	1.32
1	A	428	HIS	ND1-CE1	5.59	1.38	1.32
1	A	293	GLN	CD-OE1	5.57	1.34	1.23
1	B	495	HIS	ND1-CE1	5.50	1.38	1.32
1	E	85	GLN	CD-OE1	5.47	1.33	1.23
1	C	401	HIS	ND1-CE1	5.43	1.38	1.32
1	D	577	ASN	CG-OD1	5.41	1.33	1.23
1	C	206	HIS	ND1-CE1	5.41	1.38	1.32
1	F	262	GLN	CD-OE1	5.41	1.33	1.23
1	B	577	ASN	CG-OD1	5.40	1.33	1.23
1	D	401	HIS	ND1-CE1	5.40	1.38	1.32
1	F	206	HIS	ND1-CE1	5.39	1.38	1.32
1	B	401	HIS	ND1-CE1	5.38	1.38	1.32
1	D	293	GLN	CD-OE1	5.38	1.33	1.23
1	F	293	GLN	CD-OE1	5.38	1.33	1.23
1	B	161	HIS	ND1-CE1	5.37	1.38	1.32
1	A	401	HIS	ND1-CE1	5.35	1.38	1.32
1	E	161	HIS	ND1-CE1	5.35	1.37	1.32
1	C	161	HIS	ND1-CE1	5.33	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	501	GLN	CD-OE1	5.33	1.33	1.23
1	B	293	GLN	CD-OE1	5.32	1.33	1.23
1	D	179	HIS	ND1-CE1	5.31	1.37	1.32
1	F	161	HIS	ND1-CE1	5.29	1.37	1.32
1	A	283	GLN	CD-OE1	5.26	1.33	1.23
1	E	401	HIS	ND1-CE1	5.25	1.37	1.32
1	F	179[A]	HIS	ND1-CE1	5.25	1.37	1.32
1	F	179[B]	HIS	ND1-CE1	5.25	1.37	1.32
1	A	206	HIS	ND1-CE1	5.25	1.37	1.32
1	C	86	HIS	ND1-CE1	5.24	1.37	1.32
1	E	206	HIS	ND1-CE1	5.24	1.37	1.32
1	C	41	ASN	CG-OD1	5.24	1.33	1.23
1	F	401	HIS	ND1-CE1	5.23	1.37	1.32
1	A	143	ASN	CG-OD1	5.23	1.33	1.23
1	F	89	ASN	CG-OD1	5.23	1.33	1.23
1	F	488	ASN	CG-OD1	5.22	1.33	1.23
1	C	179	HIS	ND1-CE1	5.21	1.37	1.32
1	D	430	GLN	CD-OE1	5.21	1.33	1.23
1	D	85	GLN	CD-OE1	5.20	1.33	1.23
1	E	465	GLN	CD-OE1	5.20	1.33	1.23
1	D	3	ASN	CG-OD1	5.19	1.33	1.23
1	B	430	GLN	CD-OE1	5.18	1.33	1.23
1	E	283	GLN	CD-OE1	5.18	1.33	1.23
1	B	465	GLN	CD-OE1	5.15	1.33	1.23
1	D	489	GLN	CD-OE1	5.15	1.33	1.23
1	B	283	GLN	CD-OE1	5.14	1.33	1.23
1	E	130	GLN	CD-OE1	5.13	1.33	1.23
1	E	488	ASN	CG-OD1	5.11	1.33	1.23
1	D	388	ASN	CG-OD1	5.11	1.33	1.23
1	A	254	ASN	CG-OD1	5.11	1.33	1.23
1	A	189	GLN	CD-OE1	5.11	1.33	1.23
1	F	130	GLN	CD-OE1	5.09	1.33	1.23
1	D	187	GLN	CD-OE1	5.08	1.33	1.23
1	F	103	GLN	CD-OE1	5.08	1.33	1.23
1	F	496	ASN	CG-OD1	5.07	1.33	1.23
1	A	41	ASN	CG-OD1	5.04	1.33	1.23
1	B	388	ASN	CG-OD1	5.04	1.33	1.23

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	428	HIS	CB-CG-CD2	-6.92	122.20	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	161	HIS	CB-CG-CD2	-6.68	122.51	131.20
1	B	161	HIS	CB-CG-CD2	-6.63	122.58	131.20
1	F	161	HIS	CB-CG-CD2	-6.62	122.59	131.20
1	C	86	HIS	CB-CG-CD2	-6.60	122.62	131.20
1	A	401	HIS	CB-CG-CD2	-6.60	122.62	131.20
1	C	401	HIS	CB-CG-CD2	-6.58	122.64	131.20
1	A	351	HIS	CB-CG-CD2	-6.57	122.66	131.20
1	E	401	HIS	CB-CG-CD2	-6.57	122.66	131.20
1	D	179	HIS	CB-CG-CD2	-6.56	122.67	131.20
1	C	179	HIS	CB-CG-CD2	-6.55	122.69	131.20
1	B	401	HIS	CB-CG-CD2	-6.54	122.70	131.20
1	F	401	HIS	CB-CG-CD2	-6.54	122.70	131.20
1	A	206	HIS	CB-CG-CD2	-6.50	122.75	131.20
1	E	161	HIS	CB-CG-CD2	-6.50	122.75	131.20
1	F	179[A]	HIS	CB-CG-CD2	-6.47	122.78	131.20
1	F	179[B]	HIS	CB-CG-CD2	-6.47	122.78	131.20
1	C	206	HIS	CB-CG-CD2	-6.47	122.79	131.20
1	E	206	HIS	CB-CG-CD2	-6.47	122.80	131.20
1	D	401	HIS	CB-CG-CD2	-6.46	122.80	131.20
1	D	559	ILE	N-CA-C	6.45	117.08	110.82
1	F	206	HIS	CB-CG-CD2	-6.44	122.82	131.20
1	B	495	HIS	CB-CG-CD2	-6.28	123.04	131.20
1	A	428	HIS	CB-CG-ND1	5.96	131.65	122.70
1	E	137	GLY	CA-C-N	5.75	125.70	119.78
1	E	137	GLY	C-N-CA	5.75	125.70	119.78
1	C	161	HIS	CB-CG-ND1	5.73	131.30	122.70
1	A	351	HIS	CB-CG-ND1	5.70	131.26	122.70
1	E	161	HIS	CB-CG-ND1	5.70	131.25	122.70
1	C	86	HIS	CB-CG-ND1	5.70	131.25	122.70
1	B	161	HIS	CB-CG-ND1	5.67	131.21	122.70
1	D	179	HIS	CB-CG-ND1	5.67	131.20	122.70
1	C	401	HIS	CB-CG-ND1	5.66	131.19	122.70
1	B	401	HIS	CB-CG-ND1	5.65	131.18	122.70
