



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 08:45 pm BST

PDB ID : 4ZE5
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

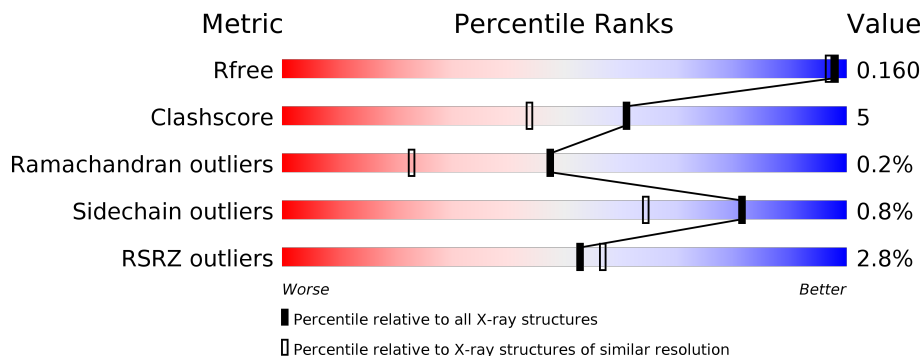
1 Overall quality at a glance

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}	130704	4690 (1.50-1.46)
Clashscore	141614	4955 (1.50-1.46)
Ramachandran outliers	138981	4846 (1.50-1.46)
Sidechain outliers	138945	4844 (1.50-1.46)
RSRZ outliers	127900	4614 (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 on 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	 4% 77% 16% • 5%
1	B	485	 2% 79% 14% • 5%
1	C	485	 2% 77% 16% • 5%
1	D	485	 2% 75% 18% • 5%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	IMD	A	505	-	-	X	-

2 Entry composition i

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-galactosidase.

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

There are 36 discrepancies between the modelled and reference sequences:

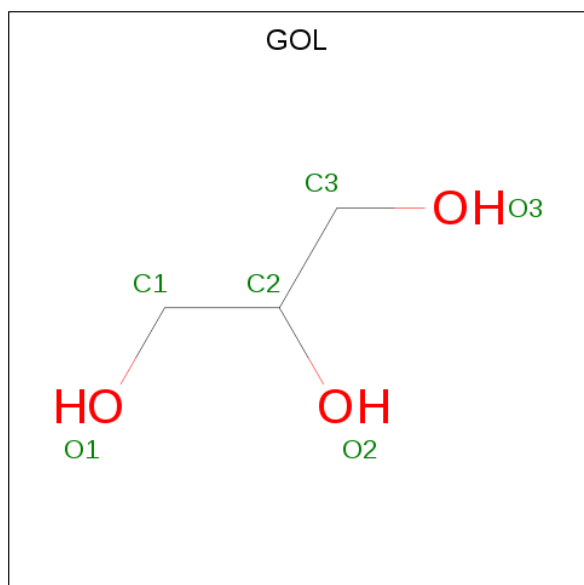
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP W8QF82
A	-5	ILE	-	expression tag	UNP W8QF82
A	-4	HIS	-	expression tag	UNP W8QF82
A	-3	HIS	-	expression tag	UNP W8QF82
A	-2	HIS	-	expression tag	UNP W8QF82
A	-1	HIS	-	expression tag	UNP W8QF82
A	0	HIS	-	expression tag	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 (three-letter code: GOL) (formula: C₃H₈O₃).



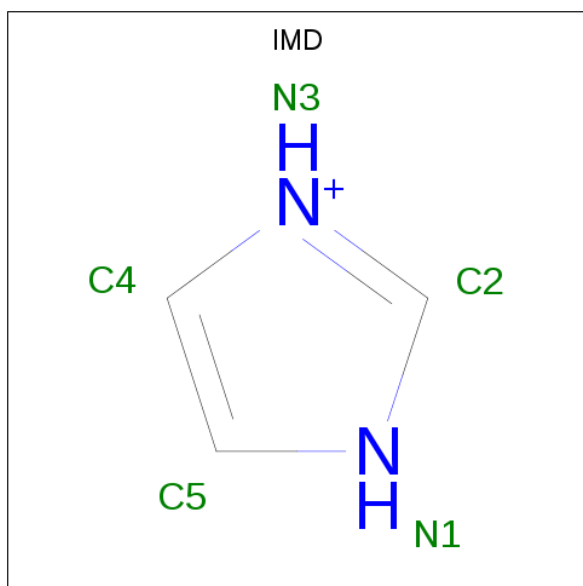
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		

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 (three-letter code: IMD) (formula: C₃H₅N₂).



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		

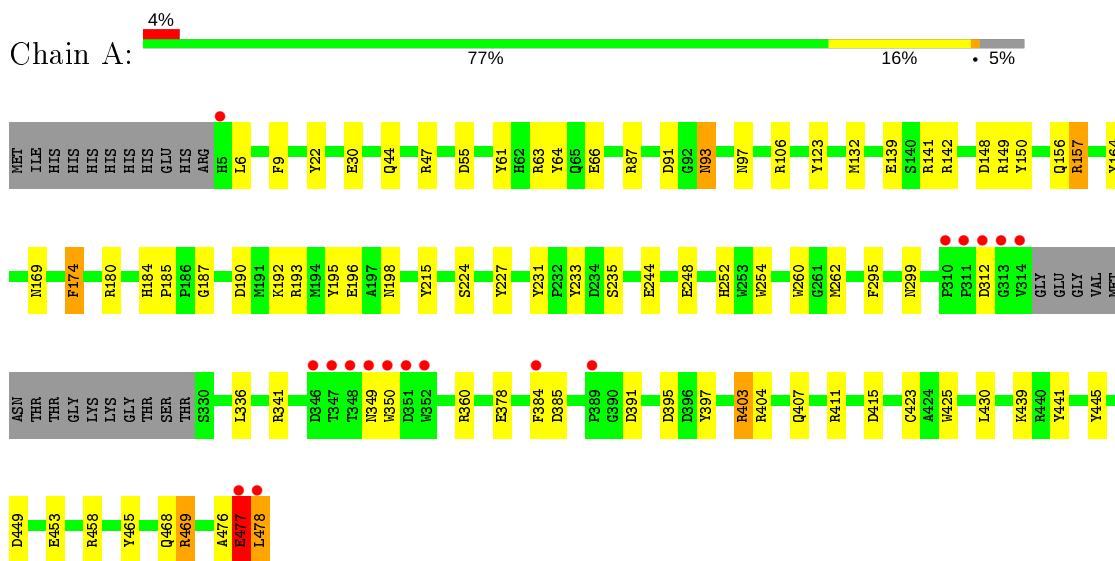
- Molecule 4 is water.

