



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:08 AM UTC

PDB ID : 2WVX / pdb_00002wvx
Title : Structure of the Family GH92 Inverting Mannosidase BT3990 from Bacteroides
thetaiotaomicron VPI-5482
Authors : Suits, M.D.L.; Zhu, Y.; Thompson, A.; Gilbert, H.J.; Davies, G.J.
Deposited on : 2009-10-21
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

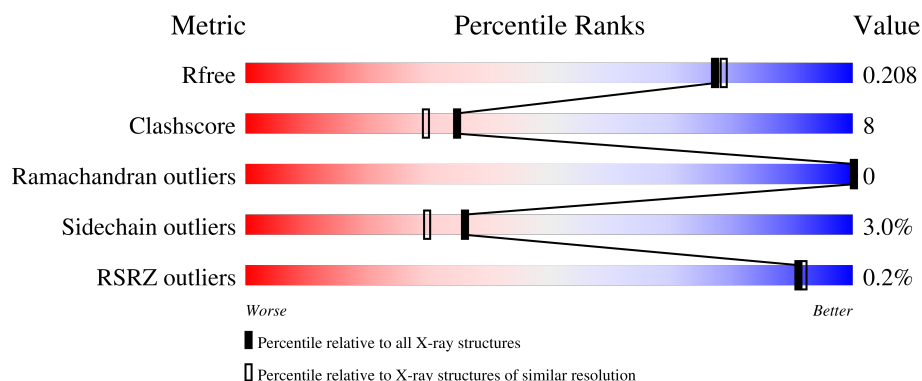
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

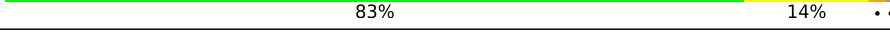
The reported resolution of this entry is 1.90 Å.

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	744	 84% 13% ..
1	C	744	 82% 15% ..
1	D	744	 84% 13% ..
2	B	744	 83% 14% ..

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
4	GOL	D	804	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 25973 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 PUTATIVE ALPHA-1,2-MANNOSIDASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	736	Total	C	N	O	S	Se	0	2	0
			5932	3801	974	1124	6	27			
1	C	736	Total	C	N	O	S	Se	0	6	0
			5972	3831	976	1129	6	30			
1	D	736	Total	C	N	O	S	Se	0	4	0
			5973	3831	982	1126	6	28			

- Molecule 2 is a protein called PUTATIVE ALPHA-1,2-MANNOSIDASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	737	Total	C	N	O	S	Se	0	5	0
			5974	3833	982	1124	6	29			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	216	GLN	ASN	conflict	UNP Q8A0N1

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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

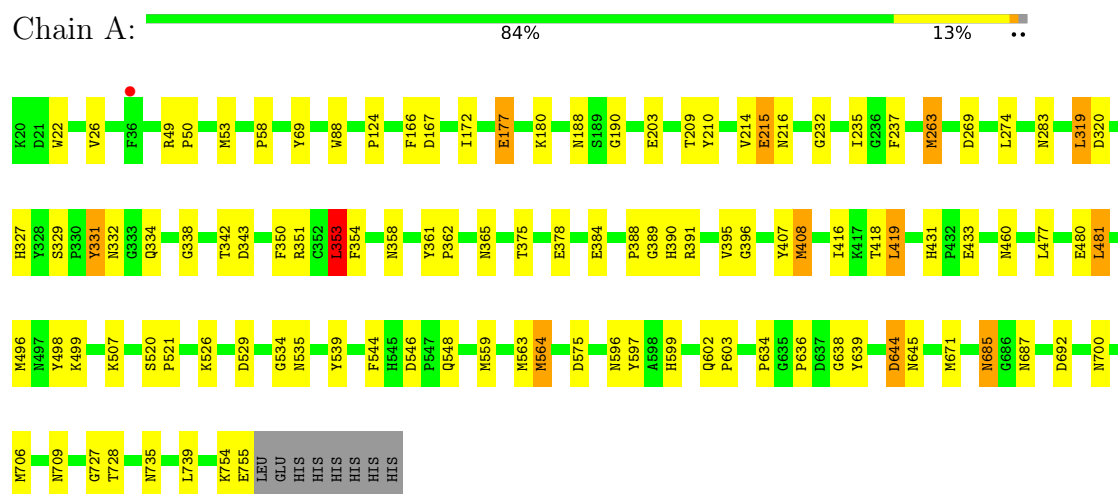
- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	529	Total	O		0	0
			529	529			
5	B	463	Total	O		0	0
			463	463			
5	C	531	Total	O		0	0
			531	531			
5	D	499	Total	O		0	0
			499	499			

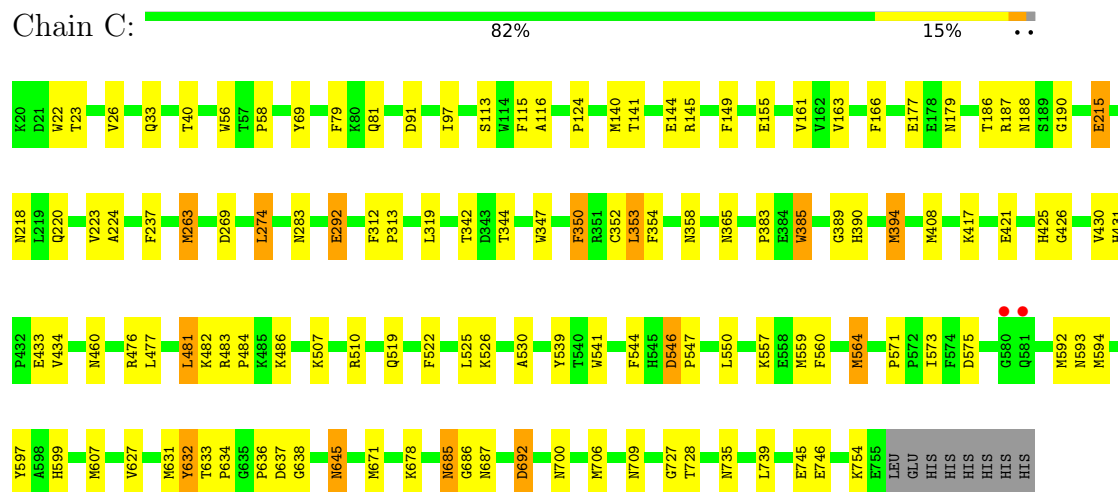
3 Residue-property plots

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.