1	A	401	HIS	CB-CG-ND1	5.65	131.18	122.70
1	F	401	HIS	CB-CG-ND1	5.65	131.18	122.70
1	C	179	HIS	CB-CG-ND1	5.65	131.17	122.70
1	F	161	HIS	CB-CG-ND1	5.64	131.17	122.70
1	E	401	HIS	CB-CG-ND1	5.64	131.16	122.70
1	F	179[A]	HIS	CB-CG-ND1	5.62	131.13	122.70
1	F	179[B]	HIS	CB-CG-ND1	5.62	131.13	122.70
1	E	206	HIS	CB-CG-ND1	5.62	131.12	122.70
1	F	206	HIS	CB-CG-ND1	5.59	131.09	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	401	HIS	CB-CG-ND1	5.58	131.08	122.70
1	A	206	HIS	CB-CG-ND1	5.58	131.07	122.70
1	C	206	HIS	CB-CG-ND1	5.54	131.01	122.70
1	B	495	HIS	CB-CG-ND1	5.46	130.89	122.70
1	A	126	SER	N-CA-C	5.11	117.24	111.11
1	B	3	ASN	CA-C-N	5.10	124.86	119.76
1	B	3	ASN	C-N-CA	5.10	124.86	119.76
1	A	242	ASN	CA-C-N	5.08	125.11	119.32
1	A	242	ASN	C-N-CA	5.08	125.11	119.32

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	4752	0	4532	31	0
1	B	4737	0	4513	38	0
1	C	4718	0	4494	32	0
1	D	4721	0	4506	57	0
1	E	4769	0	4551	41	0
1	F	4696	0	4470	46	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
3	A	24	0	32	4	0
3	B	18	0	24	2	0
3	C	42	0	56	6	0
3	D	36	0	48	16	0
3	E	24	0	32	13	0
3	F	18	0	24	5	0
4	A	8	0	6	0	0
4	D	4	0	3	3	0
4	E	4	0	3	1	0
5	A	380	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	296	0	0	3	0
5	C	350	0	0	4	0
5	D	305	0	0	3	0
5	E	295	0	0	1	0
5	F	182	0	0	1	0
All	All	30404	0	27294	242	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 4.

All (242) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:ASP:HB2	3:C:607:GOL:H32	1.41	1.01
1:D:32:ASN:HA	3:D:603:GOL:H11	1.45	0.99
1:A:434:MET:HE3	3:A:606:GOL:H2	1.48	0.94
1:D:58[A]:ILE:HD11	1:D:150:VAL:HG11	1.52	0.91
1:C:115:MET:HA	1:C:118:MET:HE2	1.60	0.83
1:D:208:SER:H	3:D:603:GOL:H32	1.46	0.81
1:E:560:SER:HA	1:E:564:TRP:HB2	1.62	0.81
1:A:113:ARG:HH21	3:A:604:GOL:H12	1.50	0.77
1:D:33:PHE:H	3:D:603:GOL:H11	1.49	0.77
1:F:113:ARG:HB3	3:F:603:GOL:H12	1.66	0.75
1:D:208:SER:H	3:D:603:GOL:C3	2.01	0.74
1:D:423:ASP:HB3	1:D:426:THR:HG22	1.69	0.74
1:D:58[A]:ILE:HD11	1:D:150:VAL:CG1	2.18	0.72
1:D:583:LEU:HD22	3:D:605:GOL:H12	1.72	0.72
1:D:157:PRO:HG3	5:D:999:HOH:O	1.90	0.71
1:D:44:ARG:HG2	5:D:836:HOH:O	1.89	0.71
1:A:59:ARG:HD2	3:A:606:GOL:H12	1.72	0.71
1:B:251:LYS:HE3	1:B:253:ASP:OD2	1.91	0.70
1:C:118:MET:HE3	1:C:257:LEU:HG	1.73	0.70
1:E:32:ASN:HA	3:E:604:GOL:H32	1.73	0.69
1:D:58[A]:ILE:CD1	1:D:150:VAL:HG11	2.23	0.69
1:D:156:GLU:OE1	4:D:608:ACT:H2	1.93	0.69
1:E:208:SER:H	3:E:604:GOL:C1	2.06	0.68
1:D:33:PHE:N	3:D:603:GOL:H11	2.09	0.68
1:A:203:THR:HB	1:A:204:PRO:HD3	1.76	0.67
1:B:577:ASN:HB3	5:B:861:HOH:O	1.93	0.67
1:B:75:ARG:HG2	1:B:151:ASP:OD1	1.93	0.67
1:B:98:LEU:HA	1:B:101:MET:HE3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:ASN:CA	3:D:603:GOL:H11	2.22	0.67
1:E:75:ARG:HG3	1:E:149:LEU:HD21	1.78	0.66
1:A:104:ARG:HG2	1:A:104:ARG:HH11	1.62	0.65
1:D:557:VAL:HG13	1:D:579:GLU:HB3	1.77	0.65
1:D:61:PHE:CZ	1:D:74:ARG:HG2	2.32	0.65
1:E:333:ILE:HD13	1:E:354:VAL:HG22	1.79	0.65
1:C:183:TYR:HE2	1:C:185:GLU:HG2	1.62	0.64
1:D:392:TRP:HB3	1:D:418:LEU:HD11	1.79	0.64
1:C:112:ASP:HB2	3:C:607:GOL:C3	2.24	0.64
1:A:434:MET:CE	3:A:606:GOL:H2	2.26	0.64
1:D:32:ASN:HA	3:D:603:GOL:C1	2.26	0.64
1:C:583:LEU:HD22	3:C:603:GOL:H32	1.81	0.62
1:A:61:PHE:CZ	1:A:74:ARG:HG2	2.35	0.62
1:C:348:LEU:HB2	1:C:405:VAL:HB	1.82	0.62
1:C:552:ASN:O	3:C:606:GOL:H2	2.00	0.62
1:C:434:MET:HE1	5:C:803:HOH:O	1.99	0.62
1:D:33:PHE:H	3:D:603:GOL:C1	2.11	0.62
1:D:381:GLU:OE2	3:D:606:GOL:H11	2.00	0.62
1:E:559:ILE:O	1:E:564:TRP:HD1	1.84	0.61
1:C:58:ILE:HD11	1:C:150:VAL:HG13	1.82	0.61