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

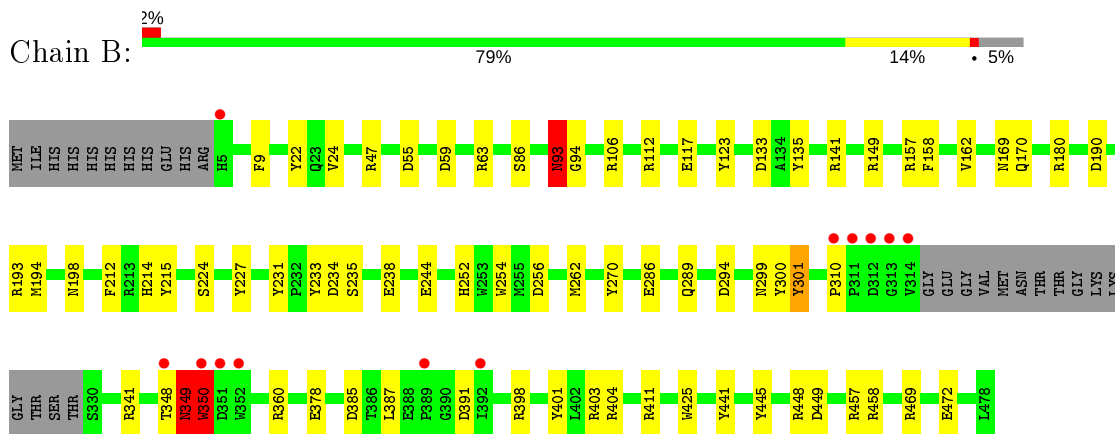
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

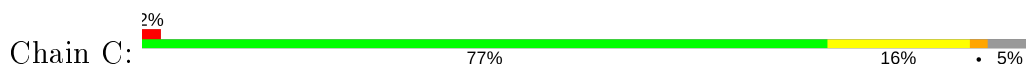
- Molecule 1: Putative 6-phospho-beta-galactobiosidase

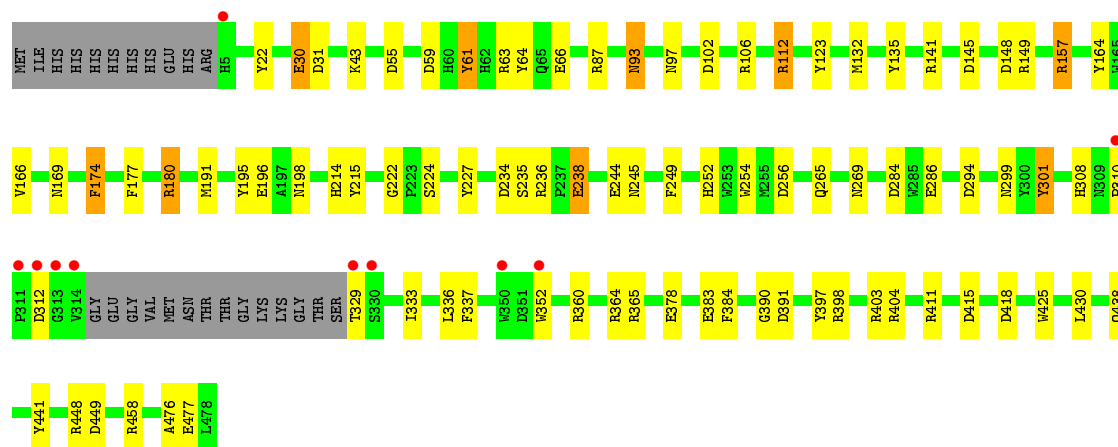


- Molecule 1: Putative 6-phospho-beta-galactobiosidase

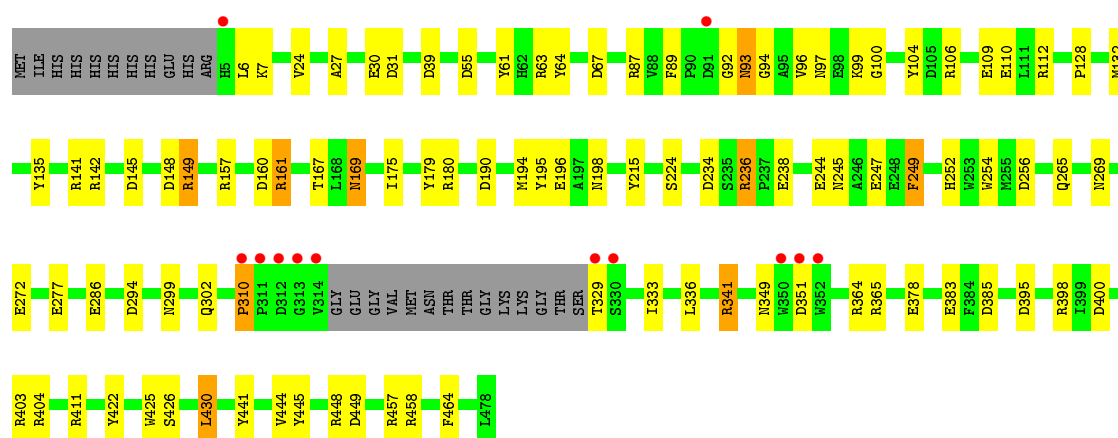
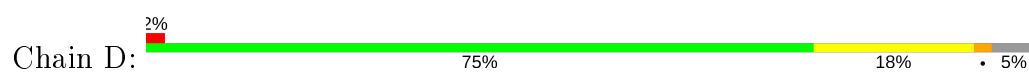