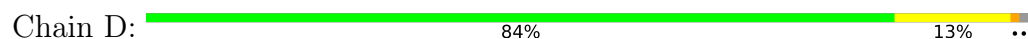
• Molecule 1: PUTATIVE ALPHA-1,2-MANNOSIDASE



• Molecule 1: PUTATIVE ALPHA-1,2-MANNOSIDASE



• Molecule 1: PUTATIVE ALPHA-1,2-MANNOSIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.23Å 190.95Å 135.10Å 90.00° 96.97° 90.00°	Depositor
Resolution (Å)	133.63 – 1.90 133.63 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.5 (133.63-1.90) 97.5 (133.63-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.70 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.4.0077	Depositor
R, R_{free}	0.155 , 0.186 0.182 , 0.208	Depositor DCC
R_{free} test set	12380 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	16.1	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25973	wwPDB-VP
Average B, all atoms (Å ²)	8.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.99	33/6086 (0.5%)	0.90	7/8226 (0.1%)
1	C	1.00	36/6141 (0.6%)	0.90	6/8292 (0.1%)
1	D	0.93	17/6136 (0.3%)	0.89	10/8283 (0.1%)
2	B	0.91	24/6136 (0.4%)	0.87	10/8282 (0.1%)
All	All	0.96	110/24499 (0.4%)	0.89	33/33083 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2

All (110) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	167	ASP	C-N	13.63	1.52	1.33
1	A	354	PHE	C-O	-10.30	1.14	1.24
2	B	394	MSE	SE-CE	-8.82	1.69	1.95
1	A	638	GLY	C-O	-8.44	1.13	1.23
1	C	342	THR	C-O	-7.94	1.16	1.24
1	D	88	TRP	C-O	-7.90	1.15	1.24
1	C	633	THR	C-O	-7.88	1.15	1.24
1	C	394	MSE	C-O	-7.54	1.14	1.24
2	B	396	GLY	C-O	-7.51	1.14	1.23
2	B	633	THR	C-O	-7.49	1.17	1.24
1	A	53	MSE	C-O	-7.36	1.15	1.24
1	D	389	GLY	C-O	-7.35	1.17	1.23
2	B	342	THR	C-O	-7.35	1.17	1.24
1	C	389	GLY	C-O	-7.31	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	215	GLU	C-O	-7.28	1.15	1.24
1	A	396	GLY	C-O	-7.27	1.14	1.23
1	C	632	TYR	C-O	-7.26	1.15	1.24
1	D	354	PHE	C-O	-7.19	1.17	1.24
1	C	425	HIS	C-O	-7.16	1.15	1.24
1	C	350	PHE	C-O	-6.96	1.15	1.24
2	B	166	PHE	C-O	-6.90	1.15	1.24
1	C	353	LEU	C-O	-6.80	1.16	1.24
1	D	390	HIS	C-O	-6.71	1.15	1.23
2	B	530	ALA	CA-CB	-6.66	1.42	1.53
1	D	351	ARG	C-O	-6.63	1.16	1.24
1	D	141	THR	C-O	-6.60	1.15	1.24
1	A	419	LEU	C-O	-6.52	1.16	1.24
1	C	144	GLU	C-O	-6.39	1.16	1.24
1	C	636	PRO	C-O	-6.38	1.16	1.24
2	B	350	PHE	C-O	-6.38	1.16	1.24
2	B	529	ASP	C-O	-6.36	1.16	1.24
2	B	544	PHE	C-O	-6.36	1.16	1.24
1	D	632	TYR	C-O	-6.35	1.16	1.24
1	D	636	PRO	C-O	-6.33	1.16	1.24
1	D	342	THR	C-O	-6.32	1.18	1.24
1	C	145	ARG	C-O	-6.30	1.16	1.24
1	C	354	PHE	C-O	-6.27	1.16	1.24
1	C	546	ASP	C-O	-6.24	1.16	1.24
1	C	141	THR	C-O	-6.22	1.16	1.24
1	C	224	ALA	C-O	-6.21	1.16	1.24
1	A	343	ASP	C-O	-6.20	1.15	1.23
1	A	390	HIS	C-O	-6.18	1.16	1.23
1	A	166	PHE	C-O	-6.17	1.16	1.24
1	C	544	PHE	C-O	-6.15	1.17	1.24
2	B	352	CYS	C-O	-6.13	1.17	1.24
1	A	342	THR	C-O	-6.08	1.18	1.24
1	C	113	SER	C-O	-6.08	1.16	1.23
1	C	163	VAL	C-O	-6.07	1.17	1.24
1	C	390	HIS	C-O	-6.04	1.16	1.23
2	B	425	HIS	C-O	-5.97	1.17	1.24
1	A	88	TRP	C-O	-5.95	1.17	1.24
2	B	88	TRP	C-O	-5.93	1.17	1.24
1	D	343	ASP	C-O	-5.91	1.16	1.23
2	B	141	THR	C-O	-5.90	1.16	1.24
1	D	352	CYS	C-O	-5.86	1.17	1.23
1	C	166	PHE	C-O	-5.81	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	384	GLU	C-O	-5.79	1.16	1.24
2	B	140	MSE	C-O	-5.77	1.16	1.23
1	A	391	ARG	C-O	-5.74	1.17	1.23
1	C	430	VAL	C-O	-5.74	1.18	1.24
1	A	215	GLU	C-O	-5.73	1.17	1.24
1	A	49	ARG	C-O	-5.71	1.16	1.23
1	A	334	GLN	C-O	-5.70	1.16	1.23
1	A	529	ASP	C-O	-5.69	1.16	1.24
1	C	634	PRO	C-O	-5.67	1.17	1.24
1	D	550	LEU	C-O	-5.65	1.17	1.24
1	C	638	GLY	C-O	-5.65	1.17	1.23
1	C	116	ALA	CA-CB	-5.61	1.39	1.54
2	B	391	ARG	C-O	-5.59	1.17	1.23
1	A	353	LEU	C-O	-5.58	1.17	1.24
1	D	359	LEU	C-O	-5.58	1.17	1.24
2	B	427	THR	C-O	-5.57	1.16	1.24
1	C	115	PHE	C-O	-5.55	1.17	1.23
1	D	638	GLY	C-O	-5.55	1.17	1.23
1	A	544	PHE	C-O	-5.53	1.17	1.24
1	A	416	ILE	C-O	-5.53	1.17	1.24
1	C	223	VAL	C-O	-5.52	1.18	1.24
1	A	639	TYR	C-O	-5.51	1.16	1.23
1	C	352	CYS	C-O	-5.51	1.17	1.23
1	A	535	ASN	C-O	-5.48	1.15	1.23
1	D	387	SER	C-O	-5.47	1.17	1.24
1	C	385	TRP	C-O	-5.45	1.17	1.24
1	A	50	PRO	C-O	-5.44	1.17	1.23
2	B	548	GLN	C-O	-5.39	1.17	1.24
1	C	383	PRO	C-O	-5.36	1.17	1.23
1	C	344	THR	C-O	-5.33	1.17	1.23
2	B	637	ASP	C-O	-5.29	1.15	1.23
1	A	548	GLN	C-O	-5.28	1.18	1.24
1	A	418	THR	C-O	-5.27	1.18	1.24
1	C	637	ASP	C-O	-5.26	1.15	1.23
1	A	351	ARG	C-O	-5.26	1.18	1.24
2	B	636	PRO	C-O	-5.24	1.17	1.24
1	A	634	PRO	C-O	-5.23	1.17	1.24
1	D	166	PHE	C-O	-5.23	1.17	1.24
1	A	546	ASP	C-O	-5.22	1.17	1.24
1	A	636	PRO	C-O	-5.21	1.17	1.24
1	C	426	GLY	C-O	-5.21	1.17	1.23
1	A	329	SER	C-O	-5.20	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	546	ASP	C-O	-5.20	1.17	1.24
2	B	354	PHE	C-O	-5.19	1.19	1.24
1	D	143	THR	C-O	-5.17	1.16	1.24
2	B	634	PRO	C-O	-5.15	1.17	1.24
1	A	332	ASN	C-O	-5.12	1.17	1.24
1	A	167	ASP	C-O	-5.11	1.16	1.24
1	A	331	TYR	C-O	-5.09	1.17	1.24
1	C	218	ASN	C-O	-5.08	1.17	1.24
1	C	530	ALA	CA-CB	-5.08	1.44	1.53
1	C	550	LEU	C-O	-5.07	1.18	1.24
1	A	214	VAL	C-O	-5.06	1.18	1.24
2	B	143	THR	C-O	-5.01	1.16	1.24

