



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:38 PM UTC

PDB ID : 4ZE5 / pdb_00004ze5
Title : Structure of Gan1D-E170Q, a catalytic mutant of a putative 6-phospho-beta-galactosidase from *Geobacillus stearothermophilus*
Authors : Lansky, S.; Zehavi, A.; Dvir, H.; Shoham, Y.; Shoham, G.
Deposited on : 2015-04-20
Resolution : 1.48 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

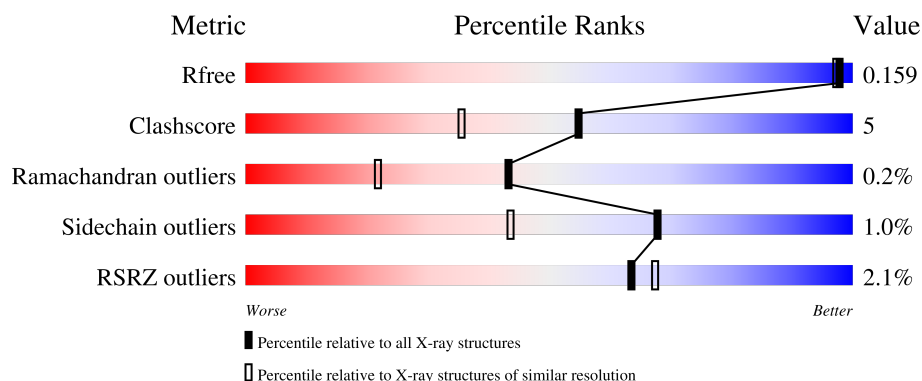
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

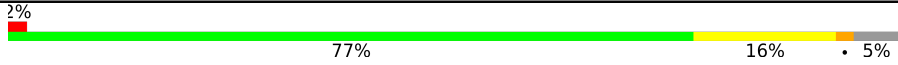
The reported resolution of this entry is 1.48 Å.

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	6779 (1.50-1.46)
Clashscore	190562	7025 (1.50-1.46)
Ramachandran outliers	187476	6917 (1.50-1.46)
Sidechain outliers	187428	6914 (1.50-1.46)
RSRZ outliers	180081	6781 (1.50-1.46)

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	485	
1	B	485	
1	C	485	
1	D	485	

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	IMD	A	505	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18228 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 6-phospho-beta-galactobiosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	0	21	0
			3902	2518	666	703	15			
1	B	459	Total	C	N	O	S	0	20	0
			3900	2515	662	709	14			
1	C	460	Total	C	N	O	S	0	23	0
			3923	2530	674	705	14			
1	D	460	Total	C	N	O	S	0	16	0
			3872	2497	664	699	12			

There are 36 discrepancies between the modelled and reference sequences:

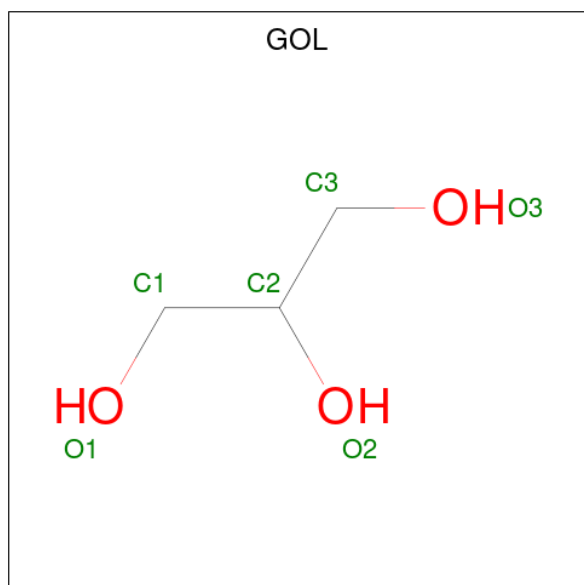
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP W8QF82
A	-5	ILE	-	expression tag	UNP W8QF82
A	-4	HIS	-	expression tag	UNP W8QF82
A	-3	HIS	-	expression tag	UNP W8QF82
A	-2	HIS	-	expression tag	UNP W8QF82
A	-1	HIS	-	expression tag	UNP W8QF82
A	0	HIS	-	expression tag	UNP W8QF82
A	1	HIS	-	expression tag	UNP W8QF82
A	170	GLN	GLU	engineered mutation	UNP W8QF82
B	-6	MET	-	initiating methionine	UNP W8QF82
B	-5	ILE	-	expression tag	UNP W8QF82
B	-4	HIS	-	expression tag	UNP W8QF82
B	-3	HIS	-	expression tag	UNP W8QF82
B	-2	HIS	-	expression tag	UNP W8QF82
B	-1	HIS	-	expression tag	UNP W8QF82
B	0	HIS	-	expression tag	UNP W8QF82
B	1	HIS	-	expression tag	UNP W8QF82
B	170	GLN	GLU	engineered mutation	UNP W8QF82
C	-6	MET	-	initiating methionine	UNP W8QF82
C	-5	ILE	-	expression tag	UNP W8QF82
C	-4	HIS	-	expression tag	UNP W8QF82

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	HIS	-	expression tag	UNP W8QF82
C	-2	HIS	-	expression tag	UNP W8QF82
C	-1	HIS	-	expression tag	UNP W8QF82
C	0	HIS	-	expression tag	UNP W8QF82
C	1	HIS	-	expression tag	UNP W8QF82
C	170	GLN	GLU	engineered mutation	UNP W8QF82
D	-6	MET	-	initiating methionine	UNP W8QF82
D	-5	ILE	-	expression tag	UNP W8QF82
D	-4	HIS	-	expression tag	UNP W8QF82
D	-3	HIS	-	expression tag	UNP W8QF82
D	-2	HIS	-	expression tag	UNP W8QF82
D	-1	HIS	-	expression tag	UNP W8QF82
D	0	HIS	-	expression tag	UNP W8QF82
D	1	HIS	-	expression tag	UNP W8QF82
D	170	GLN	GLU	engineered mutation	UNP W8QF82

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



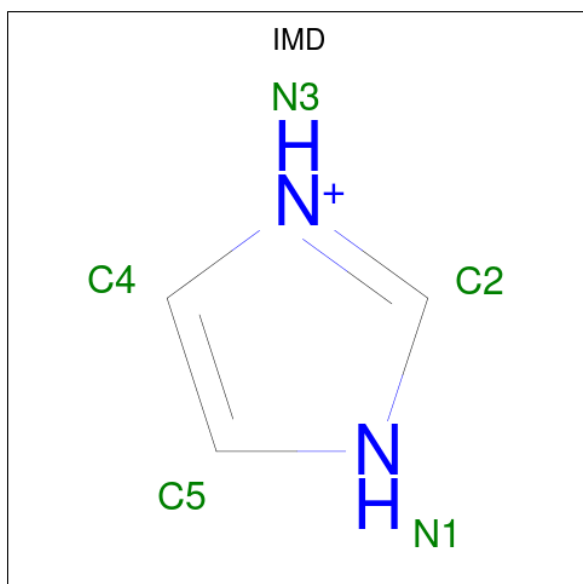
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