- Molecule 1: Putative 6-phospho-beta-galactobiosidase





• 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 27.62 – 1.48	Depositor EDS
% Data completeness (in resolution range)	99.7 (27.64-1.48) 99.7 (27.62-1.48)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.50 (at 1.48Å)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.132 , 0.159 0.132 , 0.160	Depositor DCC
R_{free} test set	16966 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	10.9	Xtrriage
Anisotropy	0.482	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.000 for l,-k,h	Xtrriage
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

Xtrriage'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 i

5.1 Standard geometry i

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	1.44	26/4091 (0.6%)	1.48	65/5559 (1.2%)
1	B	1.43	23/4076 (0.6%)	1.52	73/5543 (1.3%)
1	C	1.42	28/4117 (0.7%)	1.51	76/5597 (1.4%)
1	D	1.40	20/4041 (0.5%)	1.57	72/5496 (1.3%)
All	All	1.42	97/16325 (0.6%)	1.52	286/22195 (1.3%)

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

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

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	286	GLU	CD-OE2	10.28	1.36	1.25
1	C	238[A]	GLU	CD-OE1	9.94	1.36	1.25
1	C	238[B]	GLU	CD-OE1	9.94	1.36	1.25
1	B	238[A]	GLU	CG-CD	9.45	1.66	1.51
1	B	238[B]	GLU	CG-CD	9.45	1.66	1.51
1	C	441	TYR	CE2-CZ	-8.89	1.26	1.38
1	A	477	GLU	CG-CD	8.76	1.65	1.51
1	D	286	GLU	CD-OE2	8.68	1.35	1.25
1	D	64	TYR	CE1-CZ	-8.66	1.27	1.38
1	B	350[A]	TRP	N-CA	8.49	1.63	1.46
1	B	350[B]	TRP	N-CA	8.49	1.63	1.46
1	A	22	TYR	CD1-CE1	8.12	1.51	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	445	TYR	CE1-CZ	-8.09	1.28	1.38
1	A	469	ARG	CG-CD	-7.78	1.32	1.51
1	B	441	TYR	CE1-CZ	-7.69	1.28	1.38
1	B	238[A]	GLU	CD-OE2	7.44	1.33	1.25
1	B	238[B]	GLU	CD-OE2	7.44	1.33	1.25
1	C	286	GLU	CG-CD	7.41	1.63	1.51
1	C	63[A]	ARG	CZ-NH1	-7.12	1.23	1.33
1	C	63[B]	ARG	CZ-NH1	-7.12	1.23	1.33
1	A	244	GLU	CD-OE1	6.99	1.33	1.25
1	B	472	GLU	CD-OE1	6.98	1.33	1.25
1	C	180[A]	ARG	CZ-NH2	6.86	1.42	1.33
1	C	180[B]	ARG	CZ-NH2	6.86	1.42	1.33
1	C	180[A]	ARG	CZ-NH1	6.82	1.42	1.33
1	C	180[B]	ARG	CZ-NH1	6.82	1.42	1.33
1	C	61	TYR	CE2-CZ	-6.82	1.29	1.38
1	B	94	GLY	N-CA	6.72	1.56	1.46
1	C	215	TYR	CE1-CZ	-6.61	1.29	1.38
1	C	61	TYR	CE1-CZ	-6.61	1.29	1.38
1	B	133	ASP	CG-OD1	-6.60	1.10	1.25
1	A	66	GLU	CD-OE1	6.40	1.32	1.25
1	A	227	TYR	CE2-CZ	-6.37	1.30	1.38
1	B	401	TYR	CE2-CZ	-6.35	1.30	1.38
1	D	286	GLU	CG-CD	6.32	1.61	1.51
1	D	180[A]	ARG	CZ-NH1	6.31	1.41	1.33
1	D	180[B]	ARG	CZ-NH1	6.31	1.41	1.33
1	C	441	TYR	CZ-OH	6.28	1.48	1.37
1	C	383	GLU	CD-OE1	-6.27	1.18	1.25
1	A	196	GLU	CD-OE2	6.20	1.32	1.25
1	C	235	SER	CB-OG	6.20	1.50	1.42
1	C	301	TYR	CE2-CZ	-6.18	1.30	1.38
1	B	22	TYR	CZ-OH	6.16	1.48	1.37
1	D	110	GLU	CD-OE2	-6.14	1.18	1.25
1	D	160	ASP	CB-CG	6.11	1.64	1.51
1	C	476	ALA	C-O	6.09	1.34	1.23
1	D	249	PHE	CB-CG	-6.08	1.41	1.51
1	A	441	TYR	CE2-CZ	-6.07	1.30	1.38
1	B	106	ARG	CZ-NH2	-5.97	1.25	1.33
1	C	61	TYR	CZ-OH	5.82	1.47	1.37
1	C	390	GLY	N-CA	-5.80	1.37	1.46
1	A	430	LEU	C-O	-5.75	1.12	1.23
1	A	215	TYR	CG-CD1	5.74	1.46	1.39
1	B	270	TYR	CG-CD1	-5.72	1.31	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	196	GLU	CD-OE2	5.71	1.31	1.25
1	B	235	SER	CB-OG	5.70	1.49	1.42
1	B	117	GLU	CB-CG	-5.57	1.41	1.52
1	D	61	TYR	CE2-CZ	-5.57	1.31	1.38
1	A	164	TYR	CE1-CZ	-5.56	1.31	1.38
1	A	441	TYR	CZ-OH	5.54	1.47	1.37
1	C	301	TYR	CG-CD2	-5.53	1.31	1.39
1	A	235	SER	CB-OG	5.53	1.49	1.42
1	A	441	TYR	CD2-CE2	-5.52	1.31	1.39
1	D	238[A]	GLU	CD-OE2	5.52	1.31	1.25
1	D	238[B]	GLU	CD-OE2	5.52	1.31	1.25
1	B	301	TYR	CE1-CZ	-5.50	1.31	1.38
1	B	445	TYR	CE1-CZ	-5.47	1.31	1.38
1	A	164	TYR	CZ-OH	5.45	1.47	1.37
1	A	397	TYR	CE1-CZ	5.44	1.45	1.38
1	D	277	GLU	CD-OE2	-5.44	1.19	1.25
1	C	164	TYR	CG-CD1	-5.44	1.32	1.39
1	D	179	TYR	CE1-CZ	-5.44	1.31	1.38
1	B	286[A]	GLU	CD-OE2	5.42	1.31	1.25
1	B	286[B]	GLU	CD-OE2	5.42	1.31	1.25
1	A	248	GLU	CG-CD	-5.36	1.44	1.51
1	D	169	ASN	CG-ND2	-5.36	1.19	1.32
1	D	215	TYR	CE1-CZ	-5.27	1.31	1.38
1	A	157[A]	ARG	CZ-NH2	5.25	1.39	1.33
1	A	157[B]	ARG	CZ-NH2	5.25	1.39	1.33
1	D	444	VAL	CB-CG2	-5.25	1.41	1.52
1	D	448	ARG	CZ-NH1	5.23	1.39	1.33
1	A	64	TYR	CE1-CZ	-5.19	1.31	1.38
1	C	64	TYR	CE1-CZ	-5.17	1.31	1.38
1	D	104	TYR	CE1-CZ	-5.17	1.31	1.38
1	B	286[A]	GLU	CG-CD	5.16	1.59	1.51
1	B	286[B]	GLU	CG-CD	5.16	1.59	1.51
1	A	469	ARG	CD-NE	5.13	1.55	1.46
1	C	195	TYR	CE1-CZ	-5.13	1.31	1.38
1	A	187	GLY	N-CA	-5.10	1.38	1.46
1	A	423	CYS	CB-SG	-5.09	1.73	1.81
1	B	86	SER	CB-OG	-5.08	1.35	1.42
1	D	196	GLU	CD-OE2	5.06	1.31	1.25
1	A	61	TYR	CE1-CZ	-5.05	1.31	1.38
1	C	22	TYR	CE2-CZ	-5.04	1.31	1.38
1	A	123	TYR	CE1-CZ	-5.04	1.32	1.38
1	C	87	ARG	CB-CG	-5.04	1.39	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	247	GLU	CD-OE2	5.00	1.31	1.25