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	564	MSE	CG-SE-CE	-9.50	78.02	98.92
1	C	224	ALA	N-CA-C	8.40	120.52	111.36
1	D	564	MSE	CG-SE-CE	-7.93	81.47	98.92
1	A	638	GLY	N-CA-C	7.90	122.88	112.77
2	B	638	GLY	N-CA-C	7.74	122.02	112.73
2	B	170	SER	N-CA-C	7.57	118.78	108.56
1	C	638	GLY	N-CA-C	6.83	120.93	112.73
1	D	638	GLY	N-CA-C	6.63	121.26	112.77
1	C	263	MSE	CG-SE-CE	-6.39	84.87	98.92
1	D	224	ALA	N-CA-C	6.33	118.18	111.28
1	A	644	ASP	N-CA-C	6.25	119.87	111.24
2	B	395	VAL	N-CA-C	6.11	116.97	108.23
1	A	534	GLY	N-CA-C	6.04	119.09	110.46
1	A	342	THR	N-CA-C	5.99	116.14	108.24
1	C	91	ASP	N-CA-C	5.95	119.25	109.85
1	D	179	ASN	CB-CA-C	-5.80	103.25	111.95
1	D	342	THR	N-CA-C	5.72	115.79	108.24
2	B	645	ASN	CB-CA-C	-5.67	103.67	111.73
2	B	351	ARG	N-CA-C	5.63	117.10	111.07
1	D	330	PRO	N-CA-C	-5.58	108.87	114.68
1	C	179	ASN	CB-CA-C	-5.55	104.01	111.89
2	B	224	ALA	N-CA-C	5.53	118.23	111.82
1	D	556	GLY	N-CA-C	5.45	117.60	112.04
2	B	91	ASP	N-CA-C	5.42	117.91	109.52
1	D	395	VAL	N-CA-C	5.41	115.97	108.23
2	B	209	THR	N-CA-C	-5.39	106.63	114.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	637	ASP	CA-C-N	5.32	125.89	119.98
2	B	637	ASP	C-N-CA	5.32	125.89	119.98
1	D	644	ASP	N-CA-C	5.19	118.40	111.24
1	D	351	ARG	N-CA-C	5.18	116.61	111.07
1	A	395	VAL	N-CA-C	5.16	115.61	108.23
1	C	342	THR	N-CA-C	5.12	115.00	108.24
1	A	263	MSE	CG-SE-CE	-5.06	87.78	98.92

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	167	ASP	Mainchain

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	5932	0	5528	85	0
1	C	5972	0	5606	89	0
1	D	5973	0	5627	77	0
2	B	5974	0	5623	99	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	24	0	32	0	0
4	B	24	0	32	0	0
4	C	24	0	32	0	0
4	D	24	0	32	4	0
5	A	529	0	0	5	0
5	B	463	0	0	5	0
5	C	531	0	0	6	0
5	D	499	0	0	6	0
All	All	25973	0	22512	350	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 8.