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

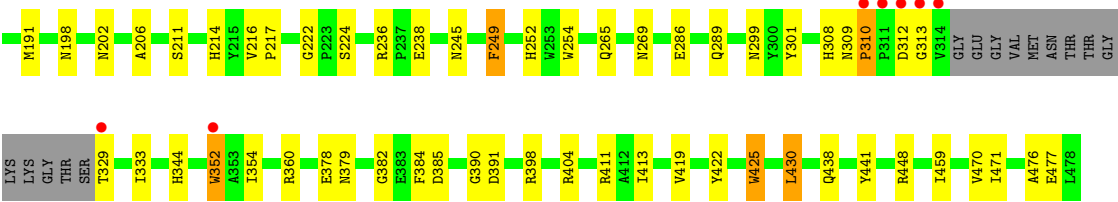
- Molecule 3 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



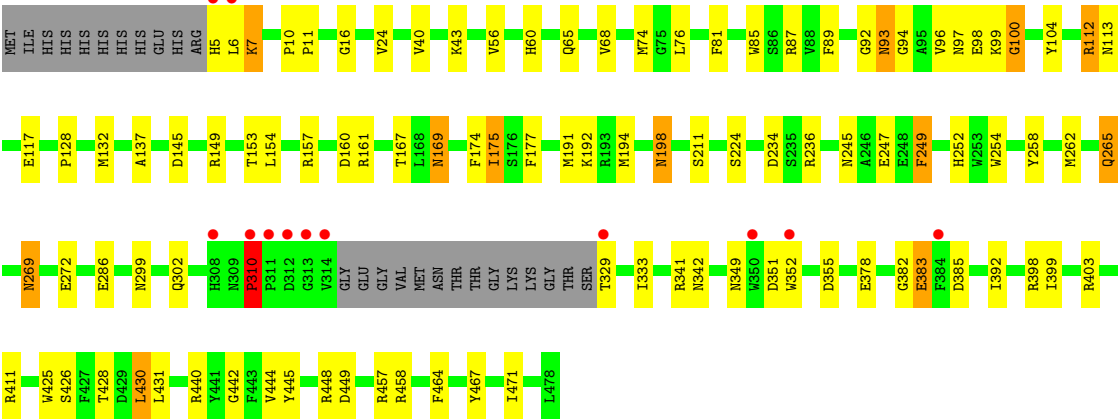
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			5	3	2		
3	C	1	Total	C	N	0	0
			5	3	2		
3	D	1	Total	C	N	0	0
			5	3	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	616	Total 616	O 616	0	0
4	B	640	Total 640	O 640	0	0
4	C	690	Total 690	O 690	0	0
4	D	610	Total 610	O 610	0	0



● Molecule 1: Putative 6-phospho-beta-galactobiosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.55Å 97.44Å 105.24Å 90.00° 97.82° 90.00°	Depositor
Resolution (Å)	27.64 – 1.48 27.64 – 1.48	Depositor EDS
% Data completeness (in resolution range)	99.7 (27.64-1.48) 99.7 (27.64-1.48)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.50 (at 1.48Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.132 , 0.159 0.132 , 0.159	Depositor DCC
R_{free} test set	16968 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	10.9	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	18228	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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 71.27 % 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 2.7039e-06. 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: GOL, IMD

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	1.70	50/4091 (1.2%)	1.47	30/5559 (0.5%)
1	B	1.65	31/4076 (0.8%)	1.48	30/5543 (0.5%)
1	C	1.63	35/4117 (0.9%)	1.44	25/5597 (0.4%)
1	D	1.70	42/4041 (1.0%)	1.56	42/5496 (0.8%)
All	All	1.67	158/16325 (1.0%)	1.49	127/22195 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	2
All	All	0	6