All (286) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	180[A]	ARG	NE-CZ-NH2	-14.57	113.02	120.30
1	B	180[B]	ARG	NE-CZ-NH2	-14.57	113.02	120.30
1	D	458	ARG	NE-CZ-NH1	13.48	127.04	120.30
1	D	403	ARG	NE-CZ-NH1	13.33	126.96	120.30
1	C	411	ARG	NE-CZ-NH2	-12.60	114.00	120.30
1	C	106	ARG	NE-CZ-NH1	12.54	126.57	120.30
1	D	411	ARG	NE-CZ-NH2	-12.10	114.25	120.30
1	B	398	ARG	NE-CZ-NH2	11.88	126.24	120.30
1	B	141[A]	ARG	NE-CZ-NH1	11.36	125.98	120.30
1	B	141[B]	ARG	NE-CZ-NH1	11.36	125.98	120.30
1	C	227	TYR	CB-CG-CD1	11.32	127.79	121.00
1	D	411	ARG	NE-CZ-NH1	11.23	125.92	120.30
1	A	395	ASP	CB-CG-OD1	11.00	128.20	118.30
1	B	449	ASP	CB-CG-OD1	11.00	128.20	118.30
1	D	180[A]	ARG	NE-CZ-NH2	-10.82	114.89	120.30
1	D	180[B]	ARG	NE-CZ-NH2	-10.82	114.89	120.30
1	C	180[A]	ARG	NE-CZ-NH2	-10.79	114.90	120.30
1	C	180[B]	ARG	NE-CZ-NH2	-10.79	114.90	120.30
1	A	180[A]	ARG	NE-CZ-NH2	-10.68	114.96	120.30
1	A	180[B]	ARG	NE-CZ-NH2	-10.68	114.96	120.30
1	D	365	ARG	NE-CZ-NH1	10.62	125.61	120.30
1	D	403	ARG	NE-CZ-NH2	-10.56	115.02	120.30
1	A	193	ARG	NE-CZ-NH1	-10.49	115.05	120.30
1	C	403	ARG	NE-CZ-NH2	-10.22	115.19	120.30
1	C	55	ASP	CB-CG-OD2	-10.21	109.11	118.30
1	B	294	ASP	CB-CG-OD2	10.18	127.47	118.30
1	A	142	ARG	NE-CZ-NH2	-9.98	115.31	120.30
1	C	87	ARG	NE-CZ-NH1	9.97	125.29	120.30
1	B	360	ARG	NE-CZ-NH2	-9.84	115.38	120.30
1	C	360	ARG	NE-CZ-NH2	-9.83	115.39	120.30
1	B	63	ARG	NE-CZ-NH1	-9.78	115.41	120.30
1	A	360	ARG	NE-CZ-NH2	-9.55	115.52	120.30
1	C	404	ARG	NE-CZ-NH2	-9.35	115.62	120.30
1	A	190	ASP	CB-CG-OD1	9.17	126.55	118.30
1	D	87	ARG	NE-CZ-NH2	-9.14	115.73	120.30
1	A	449	ASP	CB-CG-OD1	8.93	126.34	118.30
1	B	341	ARG	NE-CZ-NH2	-8.92	115.84	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	458	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	D	161	ARG	NE-CZ-NH1	8.89	124.75	120.30
1	D	194	MET	CG-SD-CE	-8.88	86.00	100.20
1	D	398	ARG	NE-CZ-NH2	8.79	124.70	120.30
1	A	469	ARG	NE-CZ-NH1	-8.78	115.91	120.30
1	A	411	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	D	141[A]	ARG	NE-CZ-NH1	8.69	124.64	120.30
1	D	141[B]	ARG	NE-CZ-NH1	8.69	124.64	120.30
1	B	411	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	B	341	ARG	NE-CZ-NH1	8.63	124.62	120.30
1	D	148	ASP	CB-CG-OD1	8.56	126.01	118.30
1	C	294	ASP	CB-CG-OD2	8.54	125.98	118.30
1	B	9	PHE	CB-CG-CD1	8.49	126.74	120.80
1	D	395	ASP	CB-CG-OD1	8.47	125.92	118.30
1	B	403	ARG	NE-CZ-NH2	-8.38	116.11	120.30
1	D	458	ARG	NE-CZ-NH2	-8.36	116.12	120.30
1	A	157[A]	ARG	NE-CZ-NH1	-8.32	116.14	120.30
1	A	157[B]	ARG	NE-CZ-NH1	-8.32	116.14	120.30
1	A	227	TYR	CB-CG-CD1	8.32	125.99	121.00
1	A	148	ASP	CB-CG-OD2	-8.27	110.86	118.30
1	D	87	ARG	NE-CZ-NH1	8.23	124.42	120.30
1	B	441	TYR	CG-CD2-CE2	-8.23	114.72	121.30
1	B	106	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	B	404	ARG	NE-CZ-NH1	8.17	124.38	120.30
1	C	411	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	D	238[A]	GLU	CG-CD-OE1	-8.13	102.03	118.30
1	D	238[B]	GLU	CG-CD-OE1	-8.13	102.03	118.30
1	D	404	ARG	NE-CZ-NH2	-8.07	116.26	120.30
1	C	403	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	C	294	ASP	CB-CG-OD1	-8.04	111.07	118.30
1	C	365	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	B	404	ARG	NE-CZ-NH2	-7.89	116.36	120.30
1	C	352	TRP	CA-CB-CG	7.89	128.69	113.70
1	D	106	ARG	NE-CZ-NH1	7.87	124.24	120.30
1	B	93	ASN	C-N-CA	-7.85	105.81	122.30
1	D	24	VAL	CG1-CB-CG2	7.84	123.44	110.90
1	C	449	ASP	CB-CG-OD1	7.78	125.30	118.30
1	B	135	TYR	CB-CG-CD2	7.78	125.67	121.00
1	A	141	ARG	NE-CZ-NH1	-7.77	116.42	120.30
1	C	364	ARG	NE-CZ-NH2	-7.73	116.43	120.30
1	D	104	TYR	CB-CG-CD2	7.68	125.61	121.00
1	A	385	ASP	CB-CG-OD1	7.66	125.19	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	458	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	A	477	GLU	N-CA-CB	7.63	124.34	110.60
1	D	106	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	D	400	ASP	CB-CG-OD1	-7.61	111.45	118.30
1	C	286	GLU	CG-CD-OE2	7.60	133.49	118.30
1	B	55	ASP	CB-CG-OD2	-7.58	111.48	118.30
1	D	149	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	C	364	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	C	398	ARG	NE-CZ-NH2	7.46	124.03	120.30
1	B	403	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	D	457	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	D	441	TYR	CB-CG-CD2	-7.38	116.57	121.00