1:E:392:TRP:HB3	1:E:418:LEU:HD11	1.84	0.60
1:D:208:SER:N	3:D:603:GOL:H32	2.16	0.60
1:F:348:LEU:HB2	1:F:405:VAL:HB	1.84	0.59
1:A:464:TYR:CD1	1:A:466:MET:HG2	2.37	0.59
1:B:294:ASN:HA	3:B:604:GOL:H11	1.85	0.59
1:E:113:ARG:HE	3:E:603:GOL:H32	1.66	0.59
1:B:175:GLU:HB3	1:B:176:PRO:HA	1.84	0.59
1:E:395:LYS:HD3	1:E:414:ASP:CG	2.28	0.59
1:B:341:THR:HA	1:B:348:LEU:HD23	1.85	0.59
1:B:559:ILE:O	1:B:564:TRP:HD1	1.85	0.58
1:E:102:ARG:HH12	3:E:603:GOL:H12	1.69	0.58
1:C:233:TRP:HZ3	1:C:244:LEU:HD12	1.69	0.58
1:C:412:PRO:HB2	1:C:415:LEU:HG	1.84	0.58
1:D:365:LYS:HD3	3:D:606:GOL:H2	1.86	0.58
1:F:67:GLU:HG3	1:F:162:HIS:ND1	2.18	0.58
1:E:542:ASN:HB2	1:E:586:ASP:OD1	2.05	0.57
1:F:113:ARG:CB	3:F:603:GOL:H12	2.34	0.57
1:E:156:GLU:HG2	1:E:159:HIS:HB2	1.86	0.57
1:F:233:TRP:HZ3	1:F:244:LEU:HD23	1.70	0.56
1:B:333:ILE:HD13	1:B:354:VAL:HG22	1.86	0.56
1:D:65:LEU:HD21	1:D:74:ARG:NH1	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:575:GLU:HG3	1:D:578:VAL:HG21	1.88	0.56
1:A:74:ARG:HD2	1:A:152:ALA:HB3	1.88	0.55
1:B:500:LYS:HE3	1:B:571:TYR:CZ	2.42	0.55
1:E:449:TYR:OH	1:E:452:GLY:HA2	2.07	0.55
1:F:280:ILE:HD11	5:F:805:HOH:O	2.07	0.55
1:D:276:TYR:HB2	1:D:426:THR:OG1	2.06	0.55
1:E:377:ARG:CZ	1:E:408:LEU:HD21	2.37	0.55
1:A:395:LYS:HD2	1:A:414:ASP:CG	2.31	0.55
1:C:1:MET:N	1:C:2:PRO:CD	2.69	0.55
1:A:1:MET:N	1:A:2:PRO:CD	2.70	0.55
1:B:75:ARG:NH2	5:B:701:HOH:O	2.40	0.55
1:A:104:ARG:HG2	1:A:104:ARG:NH1	2.21	0.54
1:D:113:ARG:HH21	3:D:604:GOL:H2	1.72	0.54
1:B:52:GLU:OE1	1:B:590:ARG:NH1	2.40	0.54
1:F:166:ARG:HG3	1:F:269:GLU:OE2	2.08	0.54
1:E:208:SER:H	3:E:604:GOL:H11	1.73	0.54
1:D:41:ASN:O	1:D:44:ARG:NH1	2.41	0.54
1:E:33:PHE:H	3:E:604:GOL:H32	1.73	0.54
1:B:69:VAL:HG13	1:B:70:PRO:HD2	1.89	0.53
1:B:40:THR:HG21	1:B:210:PRO:HB3	1.89	0.53
1:C:371:ILE:HD12	1:C:372:ALA:N	2.23	0.53
1:F:539:GLU:OE1	1:F:539:GLU:N	2.34	0.53
1:A:202:ALA:HB1	5:A:713:HOH:O	2.08	0.53
1:D:58[A]:ILE:HG23	5:D:920:HOH:O	2.09	0.52
1:A:421:ILE:CD1	1:A:426:THR:HG21	2.39	0.52
1:E:75:ARG:CG	1:E:149:LEU:HD21	2.40	0.52
1:F:392:TRP:HB3	1:F:418:LEU:HD11	1.92	0.52
1:F:51:SER:HB3	1:F:57:ALA:HB2	1.91	0.51
1:E:51[A]:SER:HB2	1:E:57:ALA:HB2	1.91	0.51
1:F:203:THR:HB	1:F:204:PRO:HD3	1.93	0.50
1:B:392:TRP:HB3	1:B:418:LEU:HD11	1.93	0.50
1:B:557:VAL:HG13	1:B:579:GLU:HB3	1.93	0.50
1:B:15:SER:HA	1:B:77:TYR:CE2	2.47	0.50
1:F:263:TYR:CZ	3:F:602:GOL:H32	2.47	0.50
1:F:335:LEU:HB3	1:F:352:LEU:HG	1.93	0.50
1:B:263:TYR:CZ	3:B:602:GOL:H32	2.47	0.49
1:E:13:LEU:HD23	1:E:76:ALA:HB2	1.94	0.49
1:A:302:VAL:O	1:A:303:ASN:HB2	2.12	0.49
1:B:564:TRP:CZ2	1:E:2:PRO:HA	2.47	0.49
1:F:500:LYS:HE3	1:F:571:TYR:CZ	2.48	0.49
1:A:410:ASN:N	1:A:411:PRO:HD3	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:ILE:HD11	1:C:150:VAL:CG1	2.41	0.49
1:F:229:ALA:C	1:F:231:PRO:HD3	2.37	0.49
1:C:467:LYS:NZ	3:C:603:GOL:H11	2.28	0.49
1:F:156:GLU:N	1:F:157:PRO:HD3	2.28	0.49
1:D:449:TYR:OH	1:D:452:GLY:HA2	2.13	0.48
1:E:32:ASN:CA	3:E:604:GOL:H32	2.43	0.48
1:E:98:LEU:HB2	1:E:120:ILE:HD13	1.95	0.48
1:A:450:TRP:HD1	5:A:724:HOH:O	1.95	0.48
1:C:233:TRP:CZ3	1:C:244:LEU:HD12	2.46	0.48
1:F:340:PHE:CE2	1:F:351:HIS:HB3	2.48	0.48
1:C:263:TYR:CZ	3:C:601:GOL:H11	2.48	0.48
1:D:51[B]:SER:OG	1:D:228:PHE:HE2	1.97	0.48
1:C:183:TYR:CE2	1:C:185:GLU:HG2	2.45	0.48
1:D:184:GLN:HB3	1:D:186:LEU:HD13	1.95	0.48
1:F:114:GLU:H	3:F:603:GOL:C3	2.27	0.47
1:A:85:GLN:HG2	5:A:727:HOH:O	2.14	0.47
1:E:575:GLU:HB2	1:E:578:VAL:HG21	1.95	0.47
1:F:61:PHE:CE1	1:F:248:ILE:HD13	2.49	0.47
1:D:583:LEU:HB3	3:D:605:GOL:H32	1.95	0.47