All (158) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	430	LEU	C-O	-9.11	1.12	1.23
1	C	476	ALA	C-O	8.42	1.34	1.24
1	D	440	ARG	CA-C	-8.02	1.42	1.52
1	B	133	ASP	CG-OD1	-7.99	1.10	1.25
1	C	309	ASN	C-O	-7.96	1.17	1.24
1	B	308	HIS	C-N	-7.88	1.27	1.33
1	B	430	LEU	C-O	-7.85	1.14	1.23
1	A	477	GLU	N-CA	7.78	1.56	1.46
1	C	430	LEU	C-O	-7.71	1.14	1.23
1	C	76	LEU	CB-CG	-7.58	1.38	1.53
1	A	419	VAL	CA-CB	-7.46	1.45	1.54
1	C	249	PHE	N-CA	-7.33	1.37	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	74	MET	SD-CE	-6.98	1.62	1.79
1	B	47	ARG	N-CA	-6.96	1.37	1.46
1	D	76	LEU	CA-C	-6.94	1.43	1.52
1	D	383	GLU	CA-C	-6.83	1.44	1.52
1	D	464	PHE	C-O	-6.81	1.16	1.24
1	A	468	GLN	CA-C	6.79	1.61	1.52
1	B	74	MET	SD-CE	-6.76	1.62	1.79
1	D	310	PRO	CA-C	6.72	1.58	1.52
1	D	56	VAL	CA-C	6.67	1.59	1.52
1	A	469	ARG	CG-CD	-6.65	1.32	1.52
1	D	249	PHE	N-CA	-6.58	1.38	1.46
1	D	169	ASN	CG-ND2	-6.57	1.19	1.33
1	B	94	GLY	N-CA	6.42	1.56	1.45
1	A	469	ARG	CD-NE	6.37	1.55	1.46
1	C	74	MET	SD-CE	-6.35	1.63	1.79
1	A	398	ARG	C-O	6.34	1.31	1.24
1	C	354	ILE	C-O	6.34	1.31	1.24
1	A	406	VAL	CA-C	6.33	1.60	1.52
1	D	449	ASP	CA-C	-6.33	1.45	1.53
1	A	76	LEU	CA-C	-6.29	1.45	1.52
1	A	290	ALA	C-N	-6.28	1.25	1.33
1	B	106	ARG	CZ-NH2	-6.28	1.25	1.33
1	C	382	GLY	C-O	-6.22	1.16	1.23
1	C	76	LEU	CA-C	-6.20	1.45	1.52
1	D	98	GLU	N-CA	-6.18	1.38	1.46
1	D	449	ASP	C-O	6.18	1.29	1.24
1	B	384	PHE	C-O	6.16	1.30	1.23
1	D	392	ILE	C-O	-6.16	1.17	1.24
1	A	69	ALA	CA-C	-6.14	1.44	1.52
1	D	457	ARG	CA-CB	6.11	1.63	1.53
1	A	134	ALA	CA-CB	-6.11	1.43	1.53
1	C	286	GLU	CD-OE2	6.11	1.36	1.25
1	C	17	ALA	CA-C	-6.06	1.45	1.52
1	A	462	LYS	CA-CB	-6.02	1.43	1.53
1	D	247	GLU	CA-C	-6.01	1.45	1.52
1	D	153	THR	CA-CB	-6.00	1.44	1.53
1	C	100	GLY	N-CA	5.97	1.53	1.45
1	C	217	PRO	CA-CB	5.96	1.62	1.53
1	D	100	GLY	CA-C	-5.93	1.45	1.52
1	D	428	THR	CA-C	-5.93	1.45	1.52
1	A	407	GLN	CA-CB	-5.90	1.44	1.53
1	B	381	LEU	C-N	-5.90	1.29	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	266	ALA	N-CA	-5.90	1.39	1.46
1	B	431	LEU	C-O	-5.90	1.16	1.24
1	D	113	ASN	N-CA	5.85	1.53	1.46
1	A	435	ASN	C-O	5.82	1.32	1.23
1	C	448	ARG	N-CA	-5.76	1.39	1.46
1	C	470	VAL	CA-CB	5.76	1.60	1.54
1	D	448	ARG	N-CA	-5.75	1.39	1.46
1	A	98	GLU	N-CA	-5.75	1.39	1.46
1	C	187	GLY	C-N	-5.75	1.25	1.33
1	B	47	ARG	CA-C	5.72	1.60	1.52
1	A	446	VAL	C-O	-5.71	1.18	1.24
1	B	473	THR	CA-CB	-5.70	1.44	1.53
1	A	440	ARG	N-CA	-5.68	1.39	1.45
1	A	308	HIS	C-N	-5.66	1.29	1.33
1	A	265	GLN	CA-C	-5.65	1.45	1.52
1	C	80	ARG	N-CA	-5.64	1.39	1.46
1	B	68	VAL	CA-CB	-5.62	1.47	1.54
1	B	333	ILE	CA-C	-5.61	1.48	1.52
1	B	452	SER	C-O	5.57	1.30	1.23
1	A	16	GLY	CA-C	-5.54	1.46	1.52
1	A	301	TYR	CA-C	-5.54	1.45	1.52
1	A	463	SER	CA-C	-5.53	1.45	1.52
1	D	192	LYS	N-CA	-5.52	1.39	1.46
1	C	131	LEU	N-CA	-5.52	1.39	1.46