All (350) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:MSE:CE	2:B:166:PHE:HA	1.12	1.57
2:B:63:MSE:CE	2:B:166:PHE:CA	1.90	1.48
2:B:592:MSE:HE2	2:B:631[B]:MSE:SE	1.64	1.46
1:A:496:MSE:CE	1:A:499:LYS:HE3	1.41	1.44
2:B:63:MSE:HE1	2:B:166:PHE:CA	1.51	1.37
2:B:63:MSE:HE2	2:B:166:PHE:CB	1.55	1.35
1:D:288:LYS:NZ	4:D:804:GOL:O1	1.64	1.31
1:A:507:LYS:CD	1:A:559:MSE:HE2	1.62	1.29
1:A:496:MSE:HE3	1:A:499:LYS:CE	1.74	1.17
1:A:496:MSE:CE	1:A:499:LYS:CE	2.20	1.17
2:B:63:MSE:HE2	2:B:166:PHE:CG	1.78	1.16
1:C:671:MSE:HE3	1:C:706:MSE:SE	1.94	1.16
1:A:407:TYR:CD1	1:A:408:MSE:HE3	1.83	1.13
1:A:507:LYS:HD2	1:A:559:MSE:HE2	1.25	1.12
2:B:63:MSE:HE3	2:B:166:PHE:HA	1.29	1.11
1:C:592:MSE:HE2	1:C:631[B]:MSE:HE3	1.32	1.11
1:D:587[A]:ARG:HH11	1:D:587[A]:ARG:HG2	1.03	1.09
1:A:408:MSE:HE2	1:A:408:MSE:HA	1.34	1.09
2:B:592:MSE:HE2	2:B:631[A]:MSE:CE	1.79	1.08
1:D:684:GLU:OE2	4:D:804:GOL:H11	1.54	1.07
1:A:407:TYR:HD1	1:A:408:MSE:CE	1.66	1.07
1:C:79:PHE:CD2	1:C:140[B]:MSE:CE	2.38	1.06
1:A:407:TYR:HD1	1:A:408:MSE:HE3	0.90	1.05
1:C:507:LYS:HD2	1:C:559:MSE:HE3	1.35	1.04
1:C:79:PHE:CD2	1:C:140[B]:MSE:HE1	1.91	1.04
2:B:63:MSE:CE	2:B:166:PHE:CG	2.41	1.02
2:B:592:MSE:CE	2:B:631[B]:MSE:SE	2.57	1.01
2:B:592:MSE:HE2	2:B:631[A]:MSE:HE3	1.38	0.95
1:C:592:MSE:HE2	1:C:631[B]:MSE:CE	1.83	0.93
2:B:188:ASN:HD22	2:B:190:GLY:H	1.05	0.92
2:B:63:MSE:HE1	2:B:166:PHE:C	1.94	0.92
2:B:419:LEU:HD13	2:B:419:LEU:C	1.94	0.91
2:B:63:MSE:CE	2:B:166:PHE:CB	2.28	0.91
1:A:358:ASN:HD21	1:A:365:ASN:HD22	1.19	0.90
2:B:631[B]:MSE:HG3	2:B:640:CYS:HB3	1.53	0.90
1:D:188:ASN:HD22	1:D:190:GLY:H	1.20	0.90
1:C:627:VAL:HG13	1:C:631[B]:MSE:HG3	1.54	0.90
1:D:288:LYS:NZ	4:D:804:GOL:HO1	1.68	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:MSE:HE2	2:B:166:PHE:HB3	1.52	0.89
1:C:79:PHE:HD2	1:C:140[B]:MSE:HE1	1.33	0.89
1:D:203:GLU:CD	1:D:263[B]:MSE:CE	2.46	0.89
1:A:188:ASN:HD22	1:A:190:GLY:H	1.19	0.87
1:D:587[A]:ARG:HH11	1:D:587[A]:ARG:CG	1.86	0.87
1:C:358:ASN:HD21	1:C:365:ASN:HD22	1.23	0.86
1:A:507:LYS:HD3	1:A:559:MSE:HE2	1.55	0.85
1:D:587[A]:ARG:HG2	1:D:587[A]:ARG:NH1	1.84	0.84
2:B:631[B]:MSE:HG3	2:B:640:CYS:CB	2.07	0.83
1:C:188:ASN:HD22	1:C:190:GLY:H	1.25	0.83
1:A:496:MSE:HE2	1:A:499:LYS:CE	2.09	0.82
1:A:496:MSE:HE2	1:A:499:LYS:NZ	1.93	0.82
1:A:407:TYR:CD1	1:A:408:MSE:CE	2.51	0.82
2:B:358:ASN:HD21	2:B:365:ASN:HD22	1.28	0.82
1:C:507:LYS:CD	1:C:559:MSE:HE3	2.09	0.82
1:C:507:LYS:HE3	1:C:559:MSE:HE2	1.60	0.81
2:B:63:MSE:HE1	2:B:166:PHE:HA	0.81	0.80
2:B:63:MSE:HE3	2:B:166:PHE:CD1	2.16	0.79
1:D:358:ASN:HD21	1:D:365:ASN:HD22	1.30	0.79
1:D:72[A]:THR:HG23	5:D:2052:HOH:O	1.82	0.79
1:A:358:ASN:ND2	1:A:365:ASN:HD22	1.81	0.78
1:A:507:LYS:CD	1:A:559:MSE:CE	2.56	0.78
1:C:79:PHE:HB3	1:C:140[B]:MSE:HE1	1.65	0.78
1:A:408:MSE:HA	1:A:408:MSE:CE	2.14	0.78
1:C:79:PHE:HD2	1:C:140[B]:MSE:CE	1.85	0.77
1:A:559:MSE:HE3	1:A:563:MSE:CG	2.16	0.76
1:C:507:LYS:CE	1:C:559:MSE:HE2	2.16	0.76
2:B:188:ASN:ND2	2:B:190:GLY:H	1.84	0.75
2:B:431:HIS:HD2	2:B:433:GLU:H	1.34	0.75
1:D:746:GLU:CD	1:D:746:GLU:H	1.94	0.75
1:A:507:LYS:HD2	1:A:559:MSE:CE	2.12	0.74
2:B:594:MSE:SE	2:B:631[B]:MSE:HE1	2.37	0.74
1:D:477:LEU:HG	1:D:481:LEU:HD22	1.70	0.74
1:A:559:MSE:HE3	1:A:563:MSE:HG2	1.71	0.73
1:A:496:MSE:HE3	1:A:499:LYS:HE3	0.77	0.73
1:A:22:TRP:H	1:A:283:ASN:ND2	1.88	0.72
1:D:431:HIS:HD2	1:D:433:GLU:H	1.36	0.72
2:B:63:MSE:HE3	2:B:166:PHE:CG	2.26	0.71
1:C:709:ASN:HD21	1:C:727:GLY:HA3	1.55	0.71
1:A:709:ASN:ND2	1:A:728:THR:H	1.88	0.71
2:B:419:LEU:C	2:B:419:LEU:CD1	2.64	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:MSE:O	1:C:263:MSE:HG3	1.89	0.71
1:C:358:ASN:ND2	1:C:365:ASN:HD22	1.88	0.71
1:D:203:GLU:CD	1:D:263[B]:MSE:HE3	2.15	0.71
1:C:431:HIS:HD2	1:C:433:GLU:H	1.37	0.71
2:B:263:MSE:O	2:B:263:MSE:HG3	1.91	0.70
2:B:431:HIS:CD2	2:B:433:GLU:H	2.09	0.70
1:C:507:LYS:HE3	1:C:559:MSE:CE	2.21	0.70
1:C:671:MSE:HE1	1:C:706:MSE:HE1	1.71	0.70
1:C:685:ASN:ND2	1:C:687:ASN:H	1.89	0.70
1:C:671:MSE:CE	1:C:706:MSE:HE1	2.22	0.70
1:C:431:HIS:CD2	1:C:433:GLU:H	2.09	0.70
1:C:594:MSE:SE	1:C:631[B]:MSE:SE	3.08	0.70
1:C:347:TRP:CZ3	1:C:394:MSE:HE2	2.27	0.69
1:A:644:ASP:CG	5:A:2454:HOH:O	2.34	0.69
1:A:203:GLU:CD	1:A:263:MSE:HE3	2.17	0.69
1:D:216[A]:ASN:HD21	1:D:230:HIS:H	1.41	0.69
1:D:358:ASN:ND2	1:D:365:ASN:HD22	1.90	0.69
1:A:22:TRP:H	1:A:283:ASN:HD21	1.40	0.68
1:D:38:LEU:HD12	1:D:588:GLU:HG3	1.76	0.68
1:A:597:TYR:OH	1:A:599:HIS:HD2	1.76	0.68
1:D:431:HIS:CD2	1:D:433:GLU:H	2.12	0.67
2:B:358:ASN:ND2	2:B:365:ASN:HD22	1.92	0.67
1:D:263[A]:MSE:HE2	1:D:266:LEU:HD12	1.75	0.67
1:D:709:ASN:HD21	1:D:727:GLY:HA3	1.59	0.67
1:C:507:LYS:CE	1:C:559:MSE:CE	2.73	0.67
1:D:525:LEU:HD13	1:D:573:ILE:HG13	1.76	0.67
1:D:203:GLU:OE1	1:D:263[B]:MSE:HE3	1.94	0.67
1:C:155:GLU:OE1	5:C:2113:HOH:O	2.12	0.66
1:C:22:TRP:H	1:C:283:ASN:ND2	1.94	0.66
1:C:269:ASP:HB2	1:C:274:LEU:HD13	1.77	0.66
1:A:431:HIS:HD2	1:A:433[A]:GLU:H	1.42	0.66
2:B:203:GLU:CD	2:B:263:MSE:HE3	2.20	0.66
1:C:269:ASP:CB	1:C:274:LEU:HD13	2.25	0.66
1:C:564[A]:MSE:HE1	1:C:607:MSE:HG2	1.77	0.66
1:C:597:TYR:OH	1:C:599:HIS:HD2	1.79	0.66
2:B:419:LEU:HD13	2:B:419:LEU:O	1.96	0.65
1:A:431:HIS:HD2	1:A:433[B]:GLU:H	1.42	0.65
2:B:63:MSE:HE1	2:B:167:ASP:N	2.12	0.65
1:C:79:PHE:CG	1:C:140[B]:MSE:HE1	2.32	0.65