1:E:149:LEU:HD13	1:E:149:LEU:C	2.40	0.47
1:B:60:PHE:CD2	1:B:229:ALA:HA	2.50	0.47
1:D:426:THR:HG23	1:D:427:THR:N	2.30	0.47
1:F:61:PHE:CD1	1:F:248:ILE:HD13	2.48	0.47
1:E:131:ARG:HA	5:E:866:HOH:O	2.14	0.47
1:E:208:SER:O	3:E:604:GOL:H11	2.14	0.47
1:F:67:GLU:CG	1:F:162:HIS:ND1	2.78	0.47
1:D:426:THR:HG23	1:D:427:THR:H	1.80	0.47
1:E:33:PHE:H	3:E:604:GOL:C3	2.28	0.47
1:C:1:MET:HE3	1:C:192:ASP:CG	2.40	0.47
1:D:554:GLN:O	1:D:569:SER:HA	2.15	0.47
1:A:67:GLU:HG3	1:A:165:GLY:O	2.15	0.46
1:C:40:THR:O	1:C:41:ASN:C	2.58	0.46
1:F:493:PHE:CD1	1:F:514:HIS:HB3	2.49	0.46
1:B:465:GLN:HG2	5:B:995:HOH:O	2.15	0.46
1:D:113:ARG:NH2	3:D:604:GOL:H2	2.29	0.46
1:E:271:GLU:HG2	1:E:430:GLN:NE2	2.30	0.46
1:B:242:ASN:HB3	1:B:245:ASP:OD2	2.15	0.46
1:F:35:GLU:HG2	1:F:210:PRO:HG3	1.96	0.46
1:E:33:PHE:N	3:E:604:GOL:H32	2.30	0.46
1:A:434:MET:HE1	5:A:823:HOH:O	2.15	0.46
1:B:348:LEU:HB2	1:B:405:VAL:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:LEU:HB2	1:A:405:VAL:HB	1.98	0.46
1:E:554:GLN:O	1:E:569:SER:HA	2.16	0.46
1:E:273:THR:HG21	1:E:431:PHE:HB2	1.98	0.46
1:C:1:MET:H3	1:C:2:PRO:HD3	1.81	0.45
1:A:393:ASN:HA	1:A:415:LEU:HD23	1.98	0.45
1:B:58:ILE:HG22	1:B:58:ILE:O	2.15	0.45
1:D:500:LYS:HE3	1:D:571:TYR:CZ	2.52	0.45
1:E:557:VAL:HG13	1:E:579:GLU:HB3	1.99	0.45
1:A:280:ILE:HD13	1:A:280:ILE:HA	1.79	0.45
1:F:423:ASP:C	1:F:423:ASP:OD1	2.60	0.45
1:B:576:SER:O	1:B:577:ASN:HB2	2.18	0.44
1:F:554:GLN:O	1:F:569:SER:HA	2.18	0.44
1:F:341:THR:HA	1:F:348:LEU:HD23	1.98	0.44
1:F:449:TYR:OH	1:F:452:GLY:HA2	2.17	0.44
1:A:71:GLU:HA	1:A:71:GLU:OE1	2.17	0.44
1:B:107:VAL:HG11	1:D:153:VAL:HG12	1.99	0.44
1:B:280:ILE:HD11	1:B:419:GLN:CD	2.43	0.44
1:B:365:LYS:HD2	1:B:381:GLU:OE2	2.18	0.44
1:A:554:GLN:O	1:A:569:SER:HA	2.18	0.44
1:B:251:LYS:HE3	1:B:253:ASP:CG	2.42	0.44
1:D:424:GLU:HG2	4:D:608:ACT:H3	1.99	0.44
1:E:51[B]:SER:OG	1:E:56:ALA:HB3	2.18	0.44
1:E:233:TRP:CH2	1:E:244:LEU:HD12	2.53	0.44
1:A:421:ILE:HD11	1:A:426:THR:HG21	1.99	0.43
1:B:564:TRP:CZ3	1:E:1:MET:N	2.80	0.43
1:D:16:PRO:O	1:D:20:PHE:HB2	2.17	0.43
1:F:365:LYS:HE3	1:F:379:SER:OG	2.18	0.43
1:A:577:ASN:CG	1:A:577:ASN:O	2.62	0.43
1:B:542:ASN:HB2	1:B:586:ASP:OD1	2.17	0.43
1:F:367:THR:HA	1:F:368:PRO:HD3	1.87	0.43
1:B:16:PRO:O	1:B:20:PHE:HB2	2.17	0.43
1:B:412:PRO:HB2	1:B:415:LEU:HG	1.99	0.43
1:F:233:TRP:CZ3	1:F:243:PRO:HB2	2.52	0.43
1:D:51[A]:SER:OG	1:D:56:ALA:HB3	2.17	0.43
1:D:424:GLU:HG2	4:D:608:ACT:CH3	2.49	0.43
1:B:341:THR:HA	1:B:348:LEU:CD2	2.48	0.43
1:C:78:LEU:O	1:C:147:ALA:HA	2.18	0.43
1:D:276:TYR:CB	1:D:426:THR:OG1	2.67	0.43
1:E:113:ARG:NE	3:E:603:GOL:H32	2.31	0.43
1:F:16:PRO:O	1:F:20:PHE:HB2	2.19	0.43
1:D:40:THR:O	1:D:41:ASN:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:281:LYS:HB2	1:D:416:GLU:OE1	2.18	0.43
1:D:333:ILE:HD13	1:D:354:VAL:HG22	2.00	0.43
1:C:371:ILE:HD12	1:C:371:ILE:C	2.44	0.43
1:D:198:THR:HB	1:D:199:PRO:HD2	2.00	0.43
1:D:341:THR:HA	1:D:348:LEU:HD23	2.00	0.43
1:F:114:GLU:H	3:F:603:GOL:H32	1.84	0.43
1:F:282:THR:O	1:F:283:GLN:HB2	2.19	0.43
1:F:297:VAL:HG22	1:F:352:LEU:HD13	2.01	0.42
1:A:201:ILE:HD12	1:A:201:ILE:H	1.82	0.42
1:D:273:THR:HG21	1:D:431:PHE:HB2	2.02	0.42
1:E:156:GLU:OE1	4:E:606:ACT:H3	2.19	0.42
1:A:73:PRO:HG3	5:C:833:HOH:O	2.19	0.42
1:F:333:ILE:HD13	1:F:354:VAL:HG22	2.02	0.42
1:F:373:ILE:HG22	1:F:373:ILE:O	2.20	0.42
1:D:187:GLN:OE1	1:D:187:GLN:HA	2.19	0.42
1:E:51[B]:SER:HG	1:E:56:ALA:HB3	1.83	0.42
1:E:203:THR:HB	1:E:204:PRO:HA	2.02	0.42
1:F:410:ASN:N	1:F:411:PRO:HD3	2.35	0.42
1:D:133:TRP:CZ3	1:D:190:ALA:HB1	2.55	0.42
1:F:116:ALA:O	1:F:120:ILE:HG23	2.20	0.42