1	A	171	GLN	CD-NE2	-5.51	1.21	1.33
1	B	293	PRO	C-O	5.49	1.30	1.23
1	B	57	ALA	CA-C	-5.49	1.47	1.52
1	C	175	ILE	C-O	5.48	1.30	1.24
1	C	385	ASP	C-O	-5.48	1.17	1.23
1	A	294	ASP	CA-C	-5.48	1.45	1.52
1	D	269	ASN	CA-C	-5.47	1.45	1.52
1	D	10	PRO	C-N	5.46	1.41	1.33
1	C	206	ALA	CA-CB	-5.44	1.44	1.53
1	D	431	LEU	C-O	-5.44	1.17	1.24
1	D	68	VAL	N-CA	-5.43	1.39	1.46
1	A	297	GLY	CA-C	-5.42	1.45	1.52
1	D	175	ILE	C-O	5.38	1.30	1.24
1	C	422	TYR	CA-C	-5.38	1.46	1.52
1	B	265	GLN	CA-C	-5.37	1.45	1.52
1	B	13	PHE	CA-CB	-5.34	1.45	1.53
1	A	202	ASN	CG-OD1	5.33	1.33	1.23
1	D	60	HIS	CA-C	5.33	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	444	VAL	CA-CB	-5.33	1.47	1.54
1	B	134	ALA	CA-CB	-5.32	1.45	1.53
1	D	177	PHE	C-O	5.32	1.30	1.24
1	D	154	LEU	CA-C	-5.31	1.45	1.52
1	D	258	TYR	C-O	5.30	1.30	1.24
1	A	333	ILE	CA-C	-5.30	1.48	1.52
1	D	194	MET	N-CA	5.30	1.52	1.46
1	C	391	ASP	N-CA	5.29	1.54	1.46
1	D	43	LYS	N-CA	5.29	1.53	1.46
1	A	309	ASN	CA-CB	-5.29	1.47	1.53
1	A	374	ILE	CA-CB	-5.28	1.48	1.54
1	C	29	ASN	CA-C	-5.27	1.46	1.52
1	B	62	HIS	CA-C	-5.26	1.45	1.52
1	A	469	ARG	N-CA	5.26	1.53	1.46
1	A	141	ARG	CZ-NH2	-5.26	1.26	1.33
1	D	137	ALA	C-O	-5.25	1.17	1.24
1	A	109	GLU	N-CA	5.25	1.52	1.46
1	B	112	ARG	N-CA	5.25	1.52	1.46
1	B	6	LEU	C-O	-5.25	1.17	1.23
1	C	105	ASP	CA-C	-5.25	1.46	1.52
1	C	106	ARG	CZ-NH2	-5.25	1.26	1.33
1	B	41	PHE	CA-C	-5.23	1.46	1.52
1	A	219	GLY	N-CA	5.23	1.51	1.45
1	C	419	VAL	C-O	5.22	1.29	1.24
1	A	477	GLU	CG-CD	5.22	1.65	1.52
1	C	390	GLY	N-CA	-5.20	1.37	1.45
1	A	411	ARG	CA-CB	-5.19	1.45	1.53
1	D	286	GLU	CD-OE2	5.18	1.35	1.25
1	A	384	PHE	C-O	5.17	1.29	1.23
1	C	379	ASN	CG-OD1	5.17	1.33	1.23
1	C	202	ASN	CG-OD1	5.17	1.33	1.23
1	A	47[A]	ARG	C-O	-5.15	1.17	1.24
1	A	47[B]	ARG	C-O	-5.15	1.17	1.24
1	D	198	ASN	CG-ND2	-5.14	1.22	1.33
1	D	385	ASP	N-CA	-5.14	1.39	1.46
1	A	40	VAL	C-O	5.14	1.29	1.24
1	A	476	ALA	N-CA	5.12	1.53	1.46
1	B	156	GLN	N-CA	5.12	1.52	1.46
1	C	344	HIS	N-CA	-5.12	1.40	1.46
1	A	443	PHE	N-CA	5.11	1.52	1.46
1	A	106	ARG	CZ-NH2	-5.11	1.26	1.33
1	A	344	HIS	N-CA	-5.10	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	442	GLY	C-O	5.10	1.31	1.23
1	B	401	TYR	CA-C	-5.09	1.46	1.52
1	D	398	ARG	CD-NE	-5.08	1.39	1.46
1	C	72	ALA	C-O	5.08	1.30	1.24
1	A	56	VAL	CA-C	5.07	1.57	1.52
1	D	448	ARG	CZ-NH1	5.07	1.39	1.32
1	B	240	VAL	CA-CB	-5.06	1.48	1.54
1	A	76	LEU	CB-CG	-5.05	1.43	1.53
1	C	10	PRO	CA-CB	-5.05	1.49	1.53
1	A	413	ILE	CA-C	5.04	1.59	1.52
1	C	459	ILE	CA-CB	-5.03	1.47	1.54
1	A	380	GLY	N-CA	5.03	1.51	1.45
1	B	302	GLN	CD-OE1	-5.03	1.14	1.23
1	A	169	ASN	CG-ND2	-5.03	1.22	1.33
1	C	169	ASN	CG-ND2	-5.03	1.22	1.33
1	A	375	LEU	CA-C	-5.02	1.46	1.52
1	D	403	ARG	N-CA	-5.02	1.40	1.46
1	D	160	ASP	CB-CG	5.01	1.64	1.52
1	B	446	VAL	C-O	-5.01	1.18	1.24
1	D	399	ILE	N-CA	-5.00	1.40	1.46