2:B:592:MSE:HE2	2:B:631[A]:MSE:HE1	1.75	0.63
1:C:685:ASN:C	1:C:685:ASN:HD22	2.04	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:MSE:HE3	1:A:563:MSE:SE	2.48	0.63
2:B:685:ASN:ND2	2:B:687:ASN:H	1.97	0.63
1:C:507:LYS:HD2	1:C:559:MSE:CE	2.21	0.62
1:D:685:ASN:ND2	1:D:687:ASN:H	1.98	0.62
1:C:79:PHE:CB	1:C:140[B]:MSE:HE1	2.29	0.62
1:A:709:ASN:HD21	1:A:727:GLY:HA3	1.63	0.62
1:C:557[B]:LYS:HG3	5:C:2396:HOH:O	1.98	0.61
1:A:327:HIS:HE1	1:A:378:GLU:OE2	1.83	0.61
1:D:709:ASN:ND2	1:D:728:THR:H	1.97	0.61
1:C:560:PHE:CE1	1:C:564[B]:MSE:HE2	2.35	0.61
2:B:216:GLN:N	2:B:216:GLN:OE1	2.33	0.61
2:B:216:GLN:N	2:B:216:GLN:CD	2.59	0.61
1:D:72[A]:THR:HG22	5:D:2055:HOH:O	2.01	0.60
2:B:167:ASP:O	2:B:168[A]:LYS:O	2.19	0.60
1:C:671:MSE:CE	1:C:706:MSE:SE	2.87	0.60
1:A:507:LYS:HD3	1:A:559:MSE:CE	2.27	0.60
1:A:685:ASN:HD22	1:A:685:ASN:C	2.09	0.60
2:B:597:TYR:OH	2:B:599:HIS:HD2	1.85	0.60
2:B:631[B]:MSE:HG3	2:B:640:CYS:SG	2.41	0.60
1:D:700:ASN:ND2	1:D:735:ASN:HB3	2.18	0.59
1:A:709:ASN:HD21	1:A:728:THR:H	1.49	0.59
2:B:709:ASN:HD21	2:B:727:GLY:HA3	1.68	0.59
1:A:507:LYS:CE	1:A:559:MSE:HE2	2.30	0.59
1:A:203:GLU:CD	1:A:263:MSE:CE	2.75	0.59
1:D:685:ASN:C	1:D:685:ASN:HD22	2.09	0.59
1:A:177:GLU:CD	1:A:177:GLU:H	2.09	0.59
1:C:507:LYS:CD	1:C:559:MSE:CE	2.80	0.58
1:A:477:LEU:HG	1:A:481:LEU:HD22	1.85	0.58
1:A:431:HIS:CD2	1:A:433[A]:GLU:H	2.20	0.57
1:C:22:TRP:H	1:C:283:ASN:HD21	1.50	0.57
1:C:477:LEU:HG	1:C:481:LEU:HD22	1.86	0.57
1:D:507:LYS:HB2	1:D:563:MSE:HE2	1.86	0.57
2:B:167:ASP:C	2:B:168[A]:LYS:O	2.44	0.57
2:B:685:ASN:C	2:B:685:ASN:HD22	2.11	0.57
1:D:240:ARG:HG2	1:D:243:GLU:HB2	1.86	0.57
1:D:526:LYS:HA	1:D:575:ASP:HB3	1.87	0.57
1:A:431:HIS:CD2	1:A:433[B]:GLU:H	2.21	0.57
1:D:216[A]:ASN:HD22	1:D:216[A]:ASN:H	1.50	0.57
1:A:559:MSE:CE	1:A:563:MSE:SE	3.03	0.57
2:B:347:TRP:CZ3	2:B:394:MSE:HE2	2.40	0.57
1:D:755:GLU:HG2	5:D:2493:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:347:TRP:CZ3	1:D:394:MSE:HE2	2.39	0.56
2:B:353:LEU:C	2:B:353:LEU:HD13	2.29	0.56
1:C:177:GLU:OE1	1:C:177:GLU:N	2.27	0.56
1:C:678:LYS:HE2	1:C:692:ASP:OD1	2.06	0.56
1:D:485:LYS:HD3	5:D:2341:HOH:O	2.04	0.56
1:C:347:TRP:CE3	1:C:394:MSE:HE2	2.41	0.56
1:C:417:LYS:HE2	1:C:421:GLU:OE2	2.06	0.56
1:C:79:PHE:CD2	1:C:140[B]:MSE:HE3	2.39	0.55
1:D:188:ASN:ND2	1:D:190:GLY:H	1.98	0.55
1:A:685:ASN:ND2	1:A:687:ASN:H	2.03	0.55
1:D:746:GLU:CD	1:D:746:GLU:N	2.64	0.55
1:D:214:VAL:HG22	1:D:219:LEU:HD12	1.89	0.55
1:D:700:ASN:HD22	1:D:735:ASN:HB3	1.70	0.55
1:C:353:LEU:HD13	1:C:353:LEU:C	2.33	0.54
1:A:408:MSE:HE2	1:A:408:MSE:CA	2.23	0.54
1:A:431:HIS:HE1	5:A:2275:HOH:O	1.91	0.54
1:D:248:ARG:C	1:D:263[A]:MSE:HE1	2.32	0.54
1:A:327:HIS:HD2	1:A:338:GLY:O	1.91	0.53
1:A:754:LYS:O	1:A:755:GLU:C	2.51	0.53
1:A:358:ASN:HD21	1:A:365:ASN:ND2	1.99	0.53
2:B:216:GLN:HE22	2:B:230:HIS:N	2.06	0.53
1:A:263:MSE:HG3	1:A:263:MSE:O	2.07	0.52
1:A:644:ASP:OD2	5:A:2453:HOH:O	2.19	0.52
2:B:678:LYS:HE2	2:B:692:ASP:OD1	2.08	0.52
2:B:645:ASN:HA	5:B:2059:HOH:O	2.10	0.52
1:D:203:GLU:OE2	1:D:263[B]:MSE:CE	2.58	0.52
1:C:685:ASN:HD22	1:C:686:GLY:N	2.08	0.52
1:D:597:TYR:OH	1:D:599:HIS:HD2	1.93	0.52
1:C:58:PRO:HG2	1:C:69:TYR:CD1	2.45	0.52
1:D:353:LEU:C	1:D:353:LEU:HD13	2.34	0.52
1:C:671:MSE:CE	1:C:706:MSE:CE	2.88	0.51
1:A:216:ASN:HD22	1:A:216:ASN:H	1.57	0.51
2:B:627:VAL:HG13	2:B:631[A]:MSE:HG3	1.92	0.51
1:C:671:MSE:HE3	1:C:706:MSE:CE	2.39	0.51
1:D:504:LYS:HG3	5:D:2346:HOH:O	2.11	0.51
2:B:700:ASN:HD22	2:B:735:ASN:HB3	1.76	0.51
1:D:216[A]:ASN:ND2	1:D:230:HIS:H	2.07	0.51
2:B:526:LYS:HA	2:B:575:ASP:HB3	1.93	0.50
1:A:496:MSE:HE2	1:A:499:LYS:HZ2	1.74	0.50
1:A:671:MSE:SE	1:A:706:MSE:HE1	2.62	0.50
2:B:631[B]:MSE:CG	2:B:640:CYS:SG	2.99	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:575:ASP:OD1	1:D:577:SER:OG	2.24	0.50
2:B:33:GLN:O	2:B:40:THR:OG1	2.29	0.50
2:B:709:ASN:ND2	2:B:728:THR:H	2.10	0.50
1:D:564:MSE:HE1	1:D:607:MSE:HG2	1.94	0.50
1:D:592:MSE:HE3	1:D:640:CYS:HB2	1.94	0.50
1:A:408:MSE:CE	1:A:408:MSE:CA	2.88	0.49
1:C:745:GLU:OE2	1:C:754:LYS:HE2	2.11	0.49
2:B:627:VAL:O	2:B:631[A]:MSE:HG2	2.12	0.49
1:A:203:GLU:OE1	1:A:263:MSE:HE3	2.12	0.49
2:B:63:MSE:CE	2:B:166:PHE:CD1	2.82	0.49
1:C:292:GLU:HG3	1:C:678:LYS:HB3	1.95	0.49
1:D:203:GLU:CD	1:D:263[B]:MSE:HE1	2.34	0.49
2:B:168[A]:LYS:O	2:B:229:ASP:O	2.30	0.49
2:B:331:TYR:CZ	2:B:375:THR:HG23	2.48	0.49
2:B:685:ASN:HD22	2:B:686:GLY:N	2.11	0.49
1:C:593:ASN:ND2	5:C:2424:HOH:O	2.44	0.49
1:A:180:LYS:HE2	1:A:203:GLU:HG2	1.95	0.48
2:B:203:GLU:CD	2:B:263:MSE:CE	2.85	0.48
1:D:203:GLU:OE2	1:D:263[B]:MSE:HE2	2.13	0.48
1:A:188:ASN:ND2	1:A:190:GLY:H	1.98	0.48
2:B:90:ASN:HB3	2:B:189:SER:OG	2.13	0.48
1:C:746:GLU:HG2	5:C:2517:HOH:O	2.12	0.48
1:D:546:ASP:N	1:D:547:PRO:HD3	2.29	0.48
2:B:700:ASN:ND2	2:B:735:ASN:HB3	2.28	0.48
1:C:23:THR:H	1:C:283:ASN:HD21	1.61	0.48
1:D:547:PRO:HG2	1:D:613:TYR:CE2	2.49	0.48
1:A:526:LYS:HA	1:A:575:ASP:HB3	1.96	0.48
2:B:477:LEU:HG	2:B:481:LEU:HD22	1.96	0.48
1:C:709:ASN:ND2	1:C:728:THR:H	2.10	0.48
1:D:587[A]:ARG:CG	1:D:587[A]:ARG:NH1	2.57	0.48
2:B:644:ASP:O	2:B:645:ASN:HB2	2.14	0.47
1:C:507:LYS:HE3	1:C:559:MSE:HG2	1.96	0.47
2:B:219:LEU:C	2:B:219:LEU:HD23	2.39	0.47
1:A:408:MSE:HE1	1:A:480:GLU:HG2	1.97	0.47
1:D:706:MSE:HE2	1:D:713:HIS:ND1	2.29	0.47
1:A:235:ILE:C	1:A:235:ILE:HD12	2.40	0.47