1:C:235:PRO:HA	1:C:236:PRO:HD3	1.95	0.42
1:F:365:LYS:HE3	1:F:365:LYS:HB2	1.82	0.42
1:E:353:SER:OG	3:E:605:GOL:H11	2.19	0.42
1:A:74:ARG:HD2	1:A:152:ALA:CB	2.50	0.41
1:C:242:ASN:HA	1:C:243:PRO:HD3	1.90	0.41
1:F:154:PRO:HG2	1:F:157:PRO:HG3	2.02	0.41
1:F:273:THR:HG21	1:F:431:PHE:HB2	2.02	0.41
1:F:291:ASP:HA	1:F:292:PRO:HD3	1.90	0.41
1:F:78:LEU:O	1:F:147:ALA:HA	2.20	0.41
1:B:235:PRO:HA	1:B:236:PRO:HD3	1.94	0.41
1:F:75:ARG:HD3	1:F:151:ASP:OD1	2.20	0.41
1:C:367:THR:HG23	5:C:815:HOH:O	2.21	0.41
1:B:242:ASN:HA	1:B:243:PRO:HD3	1.93	0.41
1:D:51[B]:SER:OG	1:D:228:PHE:CE2	2.74	0.41
1:B:74:ARG:C	1:B:75:ARG:HG3	2.46	0.41
1:D:61:PHE:CE1	1:D:74:ARG:HG2	2.55	0.41
1:F:408:LEU:O	1:F:411:PRO:HD3	2.21	0.41
1:D:65:LEU:CD2	1:D:74:ARG:NH1	2.83	0.41
1:C:2:PRO:HD3	1:C:536:PRO:HG3	2.03	0.41
1:C:175:GLU:HB3	1:C:176:PRO:HA	2.02	0.41
1:C:367:THR:HA	1:C:368:PRO:HD3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:113:ARG:HH21	3:E:603:GOL:H32	1.86	0.40
1:C:341:THR:HA	1:C:348:LEU:HD23	2.04	0.40
1:D:233:TRP:HZ3	1:D:244:LEU:HD23	1.85	0.40
1:C:371:ILE:HG13	5:C:845:HOH:O	2.22	0.40
1:D:32:ASN:C	3:D:603:GOL:H11	2.47	0.40
1:F:483:PHE:HB3	1:F:493:PHE:CD2	2.56	0.40
1:A:40:THR:O	1:A:41:ASN:C	2.64	0.40
1:B:302:VAL:O	1:B:303:ASN:HB2	2.21	0.40
1:D:175:GLU:OE1	1:D:175:GLU:HA	2.22	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	577/591 (98%)	558 (97%)	18 (3%)	1 (0%)	43	36
1	B	575/591 (97%)	556 (97%)	19 (3%)	0	100	100
1	C	569/591 (96%)	555 (98%)	14 (2%)	0	100	100
1	D	571/591 (97%)	554 (97%)	16 (3%)	1 (0%)	43	36
1	E	580/591 (98%)	565 (97%)	14 (2%)	1 (0%)	43	36
1	F	564/591 (95%)	540 (96%)	23 (4%)	1 (0%)	43	36
All	All	3436/3546 (97%)	3328 (97%)	104 (3%)	4 (0%)	48	40

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	THR
1	E	219	SER
1	F	432	VAL
1	D	432	VAL

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	518/524 (99%)	513 (99%)	5 (1%)	68	70
1	B	516/524 (98%)	509 (99%)	7 (1%)	59	59
1	C	514/524 (98%)	509 (99%)	5 (1%)	68	70
1	D	516/524 (98%)	509 (99%)	7 (1%)	59	59
1	E	521/524 (99%)	517 (99%)	4 (1%)	73	75
1	F	513/524 (98%)	506 (99%)	7 (1%)	59	59
All	All	3098/3144 (98%)	3063 (99%)	35 (1%)	65	67

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	193	GLN
1	A	207	LEU
1	A	349	LYS
1	A	539	GLU
1	A	586	ASP
1	B	86	HIS
1	B	146	SER
1	B	149	LEU
1	B	293	GLN
1	B	386	THR
1	B	465	GLN
1	B	574	VAL
1	C	244	LEU
1	C	262	GLN
1	C	399	SER
1	C	539	GLU
1	C	590	ARG
1	D	186	LEU
1	D	201	ILE
1	D	207	LEU
1	D	416	GLU
1	D	465	GLN

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Mol	Chain	Res	Type
1	D	478	LYS
1	D	557	VAL
1	E	175	GLU
1	E	201	ILE
1	E	408	LEU
1	E	539	GLU
1	F	75	ARG
1	F	120	ILE
1	F	146	SER
1	F	251	LYS
1	F	328	LEU
1	F	352	LEU
1	F	383	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	289	GLN
1	A	369	GLN
1	A	486	GLN
1	A	489	GLN
1	B	85	GLN
1	B	189	GLN
1	B	262	GLN
1	B	289	GLN
1	B	343	GLN
1	B	496	ASN
1	B	517	ASN
1	B	523	ASN
1	C	85	GLN
1	C	262	GLN
1	C	283	GLN
1	C	289	GLN
1	C	369	GLN
1	D	22	HIS
1	D	159	HIS
1	D	189	GLN
1	D	283	GLN
1	D	289	GLN
1	D	369	GLN
1	D	496	ASN

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Mol	Chain	Res	Type
1	D	517	ASN
1	D	523	ASN
1	E	41	ASN
1	E	343	GLN
1	E	369	GLN
1	E	517	ASN
1	F	85	GLN
1	F	262	GLN
1	F	289	GLN
1	F	293	GLN
1	F	369	GLN
1	F	489	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](#)

36 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	$\# Z > 2$
4	ACT	A	607	-	3,3,3	0.82	0	3,3,3	1.19	0
3	GOL	A	605	-	5,5,5	0.35	0	5,5,5	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	C	605	-	5,5,5	0.33	0	5,5,5	0.36	0