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	93	ASN	CA-C-N	-8.66	105.81	121.32
1	B	93	ASN	C-N-CA	-8.66	105.81	121.32
1	A	477	GLU	N-CA-CB	8.41	124.34	111.56
1	A	468	GLN	O-C-N	8.37	130.99	122.12
1	C	352	TRP	CA-CB-CG	7.94	128.69	113.60
1	B	398	ARG	NE-CZ-NH2	7.82	126.24	119.20
1	B	162	VAL	O-C-N	7.33	130.80	123.18
1	B	289	GLN	CB-CG-CD	7.17	124.79	112.60
1	D	444	VAL	O-C-N	-6.98	115.81	123.20
1	A	477	GLU	CA-C-N	6.91	134.14	121.70
1	A	477	GLU	C-N-CA	6.91	134.14	121.70
1	D	154	LEU	N-CA-C	6.83	118.72	111.28
1	D	194	MET	CG-SD-CE	-6.77	86.00	100.90
1	D	310	PRO	N-CA-C	6.64	118.81	110.70
1	A	413	ILE	O-C-N	6.60	128.27	121.87
1	D	104	TYR	CA-C-O	6.59	127.55	120.10
1	C	286	GLU	CG-CD-OE2	6.56	133.49	118.40
1	C	211	SER	CA-C-O	6.55	127.36	120.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	16	GLY	CA-C-O	6.52	127.40	121.47
1	A	133	ASP	CA-CB-CG	6.50	119.11	112.60
1	A	193	ARG	NE-CZ-NH1	-6.45	115.05	121.50
1	D	471	ILE	O-C-N	6.43	128.45	121.83
1	B	413	ILE	O-C-N	6.39	128.07	121.87
1	A	342	ASN	O-C-N	6.38	126.40	121.23
1	B	470	VAL	O-C-N	-6.35	115.69	121.91
1	C	352	TRP	CB-CA-C	-6.34	99.35	109.80
1	D	24	VAL	N-CA-C	6.33	117.44	112.12
1	D	211	SER	O-C-N	-6.28	115.47	122.12
1	C	211	SER	O-C-N	-6.25	115.02	122.15
1	D	65	GLN	O-C-N	6.21	128.71	122.12
1	A	476	ALA	CA-C-O	-6.16	111.80	119.38
1	D	11	PRO	CA-C-N	-6.16	112.81	122.73
1	D	11	PRO	C-N-CA	-6.16	112.81	122.73
1	D	355	ASP	O-C-N	-6.14	116.33	121.12
1	D	398	ARG	NE-CZ-NH2	6.11	124.70	119.20
1	B	63	ARG	NE-CZ-NH1	-6.09	115.41	121.50
1	B	94	GLY	O-C-N	-6.07	117.14	122.91
1	B	457	ARG	CA-CB-CG	6.06	126.22	114.10
1	C	413	ILE	O-C-N	6.03	127.72	121.87
1	D	85	TRP	CA-C-O	-5.99	114.16	120.63
1	D	448	ARG	CA-C-O	-5.96	115.07	121.38
1	D	174	PHE	CA-CB-CG	5.94	119.74	113.80
1	B	342	ASN	O-C-N	5.92	126.03	121.23
1	D	269	ASN	CB-CG-ND2	5.87	125.20	116.40
1	A	384	PHE	CA-C-N	5.84	129.06	120.82
1	A	384	PHE	C-N-CA	5.84	129.06	120.82
1	C	289	GLN	CB-CG-CD	5.83	122.52	112.60
1	C	100	GLY	O-C-N	-5.80	116.62	122.19
1	B	93	ASN	CB-CA-C	5.80	121.95	110.42
1	C	411	ARG	NE-CZ-NH2	-5.78	114.00	119.20
1	A	291	ALA	N-CA-CB	-5.76	103.90	110.35
1	B	350[A]	TRP	CA-CB-CG	-5.75	102.67	113.60
1	B	350[B]	TRP	CA-CB-CG	-5.75	102.67	113.60
1	D	24	VAL	CG1-CB-CG2	5.74	123.44	110.80
1	C	286	GLU	CB-CG-CD	5.74	122.36	112.60
1	D	40	VAL	N-CA-C	5.74	115.92	110.53
1	B	267	ALA	CA-C-O	-5.72	114.49	120.55
1	A	66	GLU	CG-CD-OE2	-5.71	105.26	118.40
1	C	174	PHE	CA-CB-CG	5.71	119.51	113.80
1	B	132[A]	MET	O-C-N	5.71	127.95	122.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	132[B]	MET	O-C-N	5.71	127.95	122.07
1	B	97	ASN	CA-C-O	5.69	126.45	120.54
1	D	153	THR	CA-C-O	5.68	126.98	120.90
1	C	93	ASN	CA-C-N	-5.67	111.92	120.65
1	C	93	ASN	C-N-CA	-5.67	111.92	120.65
1	B	468	GLN	O-C-N	5.65	128.11	122.12
1	B	355	ASP	O-C-N	-5.64	116.37	121.17
1	D	265	GLN	O-C-N	-5.64	114.90	122.23
1	A	443	PHE	N-CA-C	-5.64	105.28	111.82
1	D	342	ASN	O-C-N	5.60	125.76	121.23
1	A	469	ARG	NE-CZ-NH1	-5.59	115.91	121.50
1	A	16	GLY	CA-C-O	5.59	126.55	121.47
1	D	467	TYR	N-CA-C	5.57	117.36	111.28
1	D	352	TRP	CB-CA-C	-5.57	100.61	109.80
1	D	444	VAL	CA-C-O	5.56	126.18	120.39
1	D	458	ARG	NE-CZ-NH1	5.54	127.04	121.50
1	B	107	LEU	O-C-N	5.53	127.77	122.07
1	D	104	TYR	N-CA-C	5.51	118.05	111.71
1	B	410	GLN	O-C-N	5.51	127.96	122.12
1	D	411	ARG	NE-CZ-NH2	-5.50	114.25	119.20
1	D	117	GLU	CA-C-N	5.50	125.67	119.90
1	D	117	GLU	C-N-CA	5.50	125.67	119.90
1	D	403	ARG	NE-CZ-NH1	5.46	126.96	121.50
1	A	291	ALA	O-C-N	-5.44	115.70	122.83
1	A	355	ASP	O-C-N	-5.40	116.91	121.12
1	C	398	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	D	16	GLY	O-C-N	-5.35	119.83	123.95
1	B	97	ASN	O-C-N	-5.33	116.71	123.05
1	C	441	TYR	OH-CZ-CE2	-5.32	103.94	119.90
1	B	74	MET	CA-C-O	-5.32	114.09	120.10
1	C	425	TRP	O-C-N	-5.30	116.74	123.05
1	A	24	VAL	N-CA-C	5.29	116.57	112.12
1	A	468	GLN	CA-C-O	-5.29	114.92	120.63
1	C	175	ILE	O-C-N	-5.29	116.40	121.90
1	D	286	GLU	CG-CD-OE2	5.26	130.50	118.40
1	A	236	ARG	O-C-N	5.22	125.95	121.30
1	C	313	GLY	N-CA-C	5.19	120.02	112.60
1	D	211	SER	CA-C-O	5.18	126.04	120.55
1	A	25	GLU	N-CA-C	5.18	117.01	111.36
1	C	310	PRO	N-CA-C	5.18	117.02	110.70
1	A	410	GLN	O-C-N	5.17	128.27	122.22
1	D	98	GLU	O-C-N	5.16	127.59	122.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	GLU	CG-CD-OE1	5.15	130.25	118.40
1	D	467	TYR	CA-C-O	5.12	125.97	120.55
1	D	81	PHE	CA-C-O	-5.12	115.62	121.40
1	B	174	PHE	CA-CB-CG	5.12	118.92	113.80
1	C	404	ARG	NH1-CZ-NH2	5.11	125.95	119.30
1	B	403	ARG	O-C-N	5.11	127.41	122.09
1	C	216	VAL	CA-C-O	5.11	126.80	119.95
1	A	7	LYS	CA-C-N	-5.11	115.46	120.52
1	A	7	LYS	C-N-CA	-5.11	115.46	120.52
1	A	360	ARG	NH1-CZ-NH2	5.11	125.94	119.30
1	C	471	ILE	CA-C-O	-5.10	115.44	120.85
1	A	463	SER	O-C-N	-5.09	116.27	122.22
1	A	141	ARG	NE-CZ-NH1	-5.08	116.42	121.50
1	C	106	ARG	NE-CZ-NH1	5.07	126.57	121.50
1	C	360	ARG	NH1-CZ-NH2	5.05	125.87	119.30
1	D	445	TYR	CA-C-O	-5.05	115.50	121.16
1	D	398	ARG	O-C-N	-5.05	116.39	122.15
1	D	382	GLY	O-C-N	5.04	127.08	123.35
1	B	291	ALA	O-C-N	-5.03	116.86	122.55
1	A	345	VAL	O-C-N	5.03	128.35	122.97
1	D	87	ARG	N-CA-CB	5.02	117.58	110.16
1	B	112	ARG	CA-CB-CG	-5.01	104.08	114.10
1	B	47	ARG	NE-CZ-NH2	5.00	123.70	119.20
1	C	419	VAL	CA-C-O	-5.00	114.80	120.65
1	D	286	GLU	CB-CG-CD	5.00	121.10	112.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	157[A]	ARG	Sidechain
1	A	157[B]	ARG	Sidechain
1	A	476	ALA	Peptide
1	A	477	GLU	Peptide
1	B	349[A]	ASN	Peptide
1	B	349[B]	ASN	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3902	0	3768	33	0
1	B	3900	0	3731	25	0
1	C	3923	0	3783	40	0
1	D	3872	0	3716	50	0
2	A	24	0	32	3	0
2	B	18	0	24	0	0
2	C	12	0	16	0	0
2	D	6	0	8	0	0
3	A	5	0	5	6	0
3	C	5	0	5	0	0
3	D	5	0	5	1	0
4	A	616	0	0	11	0
4	B	640	0	0	9	0
4	C	690	0	0	22	0
4	D	610	0	0	18	0
All	All	18228	0	15093	147	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 5.