2:B:63:MSE:HE2	2:B:166:PHE:CD2	2.43	0.47
1:C:358:ASN:HD21	1:C:365:ASN:ND2	2.02	0.46
1:D:350:PHE:C	1:D:350:PHE:CD2	2.93	0.46
1:A:26:VAL:HG11	1:A:124:PRO:HG3	1.97	0.46
1:C:685:ASN:HD22	1:C:687:ASN:H	1.60	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:MSE:CE	2:B:167:ASP:N	2.78	0.46
1:C:220:GLN:HG3	5:C:2162:HOH:O	2.15	0.46
1:D:602:GLN:N	1:D:603:PRO:CD	2.79	0.46
1:C:685:ASN:ND2	1:C:685:ASN:C	2.72	0.46
2:B:547:PRO:HG2	2:B:613:TYR:CE2	2.50	0.46
2:B:408:MSE:HE3	2:B:476:ARG:HB3	1.98	0.46
2:B:631[B]:MSE:HB2	2:B:631[B]:MSE:HE2	1.58	0.46
1:A:671:MSE:HE2	1:A:706:MSE:SE	2.66	0.46
2:B:178:GLU:O	2:B:179:ASN:C	2.56	0.46
1:C:79:PHE:HB3	1:C:140[B]:MSE:CE	2.43	0.46
1:A:520:SER:HA	1:A:521:PRO:C	2.41	0.45
1:C:347:TRP:CH2	1:C:394:MSE:HE2	2.51	0.45
1:C:431:HIS:HD2	1:C:433:GLU:N	2.11	0.45
1:D:293:GLY:HA3	1:D:677:LYS:HB2	1.99	0.45
2:B:564:MSE:HE3	2:B:564:MSE:HB2	1.92	0.45
1:D:570:VAL:O	1:D:595:GLY:HA2	2.17	0.45
2:B:592:MSE:CE	2:B:631[A]:MSE:HE3	2.29	0.45
1:D:288:LYS:HZ1	4:D:804:GOL:HO1	1.45	0.45
1:D:312:PHE:HA	1:D:313:PRO:C	2.41	0.45
1:D:366:LYS:HE2	1:D:412:LYS:O	2.17	0.44
1:D:541:TRP:CG	1:D:607:MSE:HG3	2.52	0.44
1:A:331:TYR:CZ	1:A:375:THR:HG23	2.52	0.44
2:B:49:ARG:HD3	5:B:2034:HOH:O	2.17	0.44
1:A:216:ASN:HD22	1:A:216:ASN:N	2.14	0.43
1:A:327:HIS:CE1	1:A:378:GLU:OE2	2.68	0.43
1:A:709:ASN:HD21	1:A:727:GLY:CA	2.31	0.43
1:A:350:PHE:CD2	1:A:350:PHE:C	2.96	0.43
1:A:361:TYR:N	1:A:362:PRO:CD	2.81	0.43
2:B:257:GLU:HG2	5:B:2149:HOH:O	2.19	0.43
2:B:106:PHE:CE1	2:B:232:GLY:HA3	2.54	0.43
1:C:33:GLN:O	1:C:40:THR:OG1	2.37	0.43
1:D:599:HIS:HE1	1:D:632:TYR:OH	2.01	0.43
2:B:312:PHE:HA	2:B:313:PRO:C	2.44	0.43
1:C:571:PRO:O	1:C:573:ILE:HG12	2.18	0.43
1:A:172:ILE:HG21	1:A:232:GLY:O	2.19	0.43
2:B:350:PHE:CD2	2:B:350:PHE:C	2.97	0.43
2:B:594:MSE:SE	2:B:631[B]:MSE:CE	3.13	0.43
1:C:564[A]:MSE:CE	1:C:607:MSE:HG2	2.48	0.42
2:B:345:GLY:HA3	2:B:385:TRP:CE2	2.53	0.42
2:B:403:LEU:HB3	2:B:419:LEU:HD21	2.02	0.42
1:A:645[B]:ASN:CG	5:A:2255:HOH:O	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:685:ASN:ND2	2:B:685:ASN:C	2.75	0.42
1:C:97:ILE:HD11	1:C:161:VAL:HG11	2.01	0.42
1:C:140[B]:MSE:HE2	1:C:149:PHE:HE2	1.85	0.42
1:C:599:HIS:HE1	1:C:632:TYR:OH	2.03	0.42
1:A:320:ASP:HB2	5:A:2240:HOH:O	2.20	0.42
2:B:541:TRP:CG	2:B:607:MSE:HG3	2.54	0.42
2:B:709:ASN:HD21	2:B:728:THR:H	1.66	0.42
2:B:167:ASP:O	2:B:168[A]:LYS:C	2.63	0.42
1:C:312:PHE:HA	1:C:313:PRO:C	2.44	0.42
1:C:408:MSE:HE2	1:C:476:ARG:HB3	2.01	0.42
1:C:546:ASP:N	1:C:547:PRO:HD3	2.35	0.42
1:A:700:ASN:HD22	1:A:735:ASN:HB3	1.85	0.42
2:B:631[A]:MSE:HB3	2:B:631[A]:MSE:HE2	1.41	0.42
1:A:58:PRO:HG2	1:A:69:TYR:CD1	2.55	0.41
1:A:353:LEU:HD13	1:A:353:LEU:C	2.45	0.41
2:B:216:GLN:HE22	2:B:230:HIS:H	1.68	0.41
1:A:709:ASN:HD21	1:A:728:THR:N	2.17	0.41
1:C:483:ARG:HB3	1:C:484:PRO:HD2	2.01	0.41
1:D:374:ASN:HD22	1:D:374:ASN:HA	1.69	0.41
1:D:547:PRO:HB2	1:D:613:TYR:CD2	2.55	0.41
2:B:188:ASN:HD22	2:B:190:GLY:N	1.90	0.41
2:B:216:GLN:NE2	2:B:216:GLN:HA	2.34	0.41
2:B:575:ASP:OD1	2:B:575:ASP:C	2.63	0.41
1:C:431:HIS:HD2	1:C:434:VAL:H	1.68	0.41
1:C:645[B]:ASN:HB2	5:C:2263:HOH:O	2.20	0.41
1:D:685:ASN:ND2	1:D:685:ASN:C	2.74	0.41
1:A:180:LYS:HE3	1:A:180:LYS:HB2	1.85	0.41
1:A:210:TYR:CD1	1:A:210:TYR:C	2.98	0.41
2:B:431:HIS:HE1	5:B:2230:HOH:O	2.03	0.41
1:D:685:ASN:HD22	1:D:687:ASN:H	1.66	0.41
1:A:388:PRO:CD	1:A:389:GLY:H	2.34	0.41
1:A:407:TYR:CD1	1:A:408:MSE:HE1	2.49	0.41
1:C:186:THR:O	1:C:187:ARG:C	2.63	0.41
1:C:709:ASN:HD21	1:C:728:THR:H	1.69	0.41
2:B:387:SER:HA	2:B:388:PRO:HA	1.82	0.41
2:B:444:TYR:HB3	2:B:452:PRO:HD3	2.02	0.41
2:B:483:ARG:HB3	2:B:484:PRO:HD2	2.03	0.41
1:C:26:VAL:HG11	1:C:124:PRO:HG3	2.02	0.41
1:D:331:TYR:CZ	1:D:375:THR:HG23	2.55	0.41
1:C:56:TRP:CZ2	1:C:81:GLN:HB2	2.56	0.41
1:C:541:TRP:CG	1:C:607:MSE:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:MSE:HE1	1:A:498:TYR:OH	2.21	0.40
2:B:86:SER:HB2	2:B:87:PRO:HD2	2.02	0.40
1:C:350:PHE:CD2	1:C:350:PHE:C	2.98	0.40
1:C:700:ASN:HD22	1:C:735:ASN:HB3	1.86	0.40
1:A:602:GLN:N	1:A:603:PRO:CD	2.84	0.40
2:B:167:ASP:HB2	5:B:2104:HOH:O	2.20	0.40
2:B:186:THR:O	2:B:187:ARG:C	2.64	0.40
2:B:564:MSE:HG2	2:B:611:TYR:CZ	2.55	0.40
1:C:510:ARG:HG3	1:C:522:PHE:CD1	2.57	0.40
1:C:525:LEU:HD13	1:C:573:ILE:HG13	2.02	0.40
1:C:526:LYS:HA	1:C:575:ASP:HB3	2.04	0.40
1:D:58:PRO:HG2	1:D:69:TYR:CD1	2.57	0.40
1:D:419:LEU:CD1	1:D:419:LEU:C	2.95	0.40
1:D:685:ASN:HD22	1:D:686:GLY:N	2.18	0.40
1:A:269:ASP:HB3	1:A:274:LEU:HG	2.04	0.40
1:A:319:LEU:HD12	1:A:319:LEU:HA	1.90	0.40
2:B:238:LYS:HB3	2:B:238:LYS:HE2	1.51	0.40
2:B:627:VAL:HG13	2:B:631[A]:MSE:CG	2.51	0.40
1:D:431:HIS:HE1	5:D:2275:HOH:O	2.04	0.40
1:D:616:GLN:HG2	1:D:618:TRP:CZ2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	736/744 (99%)	716 (97%)	20 (3%)	0	100	100
1	C	740/744 (100%)	719 (97%)	21 (3%)	0	100	100
1	D	738/744 (99%)	718 (97%)	20 (3%)	0	100	100
2	B	740/744 (100%)	722 (98%)	18 (2%)	0	100	100
All	All	2954/2976 (99%)	2875 (97%)	79 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	623/616 (101%)	607 (97%)	16 (3%)	40	35
1	C	632/616 (103%)	613 (97%)	19 (3%)	36	30
1	D	633/616 (103%)	609 (96%)	24 (4%)	29	21
2	B	631/616 (102%)	610 (97%)	21 (3%)	33	26
All	All	2519/2464 (102%)	2439 (97%)	80 (3%)	36	27