3	GOL	D	602	-	5,5,5	0.36	0	5,5,5	0.59	0
2	SO4	B	601	-	4,4,4	0.28	0	6,6,6	0.08	0
3	GOL	A	604	-	5,5,5	0.35	0	5,5,5	0.34	0
3	GOL	C	604	-	5,5,5	0.36	0	5,5,5	0.33	0
3	GOL	C	607	-	5,5,5	0.36	0	5,5,5	0.98	0
3	GOL	C	606	-	5,5,5	0.34	0	5,5,5	0.53	0
2	SO4	A	601	-	4,4,4	0.30	0	6,6,6	0.24	0
3	GOL	D	607	-	5,5,5	0.34	0	5,5,5	0.37	0
3	GOL	F	601	-	5,5,5	0.40	0	5,5,5	0.33	0
4	ACT	E	606	-	3,3,3	0.81	0	3,3,3	1.18	0
3	GOL	F	603	-	5,5,5	0.32	0	5,5,5	0.29	0
4	ACT	D	608	-	3,3,3	0.83	0	3,3,3	1.16	0
3	GOL	B	602	-	5,5,5	0.47	0	5,5,5	0.20	0
4	ACT	A	608	-	3,3,3	0.73	0	3,3,3	1.35	0
3	GOL	D	606	-	5,5,5	0.39	0	5,5,5	0.28	0
3	GOL	D	604	-	5,5,5	0.35	0	5,5,5	0.31	0
3	GOL	D	605	-	5,5,5	0.35	0	5,5,5	0.26	0
3	GOL	C	603	-	5,5,5	0.41	0	5,5,5	0.43	0
3	GOL	A	606	-	5,5,5	0.34	0	5,5,5	0.78	0
3	GOL	B	604	-	5,5,5	0.41	0	5,5,5	0.45	0
2	SO4	A	602	-	4,4,4	0.22	0	6,6,6	0.16	0
3	GOL	C	601	-	5,5,5	0.40	0	5,5,5	0.44	0
3	GOL	D	603	-	5,5,5	0.36	0	5,5,5	0.69	0
3	GOL	E	602	-	5,5,5	0.42	0	5,5,5	0.32	0
2	SO4	D	601	-	4,4,4	0.81	0	6,6,6	1.35	1 (16%)
3	GOL	B	603	-	5,5,5	0.42	0	5,5,5	0.31	0
3	GOL	A	603	-	5,5,5	0.44	0	5,5,5	0.34	0
3	GOL	E	603	-	5,5,5	0.37	0	5,5,5	0.31	0
3	GOL	E	604	-	5,5,5	0.55	0	5,5,5	0.89	0
3	GOL	F	602	-	5,5,5	0.42	0	5,5,5	0.32	0
2	SO4	E	601	-	4,4,4	0.23	0	6,6,6	0.32	0
3	GOL	C	602	-	5,5,5	0.36	0	5,5,5	0.51	0
3	GOL	E	605	-	5,5,5	0.32	0	5,5,5	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	605	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	C	605	-	-	1/4/4/4	-
3	GOL	D	602	-	-	2/4/4/4	-
3	GOL	C	604	-	-	0/4/4/4	-
3	GOL	C	607	-	-	3/4/4/4	-
3	GOL	C	606	-	-	2/4/4/4	-
3	GOL	D	607	-	-	0/4/4/4	-
3	GOL	F	601	-	-	2/4/4/4	-
3	GOL	F	603	-	-	2/4/4/4	-
3	GOL	B	602	-	-	2/4/4/4	-
3	GOL	D	606	-	-	3/4/4/4	-
3	GOL	D	604	-	-	2/4/4/4	-
3	GOL	D	605	-	-	4/4/4/4	-
3	GOL	C	603	-	-	2/4/4/4	-
3	GOL	A	606	-	-	3/4/4/4	-
3	GOL	B	604	-	-	1/4/4/4	-
3	GOL	C	601	-	-	0/4/4/4	-
3	GOL	D	603	-	-	0/4/4/4	-
3	GOL	E	602	-	-	0/4/4/4	-
3	GOL	B	603	-	-	0/4/4/4	-
3	GOL	A	603	-	-	0/4/4/4	-
3	GOL	E	603	-	-	2/4/4/4	-
3	GOL	E	604	-	-	4/4/4/4	-
3	GOL	F	602	-	-	2/4/4/4	-
3	GOL	A	604	-	-	3/4/4/4	-
3	GOL	C	602	-	-	2/4/4/4	-
3	GOL	E	605	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	SO4	O4-S-O2	3.03	125.42	109.56

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	606	GOL	C1-C2-C3-O3
3	C	602	GOL	C1-C2-C3-O3
3	C	603	GOL	O1-C1-C2-C3
3	C	606	GOL	O1-C1-C2-C3
3	C	607	GOL	O1-C1-C2-C3
3	D	602	GOL	O1-C1-C2-C3
3	D	604	GOL	C1-C2-C3-O3
3	D	604	GOL	O2-C2-C3-O3
3	D	605	GOL	O1-C1-C2-C3
3	D	605	GOL	C1-C2-C3-O3
3	D	606	GOL	C1-C2-C3-O3
3	E	603	GOL	O1-C1-C2-C3
3	E	604	GOL	O1-C1-C2-O2
3	E	604	GOL	O1-C1-C2-C3
3	E	604	GOL	C1-C2-C3-O3
3	E	605	GOL	O1-C1-C2-C3
3	F	601	GOL	C1-C2-C3-O3
3	C	607	GOL	O1-C1-C2-O2
3	D	606	GOL	O2-C2-C3-O3
3	E	603	GOL	O1-C1-C2-O2
3	A	604	GOL	C1-C2-C3-O3
3	A	605	GOL	O1-C1-C2-C3
3	C	605	GOL	O1-C1-C2-C3
3	F	603	GOL	O1-C1-C2-C3
3	C	602	GOL	O2-C2-C3-O3
3	C	606	GOL	O1-C1-C2-O2
3	E	604	GOL	O2-C2-C3-O3
3	E	605	GOL	O1-C1-C2-O2
3	F	601	GOL	O2-C2-C3-O3
3	A	606	GOL	O2-C2-C3-O3
3	C	603	GOL	O1-C1-C2-O2
3	D	602	GOL	O1-C1-C2-O2
3	D	605	GOL	O1-C1-C2-O2
3	D	605	GOL	O2-C2-C3-O3
3	F	603	GOL	O1-C1-C2-O2
3	A	604	GOL	O1-C1-C2-O2
3	B	602	GOL	O1-C1-C2-O2
3	C	607	GOL	O2-C2-C3-O3
3	D	606	GOL	O1-C1-C2-O2
3	B	604	GOL	O1-C1-C2-O2
3	A	606	GOL	O1-C1-C2-C3
3	B	602	GOL	O1-C1-C2-C3
3	A	605	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	F	602	GOL	O2-C2-C3-O3
3	F	602	GOL	O1-C1-C2-O2
3	A	604	GOL	O2-C2-C3-O3

There are no ring outliers.