All (147) 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:D:132[A]:MET:HE3	4:D:1075:HOH:O	1.54	1.08
1:A:453:GLU:OE1	3:A:505:IMD:H2	1.59	1.01
1:C:132[A]:MET:HE3	4:C:1110:HOH:O	1.60	1.01
1:B:349[B]:ASN:O	1:B:350[B]:TRP:CD1	2.15	0.99
1:C:149:ARG:HD3	4:C:1004:HOH:O	1.64	0.95
1:D:249:PHE:CE2	1:D:333:ILE:HD11	2.10	0.87
1:C:301:TYR:CD1	4:C:782:HOH:O	2.29	0.85
1:C:191[B]:MET:HE1	4:C:1227:HOH:O	1.78	0.83
1:C:112[A]:ARG:HG2	4:C:912:HOH:O	1.77	0.82
1:D:112[A]:ARG:HG2	4:D:902:HOH:O	1.79	0.82
1:B:301:TYR:CD1	4:B:635:HOH:O	2.34	0.80
1:D:191[B]:MET:HE1	4:D:1169:HOH:O	1.84	0.77
1:D:97[A]:ASN:ND2	4:D:601:HOH:O	2.17	0.77
1:B:310:PRO:HB3	4:B:632:HOH:O	1.85	0.77
1:A:198:ASN:HD21	1:A:254:TRP:HE1	1.33	0.76
1:C:477[A]:GLU:HG3	4:C:1077:HOH:O	1.85	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:LEU:N	1:D:6:LEU:HD12	2.00	0.74
1:C:198:ASN:HD21	1:C:254:TRP:HE1	1.37	0.72
1:A:477:GLU:HG3	1:A:478:LEU:H	1.55	0.71
1:D:265:GLN:HE21	1:D:269:ASN:HD21	1.39	0.71
1:A:149:ARG:HD3	4:A:866:HOH:O	1.91	0.70
1:B:350[B]:TRP:CD1	1:B:350[B]:TRP:N	2.56	0.70
1:D:341:ARG:NH2	1:D:351:ASP:OD1	2.25	0.69
1:B:349[B]:ASN:C	1:B:350[B]:TRP:CD1	2.70	0.69
1:A:477:GLU:CD	1:A:478:LEU:HD12	2.18	0.68
1:D:198:ASN:HD21	1:D:254:TRP:HE1	1.42	0.67
1:A:336:LEU:CD2	2:A:504:GOL:H2	2.24	0.67
1:B:348:THR:O	1:B:350[A]:TRP:HA	1.95	0.66
1:B:198:ASN:HD21	1:B:254:TRP:HE1	1.43	0.66
1:A:169:ASN:HD21	1:A:299:ASN:HD21	1.42	0.65
1:C:169:ASN:HD21	1:C:299:ASN:HD21	1.45	0.64
1:D:169:ASN:HD21	1:D:299:ASN:HD21	1.46	0.63
1:B:169:ASN:HD21	1:B:299:ASN:HD21	1.44	0.63
1:B:214:HIS:HD2	4:B:1087:HOH:O	1.80	0.63
1:C:236[A]:ARG:HG3	4:C:656:HOH:O	1.99	0.62
1:C:249:PHE:CE2	1:C:333:ILE:HD11	2.34	0.62
1:A:350:TRP:CZ2	1:A:384:PHE:CE2	2.88	0.61
1:C:265:GLN:HE21	1:C:269:ASN:HD21	1.46	0.61
1:B:348:THR:O	1:B:350[A]:TRP:CA	2.49	0.60
1:C:180[A]:ARG:HD3	1:C:191[A]:MET:HG2	1.85	0.58
1:D:265:GLN:HE21	1:D:269:ASN:ND2	2.01	0.58
1:A:93:ASN:C	1:A:93:ASN:HD22	2.12	0.58
1:D:132[A]:MET:CE	4:D:1075:HOH:O	2.26	0.57
1:A:336:LEU:HD21	2:A:504:GOL:H2	1.85	0.57
1:C:93:ASN:HD22	1:C:93:ASN:C	2.12	0.57
1:D:157[A]:ARG:HD2	3:D:502:IMD:C4	2.34	0.57
1:B:112:ARG:HG2	4:B:951:HOH:O	2.05	0.57
1:C:236[B]:ARG:HD2	4:C:615:HOH:O	2.04	0.57
1:D:252:HIS:HE1	4:D:851:HOH:O	1.87	0.56
1:D:249:PHE:CZ	1:D:333:ILE:HD11	2.40	0.56
1:A:156:GLN:HE22	1:B:349[A]:ASN:HD22	1.51	0.56
3:A:505:IMD:H5	4:A:603:HOH:O	2.07	0.55
1:C:249:PHE:CD1	4:C:1255:HOH:O	2.53	0.55
1:A:252:HIS:HE1	4:A:831:HOH:O	1.90	0.54
1:C:265:GLN:HE21	1:C:269:ASN:ND2	2.04	0.54
1:B:93:ASN:C	1:B:93:ASN:HD22	2.14	0.54
1:A:453:GLU:OE1	3:A:505:IMD:C2	2.46	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:ASN:HD21	1:C:254:TRP:NE1	2.05	0.53
1:A:157[A]:ARG:CD	4:A:666:HOH:O	2.56	0.53
1:C:102[B]:ASP:OD2	4:C:602:HOH:O	2.18	0.53
1:C:214[A]:HIS:HE1	1:D:383:GLU:HG2	1.73	0.53
1:D:6:LEU:HD12	1:D:6:LEU:H	1.74	0.53
1:A:157[A]:ARG:HD2	4:A:666:HOH:O	2.10	0.52
1:D:93:ASN:HD22	1:D:93:ASN:C	2.17	0.52
1:C:169:ASN:HD22	1:C:224:SER:HB3	1.74	0.52
1:C:352:TRP:CD1	4:C:1080:HOH:O	2.63	0.51
1:D:302:GLN:CD	4:D:638:HOH:O	2.51	0.51
1:C:252:HIS:HE1	4:C:902:HOH:O	1.93	0.51
1:B:252:HIS:HE1	4:B:891:HOH:O	1.94	0.51
1:D:341:ARG:HH22	1:D:351:ASP:CG	2.19	0.51
1:D:6:LEU:N	1:D:6:LEU:CD1	2.73	0.51
1:D:132[A]:MET:HE1	4:D:691:HOH:O	2.11	0.51
1:B:149:ARG:HD3	4:B:811:HOH:O	2.11	0.50
1:B:169:ASN:HD22	1:B:224:SER:HB3	1.76	0.50
1:A:198:ASN:HD21	1:A:254:TRP:NE1	2.05	0.50
1:D:97[B]:ASN:ND2	1:D:100:GLY:H	2.10	0.50