1	A	415	ASP	CB-CG-OD2	7.36	124.92	118.30
1	D	365	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	B	194[A]	MET	CG-SD-CE	-7.34	88.46	100.20
1	B	194[B]	MET	CG-SD-CE	-7.34	88.46	100.20
1	D	149	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	D	256	ASP	CB-CG-OD2	-7.27	111.76	118.30
1	C	448	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	B	238[A]	GLU	CG-CD-OE2	7.26	132.82	118.30
1	B	238[B]	GLU	CG-CD-OE2	7.26	132.82	118.30
1	A	477	GLU	OE1-CD-OE2	-7.23	114.62	123.30
1	C	145	ASP	CB-CG-OD1	7.21	124.79	118.30
1	A	91	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	B	55	ASP	CB-CG-OD1	7.17	124.75	118.30
1	A	215	TYR	CB-CG-CD2	7.12	125.27	121.00
1	C	30	GLU	OE1-CD-OE2	7.09	131.81	123.30
1	D	31	ASP	CB-CG-OD2	7.09	124.68	118.30
1	C	112[A]	ARG	NE-CZ-NH1	7.03	123.82	120.30
1	C	112[B]	ARG	NE-CZ-NH1	7.03	123.82	120.30
1	C	141[A]	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	C	141[B]	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	C	441	TYR	CG-CD1-CE1	-7.02	115.69	121.30
1	A	9	PHE	CB-CG-CD1	7.01	125.71	120.80
1	C	418	ASP	CB-CG-OD2	-7.01	111.99	118.30
1	C	365	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	A	87	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	C	391	ASP	CB-CG-OD2	-6.95	112.04	118.30
1	A	231	TYR	CB-CG-CD1	6.83	125.10	121.00
1	B	411	ARG	NE-CZ-NH2	-6.83	116.88	120.30
1	B	47	ARG	NE-CZ-NH2	6.81	123.70	120.30
1	A	157[A]	ARG	CG-CD-NE	-6.73	97.67	111.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157[B]	ARG	CG-CD-NE	-6.73	97.67	111.80
1	C	238[A]	GLU	CG-CD-OE2	-6.71	104.88	118.30
1	C	238[B]	GLU	CG-CD-OE2	-6.71	104.88	118.30
1	B	300	TYR	CB-CG-CD2	6.71	125.02	121.00
1	D	39	ASP	CB-CG-OD2	6.67	124.31	118.30
1	B	256	ASP	CB-CG-OD2	-6.66	112.31	118.30
1	A	106	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	B	133	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	C	441	TYR	CB-CG-CD2	-6.61	117.03	121.00
1	B	469	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	A	139	GLU	OE1-CD-OE2	6.57	131.18	123.30
1	C	238[A]	GLU	CG-CD-OE1	6.54	131.37	118.30
1	C	238[B]	GLU	CG-CD-OE1	6.54	131.37	118.30
1	A	66	GLU	CG-CD-OE2	-6.52	105.26	118.30
1	D	364	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	B	141[A]	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	B	141[B]	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	B	445	TYR	CD1-CE1-CZ	6.36	125.52	119.80
1	D	236[A]	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	D	236[B]	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	A	22	TYR	CG-CD1-CE1	-6.35	116.22	121.30
1	D	63	ARG	NE-CZ-NH1	-6.33	117.14	120.30
1	C	61	TYR	CG-CD2-CE2	-6.32	116.25	121.30
1	C	112[A]	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	C	112[B]	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	B	106	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	B	385	ASP	CB-CG-OD1	6.28	123.96	118.30
1	C	31	ASP	CB-CG-OD2	6.28	123.95	118.30
1	D	148	ASP	CB-CG-OD2	-6.26	112.66	118.30
1	B	349[A]	ASN	C-N-CA	6.24	137.31	121.70
1	B	349[B]	ASN	C-N-CA	6.24	137.31	121.70
1	D	449	ASP	CB-CG-OD1	6.23	123.91	118.30
1	A	445	TYR	CD1-CE1-CZ	6.22	125.40	119.80
1	A	341	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	D	238[A]	GLU	CG-CD-OE2	6.21	130.72	118.30
1	D	238[B]	GLU	CG-CD-OE2	6.21	130.72	118.30
1	D	67	ASP	CB-CG-OD2	6.18	123.86	118.30
1	A	403[A]	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	A	403[B]	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	A	404	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	C	145	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	D	109	GLU	OE1-CD-OE2	-6.12	115.96	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	286	GLU	CG-CD-OE2	6.10	130.50	118.30
1	B	350[A]	TRP	CA-CB-CG	6.09	125.27	113.70
1	B	350[B]	TRP	CA-CB-CG	6.09	125.27	113.70
1	D	341	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	B	238[A]	GLU	CG-CD-OE1	-6.02	106.26	118.30
1	B	238[B]	GLU	CG-CD-OE1	-6.02	106.26	118.30
1	A	441	TYR	CD1-CE1-CZ	-6.00	114.41	119.80
1	B	244	GLU	OE1-CD-OE2	5.99	130.49	123.30
1	D	141[A]	ARG	NE-CZ-NH2	-5.99	117.30	120.30
1	D	141[B]	ARG	NE-CZ-NH2	-5.99	117.30	120.30
1	C	441	TYR	OH-CZ-CE2	-5.99	103.94	120.10
1	A	66	GLU	CG-CD-OE1	5.98	130.25	118.30