19 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	604	GOL	1	0
3	C	607	GOL	2	0
3	C	606	GOL	1	0
4	E	606	ACT	1	0
3	F	603	GOL	4	0
4	D	608	ACT	3	0
3	B	602	GOL	1	0
3	D	606	GOL	2	0
3	D	604	GOL	2	0
3	D	605	GOL	2	0
3	C	603	GOL	2	0
3	A	606	GOL	3	0
3	B	604	GOL	1	0
3	C	601	GOL	1	0
3	D	603	GOL	10	0
3	E	603	GOL	4	0
3	E	604	GOL	8	0
3	F	602	GOL	1	0
3	E	605	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	582/591 (98%)	-0.10	27 (4%)	37	40	9, 19, 43, 65	1 (0%)
1	B	580/591 (98%)	0.27	47 (8%)	18	19	12, 24, 51, 75	1 (0%)
1	C	577/591 (97%)	-0.09	22 (3%)	44	47	12, 21, 44, 65	0
1	D	577/591 (97%)	0.08	29 (5%)	34	36	11, 23, 48, 74	2 (0%)
1	E	582/591 (98%)	0.12	32 (5%)	30	32	11, 26, 52, 78	4 (0%)
1	F	573/591 (96%)	0.55	42 (7%)	21	22	18, 31, 56, 84	1 (0%)
All	All	3471/3546 (97%)	0.14	199 (5%)	29	31	9, 24, 50, 84	9 (0%)

All (199) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	203	THR	7.1
1	C	345	ALA	5.6
1	D	201	ILE	5.5
1	E	236	PRO	5.3
1	B	70	PRO	5.2
1	F	574	VAL	5.2
1	B	72	HIS	5.0
1	F	564	TRP	5.0
1	A	464	TYR	4.9
1	A	345	ALA	4.9
1	B	69	VAL	4.6
1	B	201	ILE	4.6
1	A	236	PRO	4.6
1	F	72	HIS	4.5
1	E	344	TYR	4.4
1	D	202	ALA	4.3
1	D	70	PRO	4.3
1	E	201	ILE	4.3
1	B	308	SER	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	564	TRP	4.1
1	F	573	LYS	4.1
1	F	203	THR	4.0
1	C	204	PRO	4.0
1	F	559	ILE	3.9
1	A	204	PRO	3.9
1	C	2	PRO	3.8
1	F	236	PRO	3.8
1	E	371	ILE	3.8
1	D	236	PRO	3.8
1	E	1	MET	3.8
1	F	179[A]	HIS	3.8
1	B	202	ALA	3.8
1	F	71	GLU	3.8
1	D	72	HIS	3.7
1	E	564	TRP	3.7
1	D	561	GLY	3.7
1	B	236	PRO	3.7
1	C	573	LYS	3.7
1	E	70	PRO	3.6
1	A	1	MET	3.5
1	E	72	HIS	3.5
1	A	68	TYR	3.5
1	F	198	THR	3.4
1	C	1	MET	3.4
1	D	68	TYR	3.4
1	A	450	TRP	3.4
1	D	564	TRP	3.3
1	D	343	GLN	3.3
1	F	343	GLN	3.3
1	B	200	GLY	3.3
1	C	236	PRO	3.3
1	B	559	ILE	3.2
1	C	308	SER	3.2
1	D	425	CYS	3.2
1	B	151	ASP	3.2
1	B	68	TYR	3.2
1	E	202	ALA	3.2
1	C	242	ASN	3.1
1	D	559	ILE	3.1
1	F	70	PRO	3.1
1	D	413	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	179[A]	HIS	3.1
1	C	198	THR	3.1
1	D	186	LEU	3.1
1	B	345	ALA	3.1
1	D	560	SER	3.1
1	F	3	ASN	3.1
1	B	233	TRP	3.0
1	A	201	ILE	3.0
1	C	413	SER	3.0
1	D	562	SER	3.0
1	B	27	LEU	2.9
1	E	560	SER	2.9
1	B	303	ASN	2.9
1	A	69	VAL	2.9
1	A	303	ASN	2.9
1	F	347	GLN	2.9
1	A	573	LYS	2.9
1	C	344	TYR	2.9
1	F	576	SER	2.9
1	B	280	ILE	2.9
1	E	413	SER	2.8
1	C	574	VAL	2.8
1	B	41	ASN	2.8
1	D	577	ASN	2.8
1	B	574	VAL	2.8
1	D	308	SER	2.7
1	B	149	LEU	2.7
1	B	199	PRO	2.7
1	B	560	SER	2.7
1	A	574	VAL	2.7
1	D	69	VAL	2.7
1	E	574	VAL	2.7
1	B	346	GLY	2.7
1	E	561	GLY	2.7
1	F	293	GLN	2.7
1	A	308	SER	2.7
1	F	560	SER	2.7
1	D	303	ASN	2.7
1	D	424	GLU	2.6
1	D	576	SER	2.6
1	C	538	VAL	2.6
1	E	562	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	577	ASN	2.6
1	B	176	PRO	2.6
1	C	309	SER	2.6
1	E	234	SER	2.6
1	F	462	TRP	2.6
1	C	74	ARG	2.6
1	C	244	LEU	2.5
1	F	450	TRP	2.5
1	A	503	GLY	2.5
1	B	246	LYS	2.5
1	C	346	GLY	2.5
1	F	74	ARG	2.5
1	B	71	GLU	2.5
1	D	574	VAL	2.5
1	B	344	TYR	2.5
1	F	244	LEU	2.5
1	F	591	PHE	2.5