1:A:174:PHE:HA	4:A:602:HOH:O	2.11	0.49
1:D:149:ARG:NE	4:D:615:HOH:O	2.43	0.49
1:C:43:LYS:HE3	4:C:796:HOH:O	2.12	0.49
3:A:505:IMD:H4	4:A:1070:HOH:O	2.12	0.49
1:C:249:PHE:HD1	4:C:1255:HOH:O	1.95	0.49
1:D:272:GLU:CD	4:D:604:HOH:O	2.56	0.49
1:D:89:PHE:CZ	1:D:96[B]:VAL:HG22	2.48	0.48
1:A:47[A]:ARG:NH2	4:A:612:HOH:O	2.45	0.48
1:B:262[A]:MET:HE3	4:B:772:HOH:O	2.14	0.48
1:A:350:TRP:CE3	1:A:350:TRP:N	2.82	0.48
1:C:249:PHE:CE2	1:C:333:ILE:CD1	2.96	0.48
1:C:61:TYR:OH	4:C:603:HOH:O	2.20	0.48
1:D:94:GLY:N	1:D:149:ARG:NH2	2.61	0.48
1:D:169:ASN:HD22	1:D:224:SER:HB3	1.79	0.47
1:A:169:ASN:HD22	1:A:224:SER:HB3	1.80	0.47
1:A:350:TRP:CE2	1:A:439:LYS:HD2	2.49	0.47
1:A:378:GLU:HG3	1:A:425:TRP:HB2	1.95	0.47
1:D:349:ASN:ND2	4:D:610:HOH:O	2.39	0.47
3:A:505:IMD:C4	4:A:1070:HOH:O	2.62	0.47
1:D:149:ARG:HD3	4:D:615:HOH:O	2.14	0.46
1:A:407:GLN:HG2	4:A:762:HOH:O	2.14	0.46
1:C:198:ASN:ND2	1:C:254:TRP:HE1	2.10	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308[B]:HIS:CE1	4:C:689:HOH:O	2.69	0.46
1:B:198:ASN:HD21	1:B:254:TRP:NE1	2.11	0.46
1:A:44:GLN:OE1	1:A:47[A]:ARG:NE	2.32	0.46
1:A:349:ASN:HB2	1:A:350:TRP:CZ3	2.52	0.45
1:B:310:PRO:CB	4:B:632:HOH:O	2.55	0.45
1:B:170:GLN:NE2	4:B:620:HOH:O	2.50	0.45
1:D:7:LYS:HB3	1:D:7:LYS:HE3	1.71	0.44
1:D:93:ASN:HA	1:D:149:ARG:HH21	1.83	0.44
1:C:301:TYR:CE1	4:C:782:HOH:O	2.59	0.44
1:A:260:TRP:O	1:A:262[B]:MET:HG3	2.18	0.44
1:B:430:LEU:HD12	1:B:430:LEU:C	2.43	0.44
1:D:378:GLU:HG3	1:D:425:TRP:HB2	1.99	0.44
1:A:194[B]:MET:HE2	1:A:194[B]:MET:HB3	1.63	0.44
1:B:378:GLU:HG3	1:B:425:TRP:HB2	1.99	0.44
1:D:198:ASN:HD21	1:D:254:TRP:NE1	2.10	0.44
1:A:336:LEU:HD22	2:A:504:GOL:H2	1.96	0.44
1:A:453:GLU:CD	3:A:505:IMD:H2	2.38	0.44
1:A:403[B]:ARG:CZ	1:A:403[B]:ARG:HB3	2.48	0.43
1:D:92:GLY:HA2	1:D:128:PRO:HG2	2.00	0.43
1:D:97[B]:ASN:HD21	1:D:99:LYS:HB2	1.82	0.43
1:A:184:HIS:HB3	1:A:185:PRO:HD2	2.00	0.43
1:B:157[A]:ARG:HG3	1:B:158:PHE:CE1	2.53	0.43
1:D:112[A]:ARG:HD3	1:D:161:ARG:HB3	1.99	0.43
1:C:378:GLU:HG3	1:C:425:TRP:HB2	2.00	0.43
1:D:430:LEU:C	1:D:430:LEU:HD12	2.44	0.43
1:C:132[A]:MET:HE1	4:C:752:HOH:O	2.17	0.42
1:B:387:LEU:HD11	1:B:391:ASP:HA	2.01	0.42
1:D:262:MET:HE2	4:D:880:HOH:O	2.19	0.42
1:C:238[A]:GLU:HG3	4:C:1137:HOH:O	2.19	0.42
1:D:149:ARG:CD	4:D:615:HOH:O	2.68	0.42
1:D:89:PHE:CE1	1:D:96[B]:VAL:HG22	2.55	0.42
1:A:350:TRP:CZ2	1:A:384:PHE:CZ	3.09	0.41
1:C:166:VAL:HA	1:C:222:GLY:O	2.20	0.41
1:D:245:ASN:ND2	4:D:630:HOH:O	2.53	0.41
1:D:175:ILE:HG21	1:D:198:ASN:HB2	2.03	0.41
1:D:234:ASP:OD2	1:D:236[B]:ARG:NH1	2.54	0.41
1:D:310:PRO:HG3	4:D:651:HOH:O	2.20	0.41
1:C:157[A]:ARG:HD2	4:D:620:HOH:O	2.21	0.41
1:C:174:PHE:HA	4:C:634:HOH:O	2.20	0.41
1:D:425:TRP:HA	1:D:426:SER:HA	1.90	0.41
1:A:312:ASP:HA	4:A:863:HOH:O	2.19	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:GLU:HG3	4:C:612:HOH:O	2.22	0.40
1:C:214[A]:HIS:CE1	1:D:383:GLU:HG2	2.55	0.40
1:C:214[A]:HIS:HE1	1:D:383:GLU:CG	2.34	0.40
1:C:245:ASN:ND2	4:C:630:HOH:O	2.53	0.40
1:D:145:ASP:HB3	4:D:1038:HOH:O	2.20	0.40
1:C:384:PHE:CD1	1:C:438[B]:GLN:HG2	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	478/485 (99%)	462 (97%)	16 (3%)	0	100	100
1	B	476/485 (98%)	461 (97%)	15 (3%)	0	100	100
1	C	480/485 (99%)	462 (96%)	17 (4%)	1 (0%)	43	22
1	D	472/485 (97%)	456 (97%)	14 (3%)	2 (0%)	30	11
All	All	1906/1940 (98%)	1841 (97%)	62 (3%)	3 (0%)	43	22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	310	PRO
1	C	310	PRO
1	D	167	THR