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	177	GLU
1	A	209	THR
1	A	215	GLU
1	A	237	PHE
1	A	319	LEU
1	A	353	LEU
1	A	408	MSE
1	A	419	LEU
1	A	460	ASN
1	A	481	LEU
1	A	539	TYR
1	A	564	MSE
1	A	596	ASN
1	A	685	ASN
1	A	692	ASP
1	A	739	LEU
2	B	77	ARG
2	B	109	GLU
2	B	185	THR
2	B	215	GLU
2	B	216	GLN
2	B	220	GLN

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Mol	Chain	Res	Type
2	B	237	PHE
2	B	238	LYS
2	B	257	GLU
2	B	319	LEU
2	B	385	TRP
2	B	419	LEU
2	B	460	ASN
2	B	481	LEU
2	B	482	LYS
2	B	519	GLN
2	B	539	TYR
2	B	631[A]	MSE
2	B	631[B]	MSE
2	B	685	ASN
2	B	725	LYS
1	C	215	GLU
1	C	237	PHE
1	C	274	LEU
1	C	292	GLU
1	C	319	LEU
1	C	385	TRP
1	C	460	ASN
1	C	481	LEU
1	C	482	LYS
1	C	486	LYS
1	C	519	GLN
1	C	539	TYR
1	C	564[A]	MSE
1	C	564[B]	MSE
1	C	645[A]	ASN
1	C	645[B]	ASN
1	C	685	ASN
1	C	692	ASP
1	C	739	LEU
1	D	34	SER
1	D	215	GLU
1	D	237	PHE
1	D	263[A]	MSE
1	D	263[B]	MSE
1	D	284	GLN
1	D	350	PHE
1	D	385	TRP