1	D	3	ASN	2.5
1	B	450	TRP	2.5
1	E	2	PRO	2.5
1	B	394	THR	2.4
1	F	409	LYS	2.4
1	A	538	VAL	2.4
1	B	561	GLY	2.4
1	B	244	LEU	2.4
1	E	559	ILE	2.4
1	E	345	ALA	2.4
1	B	73	PRO	2.4
1	B	235	PRO	2.4
1	E	71	GLU	2.4
1	C	343	GLN	2.4
1	B	576	SER	2.4
1	B	281	LYS	2.4
1	F	453	TYR	2.4
1	A	29	ASP	2.4
1	A	424	GLU	2.4
1	B	413	SER	2.4
1	B	409	LYS	2.4
1	D	504	TYR	2.3
1	B	399	SER	2.3
1	B	505	SER	2.3
1	E	244	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	3	ASN	2.3
1	B	371	ILE	2.3
1	B	150	VAL	2.3
1	A	72	HIS	2.3
1	F	22	HIS	2.3
1	B	178	MET	2.3
1	F	280	ILE	2.3
1	C	293	GLN	2.3
1	F	69	VAL	2.3
1	B	174	ASN	2.3
1	F	242	ASN	2.3
1	A	397	GLY	2.2
1	F	558	ILE	2.2
1	B	410	ASN	2.2
1	E	424	GLU	2.2
1	A	413	SER	2.2
1	F	204	PRO	2.2
1	D	280	ILE	2.2
1	E	505	SER	2.2
1	F	397	GLY	2.2
1	A	2	PRO	2.2
1	E	243	PRO	2.2
1	E	425	CYS	2.2
1	F	562	SER	2.2
1	E	346	GLY	2.2
1	E	412	PRO	2.2
1	A	202	ALA	2.2
1	A	344	TYR	2.1
1	B	234	SER	2.1
1	E	308	SER	2.1
1	F	561	GLY	2.1
1	C	243	PRO	2.1
1	D	6	ARG	2.1
1	F	21	GLU	2.1
1	F	187	GLN	2.1
1	A	576	SER	2.1
1	D	203	THR	2.1
1	D	75	ARG	2.1
1	F	302	VAL	2.1
1	E	303	ASN	2.1
1	A	414	ASP	2.1
1	C	151	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	573	LYS	2.1
1	F	575	GLU	2.1
1	F	504	TYR	2.0
1	D	466	MET	2.0
1	B	242	ASN	2.0
1	F	303	ASN	2.0
1	F	506	TRP	2.0
1	C	505	SER	2.0
1	E	576	SER	2.0
1	F	399	SER	2.0
1	F	505	SER	2.0
1	B	77	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	E	603	6/6	0.70	0.16	36,39,43,47	0
3	GOL	F	603	6/6	0.70	0.19	29,33,35,41	6
2	SO4	D	601	5/5	0.75	0.15	32,34,40,43	5
3	GOL	F	601	6/6	0.79	0.16	29,30,31,32	6
3	GOL	C	602	6/6	0.80	0.14	19,23,26,28	6
3	GOL	D	604	6/6	0.81	0.16	30,34,41,43	0
3	GOL	B	604	6/6	0.81	0.15	26,31,37,39	6
3	GOL	D	607	6/6	0.83	0.14	30,35,37,43	6
3	GOL	B	603	6/6	0.84	0.15	21,22,24,24	6
3	GOL	A	605	6/6	0.84	0.15	16,28,31,32	6
3	GOL	A	606	6/6	0.85	0.15	9,18,19,19	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	D	606	6/6	0.85	0.17	28,36,37,38	6
3	GOL	C	603	6/6	0.86	0.16	18,26,27,30	6
3	GOL	C	607	6/6	0.86	0.16	22,26,39,40	6
3	GOL	C	606	6/6	0.87	0.12	27,29,32,32	6
3	GOL	E	605	6/6	0.88	0.14	25,29,30,39	6
2	SO4	B	601	5/5	0.89	0.11	32,35,37,41	5
3	GOL	A	604	6/6	0.89	0.13	29,35,36,37	6
3	GOL	C	605	6/6	0.89	0.12	23,29,32,37	6
3	GOL	D	603	6/6	0.90	0.12	20,22,30,34	6
3	GOL	C	604	6/6	0.90	0.11	31,38,44,50	0
4	ACT	E	606	4/4	0.90	0.12	27,33,34,34	4
2	SO4	A	602	5/5	0.91	0.10	30,30,35,37	5
3	GOL	E	604	6/6	0.91	0.13	19,27,32,32	6
4	ACT	A	608	4/4	0.91	0.09	15,19,20,22	4
3	GOL	E	602	6/6	0.91	0.09	20,23,28,29	6
3	GOL	D	602	6/6	0.92	0.08	21,24,30,31	6
3	GOL	D	605	6/6	0.92	0.10	23,30,34,35	6
3	GOL	C	601	6/6	0.92	0.09	17,21,21,23	6
3	GOL	F	602	6/6	0.93	0.08	25,29,32,32	6
3	GOL	A	603	6/6	0.93	0.08	16,20,26,30	6
4	ACT	D	608	4/4	0.94	0.09	23,28,31,33	4
3	GOL	B	602	6/6	0.94	0.08	17,23,23,26	6
4	ACT	A	607	4/4	0.97	0.05	20,25,26,26	0
2	SO4	E	601	5/5	0.99	0.03	17,18,22,23	0
2	SO4	A	601	5/5	0.99	0.03	15,15,19,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.