5.3.2 Protein sidechains [i](#)

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	413/412 (100%)	410 (99%)	3 (1%)	76	56
1	B	411/412 (100%)	408 (99%)	3 (1%)	76	56
1	C	415/412 (101%)	411 (99%)	4 (1%)	68	43
1	D	407/412 (99%)	400 (98%)	7 (2%)	53	24
All	All	1646/1648 (100%)	1629 (99%)	17 (1%)	68	43

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	93	ASN
1	A	478	LEU
1	B	93	ASN
1	B	350[A]	TRP
1	B	350[B]	TRP
1	C	93	ASN
1	C	312	ASP
1	C	329	THR
1	C	430	LEU
1	D	5	HIS
1	D	7	LYS
1	D	93	ASN
1	D	112[A]	ARG
1	D	112[B]	ARG
1	D	329	THR
1	D	430	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	169	ASN
1	A	171	GLN
1	A	198	ASN
1	A	202	ASN
1	A	205	ASN
1	A	210	GLN
1	A	250	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	251	ASN
1	A	252	HIS
1	A	265	GLN
1	A	269	ASN
1	A	274	GLN
1	B	93	ASN
1	B	169	ASN
1	B	170	GLN
1	B	171	GLN
1	B	198	ASN
1	B	202	ASN
1	B	205	ASN
1	B	252	HIS
1	B	265	GLN
1	B	269	ASN
1	B	274	GLN
1	B	289	GLN
1	C	93	ASN
1	C	129	GLN
1	C	169	ASN
1	C	170	GLN
1	C	171	GLN
1	C	198	ASN
1	C	202	ASN
1	C	205	ASN
1	C	251	ASN
1	C	252	HIS
1	C	269	ASN
1	C	274	GLN
1	C	289	GLN
1	C	394	ASN
1	C	468	GLN
1	D	5	HIS
1	D	93	ASN
1	D	129	GLN
1	D	169	ASN
1	D	171	GLN
1	D	198	ASN
1	D	202	ASN
1	D	205	ASN
1	D	245	ASN
1	D	251	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	252	HIS
1	D	269	ASN
1	D	274	GLN
1	D	289	GLN
1	D	349	ASN
1	D	410	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](#)

13 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	B	501	-	5,5,5	0.49	0	5,5,5	1.72	2 (40%)
2	GOL	D	501	-	5,5,5	0.44	0	5,5,5	0.94	0
2	GOL	B	502	-	5,5,5	0.68	0	5,5,5	0.92	0
2	GOL	A	501	-	5,5,5	0.77	0	5,5,5	1.31	0
3	IMD	C	503	-	5,5,5	0.86	0	5,5,5	0.65	0
2	GOL	C	501	-	5,5,5	0.68	0	5,5,5	1.20	1 (20%)
2	GOL	A	503	-	5,5,5	0.41	0	5,5,5	1.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	C	502	-	5,5,5	0.49	0	5,5,5	1.01	0
3	IMD	D	502	-	5,5,5	0.93	0	5,5,5	0.73	0
3	IMD	A	505	-	5,5,5	0.74	0	5,5,5	1.48	1 (20%)
2	GOL	A	502	-	5,5,5	0.36	0	5,5,5	1.03	1 (20%)
2	GOL	A	504	-	5,5,5	0.65	0	5,5,5	1.01	0
2	GOL	B	503	-	5,5,5	0.50	0	5,5,5	1.00	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
2	GOL	B	501	-	-	0/4/4/4	-
2	GOL	D	501	-	-	0/4/4/4	-
2	GOL	B	502	-	-	0/4/4/4	-
2	GOL	A	501	-	-	0/4/4/4	-
3	IMD	C	503	-	-	-	0/1/1/1
2	GOL	C	501	-	-	2/4/4/4	-
2	GOL	A	503	-	-	0/4/4/4	-
2	GOL	C	502	-	-	2/4/4/4	-
3	IMD	D	502	-	-	-	0/1/1/1
3	IMD	A	505	-	-	-	0/1/1/1
2	GOL	A	502	-	-	0/4/4/4	-
2	GOL	A	504	-	-	3/4/4/4	-
2	GOL	B	503	-	-	0/4/4/4	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	GOL	C3-C2-C1	-2.93	101.05	111.80
2	C	501	GOL	C3-C2-C1	-2.50	102.62	111.80
2	B	501	GOL	O1-C1-C2	2.36	120.99	110.38
2	A	502	GOL	O3-C3-C2	2.22	120.38	110.38
3	A	505	IMD	C5-N1-C2	-2.05	102.77	107.19

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	GOL	O1-C1-C2-C3
2	C	501	GOL	O1-C1-C2-O2
2	A	504	GOL	C1-C2-C3-O3
2	A	504	GOL	O2-C2-C3-O3
2	A	504	GOL	O1-C1-C2-O2
2	C	502	GOL	C1-C2-C3-O3
2	C	502	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	502	IMD	1	0
3	A	505	IMD	6	0
2	A	504	GOL	3	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	459/485 (94%)	-0.33	12 (2%) 57 61	5, 11, 28, 67	21 (4%)
1	B	459/485 (94%)	-0.41	7 (1%) 72 76	4, 10, 23, 61	20 (4%)
1	C	460/485 (94%)	-0.49	8 (1%) 69 73	4, 9, 21, 80	23 (5%)
1	D	460/485 (94%)	-0.32	12 (2%) 57 61	5, 11, 25, 90	16 (3%)
All	All	1838/1940 (94%)	-0.38	39 (2%) 63 67	4, 10, 25, 90	80 (4%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	350	TRP	6.6
1	D	352	TRP	5.6
1	B	352	TRP	5.2
1	A	352	TRP	5.1
1	C	313	GLY	5.0
1	D	313	GLY	4.9
1	C	352	TRP	4.8
1	C	314	VAL	4.4
1	C	311	PRO	4.2
1	B	5	HIS	4.1
1	D	311	PRO	4.0
1	B	351[A]	ASP	4.0
1	A	477	GLU	3.9
1	B	350[A]	TRP	3.8
1	D	314	VAL	3.7
1	A	5	HIS	3.5
1	D	310	PRO	3.5
1	A	313	GLY	3.5
1	D	5	HIS	3.5
1	C	5	HIS	3.4
1	C	329	THR	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	310	PRO	3.3
1	C	312	ASP	3.2
1	D	312	ASP	3.1
1	D	329	THR	3.0
1	A	478	LEU	2.7
1	A	351	ASP	2.6
1	B	312	ASP	2.5
1	D	350	TRP	2.4
1	A	6	LEU	2.4
1	A	384	PHE	2.4
1	D	384[A]	PHE	2.4
1	B	348	THR	2.3
1	D	6	LEU	2.3
1	A	476	ALA	2.3
1	D	308	HIS	2.2
1	A	312	ASP	2.2
1	A	311	PRO	2.1
1	B	311	PRO	2.1

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	IMD	D	502	5/5	0.77	0.16	19,25,31,32	5
2	GOL	B	503	6/6	0.80	0.13	29,34,35,35	0
3	IMD	A	505	5/5	0.81	0.13	33,38,42,45	0
2	GOL	A	503	6/6	0.81	0.14	31,32,35,35	0
2	GOL	D	501	6/6	0.82	0.14	34,35,37,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	C	502	6/6	0.86	0.10	30,31,32,33	0
3	IMD	C	503	5/5	0.87	0.13	22,26,31,35	0
2	GOL	A	504	6/6	0.87	0.12	38,40,43,47	0
2	GOL	C	501	6/6	0.93	0.10	17,26,33,44	0
2	GOL	B	502	6/6	0.97	0.07	13,15,21,23	0
2	GOL	A	501	6/6	0.97	0.07	13,15,20,22	0
2	GOL	A	502	6/6	0.97	0.07	13,17,20,22	0
2	GOL	B	501	6/6	0.97	0.08	13,17,22,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.