1	B	227	TYR	CB-CG-CD1	5.97	124.58	121.00
1	D	55	ASP	CB-CG-OD1	5.97	123.67	118.30
1	B	256	ASP	CB-CG-OD1	5.97	123.67	118.30
1	C	87	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	C	397	TYR	CB-CG-CD2	5.96	124.58	121.00
1	C	404	ARG	NH1-CZ-NH2	5.95	125.95	119.40
1	A	360	ARG	NH1-CZ-NH2	5.95	125.94	119.40
1	C	61	TYR	CE1-CZ-CE2	5.92	129.27	119.80
1	D	135	TYR	CB-CG-CD2	5.90	124.54	121.00
1	C	360	ARG	NH1-CZ-NH2	5.88	125.87	119.40
1	B	190[A]	ASP	CB-CG-OD1	5.88	123.59	118.30
1	B	190[B]	ASP	CB-CG-OD1	5.88	123.59	118.30
1	D	195	TYR	CB-CG-CD2	5.85	124.51	121.00
1	A	195	TYR	CB-CG-CD2	5.85	124.51	121.00
1	B	233	TYR	CB-CG-CD2	-5.85	117.49	121.00
1	B	457	ARG	CA-CB-CG	5.83	126.22	113.40
1	D	190	ASP	CB-CG-OD1	5.81	123.53	118.30
1	C	336	LEU	CB-CG-CD1	-5.81	101.12	111.00
1	B	22	TYR	CB-CG-CD2	-5.80	117.52	121.00
1	B	193	ARG	NE-CZ-NH1	-5.79	117.41	120.30
1	B	93	ASN	CB-CA-C	5.78	121.95	110.40
1	B	458	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	D	445	TYR	CB-CG-CD2	5.76	124.45	121.00
1	A	391	ASP	CB-CG-OD1	5.75	123.48	118.30
1	A	295	PHE	CB-CG-CD2	5.73	124.81	120.80
1	A	22	TYR	CZ-CE2-CD2	-5.73	114.64	119.80
1	C	148	ASP	CB-CG-OD1	5.73	123.45	118.30
1	A	63[A]	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	A	63[B]	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	B	469	ARG	NE-CZ-NH2	-5.71	117.45	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	142	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	B	135	TYR	CG-CD2-CE2	5.69	125.85	121.30
1	C	141[A]	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	C	141[B]	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	B	449	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	C	215	TYR	CD1-CE1-CZ	5.67	124.90	119.80
1	B	212	PHE	CB-CG-CD2	5.66	124.76	120.80
1	A	231	TYR	CB-CG-CD2	-5.65	117.61	121.00
1	D	294	ASP	CB-CG-OD1	-5.65	113.22	118.30
1	D	27	ALA	CB-CA-C	5.61	118.51	110.10
1	D	422	TYR	CB-CG-CD1	5.60	124.36	121.00
1	C	415	ASP	CB-CG-OD1	5.56	123.30	118.30
1	A	465	TYR	CB-CG-CD2	-5.55	117.67	121.00
1	D	464	PHE	CB-CG-CD2	-5.55	116.91	120.80
1	D	215	TYR	CZ-CE2-CD2	-5.53	114.82	119.80
1	C	352	TRP	CB-CA-C	-5.53	99.35	110.40
1	C	59	ASP	CB-CG-OD1	5.52	123.27	118.30
1	C	66	GLU	CG-CD-OE2	-5.51	107.27	118.30
1	C	61	TYR	CB-CG-CD2	-5.48	117.71	121.00
1	C	458	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	B	234	ASP	CB-CG-OD1	5.47	123.22	118.30
1	C	157[A]	ARG	CG-CD-NE	-5.46	100.34	111.80
1	C	157[B]	ARG	CG-CD-NE	-5.46	100.34	111.80
1	A	341	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	C	177	PHE	CB-CG-CD2	-5.42	117.00	120.80
1	A	411	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	C	441	TYR	CE1-CZ-CE2	5.41	128.46	119.80
1	D	64	TYR	CB-CG-CD1	-5.39	117.77	121.00
1	C	244	GLU	OE1-CD-OE2	5.36	129.73	123.30
1	D	385	ASP	CB-CG-OD1	5.36	123.12	118.30
1	D	430	LEU	CB-CG-CD1	-5.36	101.89	111.00
1	D	30	GLU	OE1-CD-OE2	5.34	129.71	123.30
1	C	180[A]	ARG	NH1-CZ-NH2	5.34	125.27	119.40
1	C	180[B]	ARG	NH1-CZ-NH2	5.34	125.27	119.40
1	A	227	TYR	CB-CG-CD2	-5.34	117.80	121.00
1	C	284	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	B	180[A]	ARG	NH1-CZ-NH2	5.31	125.24	119.40
1	B	180[B]	ARG	NH1-CZ-NH2	5.31	125.24	119.40
1	C	256	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	403[A]	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	403[B]	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	D	161	ARG	NE-CZ-NH2	-5.30	117.65	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	215	TYR	CG-CD2-CE2	5.29	125.53	121.30
1	C	148	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	D	277	GLU	CG-CD-OE2	5.29	128.87	118.30
1	D	249	PHE	CB-CG-CD1	5.28	124.49	120.80
1	A	30[A]	GLU	OE1-CD-OE2	5.26	129.62	123.30
1	A	30[B]	GLU	OE1-CD-OE2	5.26	129.62	123.30
1	D	244	GLU	OE1-CD-OE2	5.25	129.59	123.30
1	D	336	LEU	CB-CG-CD1	-5.23	102.11	111.00
1	B	123	TYR	CB-CG-CD2	5.20	124.12	121.00
1	A	174	PHE	CB-CG-CD1	5.19	124.43	120.80
1	C	61	TYR	CD1-CE1-CZ	-5.19	115.13	119.80
1	A	468	GLN	O-C-N	5.18	130.99	122.70
1	C	337	PHE	CB-CG-CD2	-5.17	117.18	120.80
1	B	59	ASP	CB-CG-OD1	5.14	122.93	118.30
1	A	123	TYR	CB-CG-CD1	-5.13	117.92	121.00
1	A	55	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	A	55	ASP	CB-CG-OD1	5.11	122.90	118.30
1	D	364	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	B	398	ARG	NH1-CZ-NH2	-5.10	113.79	119.40