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Mol	Chain	Res	Type
1	D	419	LEU
1	D	456	LYS
1	D	481	LEU
1	D	482	LYS
1	D	485	LYS
1	D	519	GLN
1	D	539	TYR
1	D	564	MSE
1	D	573	ILE
1	D	587[A]	ARG
1	D	587[B]	ARG
1	D	596	ASN
1	D	685	ASN
1	D	692	ASP
1	D	739	LEU
1	D	746	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	188	ASN
1	A	216	ASN
1	A	226	GLN
1	A	264	ASN
1	A	283	ASN
1	A	327	HIS
1	A	358	ASN
1	A	374	ASN
1	A	398	ASN
1	A	431	HIS
1	A	513	ASN
1	A	593	ASN
1	A	599	HIS
1	A	601	ASN
1	A	626	GLN
1	A	685	ASN
1	A	700	ASN
1	A	709	ASN
1	A	740	ASN
2	B	188	ASN
2	B	222	ASN

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Mol	Chain	Res	Type
2	B	262	ASN
2	B	264	ASN
2	B	358	ASN
2	B	374	ASN
2	B	431	HIS
2	B	446	ASN
2	B	593	ASN
2	B	596	ASN
2	B	599	HIS
2	B	601	ASN
2	B	685	ASN
2	B	700	ASN
2	B	709	ASN
2	B	716	ASN
1	C	59	GLN
1	C	81	GLN
1	C	188	ASN
1	C	198	ASN
1	C	220	GLN
1	C	226	GLN
1	C	262	ASN
1	C	264	ASN
1	C	283	ASN
1	C	358	ASN
1	C	374	ASN
1	C	431	HIS
1	C	446	ASN
1	C	519	GLN
1	C	581	GLN
1	C	593	ASN
1	C	599	HIS
1	C	601	ASN
1	C	616	GLN
1	C	685	ASN
1	C	695	ASN
1	C	700	ASN
1	C	709	ASN
1	C	716	ASN
1	D	59	GLN
1	D	84	GLN
1	D	188	ASN
1	D	264	ASN

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Mol	Chain	Res	Type
1	D	358	ASN
1	D	374	ASN
1	D	431	HIS
1	D	519	GLN
1	D	593	ASN
1	D	599	HIS
1	D	601	ASN
1	D	626	GLN
1	D	685	ASN
1	D	700	ASN
1	D	709	ASN
1	D	716	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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	GOL	B	805	-	5,5,5	0.32	0	5,5,5	0.47	0
4	GOL	C	804	-	5,5,5	0.29	0	5,5,5	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	D	803	-	5,5,5	0.36	0	5,5,5	0.07	0
4	GOL	B	804	-	5,5,5	0.36	0	5,5,5	0.55	0
4	GOL	C	805	-	5,5,5	0.44	0	5,5,5	0.37	0
4	GOL	D	806	-	5,5,5	0.26	0	5,5,5	0.69	0
4	GOL	A	805	-	5,5,5	0.27	0	5,5,5	0.63	0
4	GOL	C	803	-	5,5,5	0.42	0	5,5,5	0.58	0
4	GOL	B	802	-	5,5,5	0.26	0	5,5,5	0.63	0
4	GOL	A	802	-	5,5,5	0.36	0	5,5,5	0.44	0
4	GOL	D	805	-	5,5,5	0.37	0	5,5,5	0.63	0
4	GOL	B	803	-	5,5,5	0.43	0	5,5,5	1.02	0
4	GOL	D	804	-	5,5,5	0.24	0	5,5,5	0.67	0
4	GOL	A	804	-	5,5,5	0.55	0	5,5,5	0.46	0
4	GOL	C	802	-	5,5,5	0.22	0	5,5,5	0.58	0
4	GOL	A	803	-	5,5,5	0.38	0	5,5,5	0.21	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	GOL	B	805	-	-	1/4/4/4	-
4	GOL	C	804	-	-	1/4/4/4	-
4	GOL	D	803	-	-	0/4/4/4	-
4	GOL	B	804	-	-	1/4/4/4	-
4	GOL	C	805	-	-	0/4/4/4	-
4	GOL	D	806	-	-	2/4/4/4	-
4	GOL	A	805	-	-	2/4/4/4	-
4	GOL	C	803	-	-	0/4/4/4	-
4	GOL	B	802	-	-	0/4/4/4	-
4	GOL	A	802	-	-	2/4/4/4	-
4	GOL	D	805	-	-	2/4/4/4	-
4	GOL	B	803	-	-	3/4/4/4	-
4	GOL	D	804	-	-	2/4/4/4	-
4	GOL	A	804	-	-	0/4/4/4	-
4	GOL	C	802	-	-	0/4/4/4	-
4	GOL	A	803	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	805	GOL	C1-C2-C3-O3
4	B	803	GOL	O1-C1-C2-C3
4	B	803	GOL	C1-C2-C3-O3
4	D	804	GOL	O1-C1-C2-C3
4	D	805	GOL	O1-C1-C2-C3
4	D	806	GOL	O1-C1-C2-C3
4	B	803	GOL	O1-C1-C2-O2
4	A	802	GOL	C1-C2-C3-O3
4	D	805	GOL	O1-C1-C2-O2
4	D	804	GOL	O1-C1-C2-O2
4	D	806	GOL	O1-C1-C2-O2
4	A	805	GOL	O2-C2-C3-O3
4	C	804	GOL	O2-C2-C3-O3
4	B	804	GOL	O1-C1-C2-C3
4	A	802	GOL	O2-C2-C3-O3
4	B	805	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	804	GOL	4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	709/744 (95%)	-0.56	1 (0%) 92 92	2, 7, 16, 26	2 (0%)
1	C	709/744 (95%)	-0.57	2 (0%) 90 91	2, 7, 15, 26	3 (0%)
1	D	709/744 (95%)	-0.45	0 100 100	2, 7, 16, 28	3 (0%)
2	B	710/744 (95%)	-0.17	2 (0%) 90 91	3, 8, 15, 25	3 (0%)
All	All	2837/2976 (95%)	-0.44	5 (0%) 91 92	2, 7, 16, 28	11 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	217	GLY	3.1
2	B	216	GLN	2.5
1	A	36	PHE	2.4
1	C	580	GLY	2.2
1	C	581	GLN	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
4	GOL	D	804	6/6	0.77	0.13	18,19,23,26	0
4	GOL	A	805	6/6	0.87	0.10	21,22,22,23	0
4	GOL	D	806	6/6	0.87	0.10	23,24,25,25	0
4	GOL	C	804	6/6	0.91	0.09	14,21,23,25	0
4	GOL	D	805	6/6	0.92	0.07	9,11,14,20	0
4	GOL	A	804	6/6	0.92	0.09	11,12,14,19	0
4	GOL	B	805	6/6	0.93	0.07	13,14,15,15	0
4	GOL	B	803	6/6	0.94	0.08	12,13,15,19	0
4	GOL	B	804	6/6	0.94	0.07	14,18,19,20	0
4	GOL	C	805	6/6	0.94	0.10	9,14,16,20	0
4	GOL	C	803	6/6	0.95	0.06	11,14,16,17	0
4	GOL	D	803	6/6	0.96	0.06	10,14,16,17	0
4	GOL	B	802	6/6	0.96	0.05	14,15,15,17	0
3	CA	D	801	1/1	0.96	0.09	25,25,25,25	0
4	GOL	C	802	6/6	0.96	0.05	9,12,13,14	0
4	GOL	A	803	6/6	0.97	0.06	15,16,17,17	0
3	CA	A	801	1/1	0.97	0.08	23,23,23,23	0
4	GOL	A	802	6/6	0.97	0.05	7,12,14,15	0
3	CA	C	801	1/1	0.98	0.07	19,19,19,19	0
3	CA	B	801	1/1	0.98	0.11	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.