1	A	150	TYR	CB-CG-CD2	-5.10	117.94	121.00
1	B	445	TYR	CG-CD1-CE1	-5.10	117.22	121.30
1	C	135	TYR	CD1-CE1-CZ	5.10	124.39	119.80
1	D	180[A]	ARG	NH1-CZ-NH2	5.09	125.00	119.40
1	D	180[B]	ARG	NH1-CZ-NH2	5.09	125.00	119.40
1	C	174	PHE	CB-CG-CD2	5.08	124.36	120.80
1	B	289	GLN	CB-CG-CD	5.07	124.79	111.60
1	B	162	VAL	O-C-N	5.06	130.80	122.70
1	B	24	VAL	CG1-CB-CG2	5.06	119.00	110.90
1	C	123	TYR	CB-CG-CD1	-5.06	117.96	121.00
1	C	234	ASP	CB-CG-OD1	5.06	122.85	118.30
1	D	104	TYR	CG-CD2-CE2	5.05	125.34	121.30
1	A	233	TYR	CB-CG-CD2	-5.05	117.97	121.00
1	B	448	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	395	ASP	OD1-CG-OD2	-5.03	113.75	123.30
1	C	398	ARG	NH1-CZ-NH2	-5.02	113.87	119.40
1	A	441	TYR	CG-CD1-CE1	-5.02	117.29	121.30
1	B	231	TYR	CB-CG-CD1	5.02	124.01	121.00
1	A	295	PHE	CB-CG-CD1	-5.01	117.29	120.80
1	B	458	ARG	NE-CZ-NH1	5.01	122.80	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
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	34	0
1	B	3900	0	3731	22	0
1	C	3923	0	3783	38	0
1	D	3872	0	3716	46	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	5	0
3	C	5	0	5	0	0
3	D	5	0	5	1	0
4	A	616	0	0	15	0
4	B	640	0	0	9	0
4	C	690	0	0	21	0
4	D	610	0	0	15	0
All	All	18228	0	15093	139	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 (139) 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:A:132[A]:MET:HE3	4:A:1057:HOH:O	1.42	1.20
1:D:132[A]:MET:HE3	4:D:1075:HOH:O	1.53	1.06
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:ARG:HD3	4:C:1004:HOH:O	1.64	0.95
1:A:132[A]:MET:CE	4:A:1057:HOH:O	2.06	0.91
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: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:C:97[A]:ASN:ND2	4:C:601:HOH:O	2.12	0.81
1:A:97[B]:ASN:ND2	4:A:601:HOH:O	2.15	0.80
1:B:301:TYR:CD1	4:B:635:HOH:O	2.34	0.80
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
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:N	1:B:350[B]:TRP:CD1	2.56	0.70
1:D:341:ARG:NH2	1:D:351:ASP:OD1	2.25	0.69
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:B:349[B]:ASN:C	1:B:350[B]:TRP:CD1	2.70	0.64
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:A:477:GLU:CD	1:A:478:LEU:HD12	2.18	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:336:LEU:HD21	2:A:504:GOL:H2	1.85	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236[B]:ARG:HD2	4:C:615:HOH:O	2.04	0.57
1:D:132[A]:MET:CE	4:D:1075:HOH:O	2.26	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:A:453:GLU:OE1	3:A:505:IMD:C2	2.46	0.54
1:A:157[A]:ARG:CD	4:A:666:HOH:O	2.56	0.53
1:A:93:ASN:HD22	1:A:93:ASN:C	2.12	0.53
1:C:102[B]:ASP:OD2	4:C:602:HOH:O	2.18	0.53
1:C:93:ASN:C	1:C:93:ASN:HD22	2.12	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:C:169:ASN:HD22	1:C:224:SER:HB3	1.74	0.52
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:6:LEU:N	1:D:6:LEU:CD1	2.73	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:B:93:ASN:C	1:B:93:ASN:HD22	2.14	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: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: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:D:93:ASN:HD22	1:D:93:ASN:C	2.17	0.47
1:A:378:GLU:HG3	1:A:425:TRP:HB2	1.95	0.47
1:A:350:TRP:CE2	1:A:439:LYS:HD2	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:302:GLN:CD	4:D:638:HOH:O	2.51	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
1:C:308[B]:HIS:CE1	4:C:689:HOH:O	2.69	0.46
1:A:44:GLN:OE1	1:A:47[A]:ARG:NE	2.32	0.46
1:D:341:ARG:HH22	1:D:351:ASP:CG	2.19	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:272:GLU:CD	4:D:604:HOH:O	2.56	0.44
1:D:7:LYS:HE3	1:D:7:LYS:HB3	1.71	0.44
1:B:262[A]:MET:HE3	4:B:772:HOH:O	2.17	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:D:378:GLU:HG3	1:D:425:TRP:HB2	1.99	0.44
1:B:378:GLU:HG3	1:B:425:TRP:HB2	1.99	0.44
1:A:336:LEU:HD22	2:A:504:GOL:H2	1.96	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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:425:TRP:HA	1:D:426:SER:HA	1.90	0.41
1:A:192:LYS:NZ	4:A:625:HOH:O	2.53	0.40
1:A:312:ASP:HA	4:A:863:HOH:O	2.19	0.40
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%)	47	23
1	D	472/485 (97%)	456 (97%)	14 (3%)	2 (0%)	34	13
All	All	1906/1940 (98%)	1841 (97%)	62 (3%)	3 (0%)	47	23

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%)	409 (99%)	4 (1%)	76	54
1	B	411/412 (100%)	408 (99%)	3 (1%)	84	68
1	C	415/412 (101%)	411 (99%)	4 (1%)	76	54
1	D	407/412 (99%)	404 (99%)	3 (1%)	84	68
All	All	1646/1648 (100%)	1632 (99%)	14 (1%)	81	59

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	93	ASN
1	A	469	ARG
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	93	ASN
1	D	329	THR
1	D	430	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	129	GLN
1	A	169	ASN
1	A	171	GLN
1	A	198	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	202	ASN
1	A	205	ASN
1	A	210	GLN
1	A	251	ASN
1	A	252	HIS
1	A	265	GLN
1	A	269	ASN
1	A	349	ASN
1	A	379	ASN
1	B	93	ASN
1	B	129	GLN
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	251	ASN
1	B	252	HIS
1	B	265	GLN
1	B	269	ASN
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	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	349	ASN
1	D	379	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 carbohydrates 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	$\# Z > 2$
3	IMD	A	505	-	3,5,5	0.51	0	4,5,5	1.03	0
2	GOL	B	503	-	5,5,5	0.49	0	5,5,5	0.93	0
3	IMD	C	503	-	3,5,5	0.15	0	4,5,5	0.76	0
2	GOL	A	502	-	5,5,5	0.35	0	5,5,5	0.98	1 (20%)
2	GOL	C	502	-	5,5,5	0.48	0	5,5,5	0.94	0
2	GOL	C	501	-	5,5,5	0.67	0	5,5,5	1.13	1 (20%)
2	GOL	A	501	-	5,5,5	0.73	0	5,5,5	1.24	0
2	GOL	B	501	-	5,5,5	0.49	0	5,5,5	1.62	2 (40%)
3	IMD	D	502	-	3,5,5	0.43	0	4,5,5	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	D	501	-	5,5,5	0.43	0	5,5,5	0.87	0
2	GOL	B	502	-	5,5,5	0.67	0	5,5,5	0.87	0
2	GOL	A	503	-	5,5,5	0.38	0	5,5,5	1.18	0
2	GOL	A	504	-	5,5,5	0.63	0	5,5,5	0.96	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	IMD	A	505	-	-	-	0/1/1/1
2	GOL	B	503	-	-	1/4/4/4	-
3	IMD	C	503	-	-	-	0/1/1/1
2	GOL	A	502	-	-	0/4/4/4	-
2	GOL	C	502	-	-	2/4/4/4	-
2	GOL	C	501	-	-	2/4/4/4	-
2	GOL	A	501	-	-	0/4/4/4	-
2	GOL	B	501	-	-	0/4/4/4	-
3	IMD	D	502	-	-	-	0/1/1/1
2	GOL	D	501	-	-	0/4/4/4	-
2	GOL	B	502	-	-	0/4/4/4	-
2	GOL	A	503	-	-	0/4/4/4	-
2	GOL	A	504	-	-	4/4/4/4	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	GOL	C3-C2-C1	-2.74	101.05	111.70
2	C	501	GOL	C3-C2-C1	-2.34	102.62	111.70
2	B	501	GOL	O1-C1-C2	2.25	120.99	110.20
2	A	502	GOL	O3-C3-C2	2.12	120.38	110.20

There are no chirality outliers.

All (9) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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
2	B	503	GOL	O1-C1-C2-C3
2	A	504	GOL	O1-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	505	IMD	5	0
3	D	502	IMD	1	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%)	-0.14	17 (3%) 41 45	6, 11, 28, 67	0
1	B	459/485 (94%)	-0.21	12 (2%) 56 60	6, 11, 24, 61	0
1	C	460/485 (94%)	-0.21	10 (2%) 62 66	5, 9, 22, 80	0
1	D	460/485 (94%)	-0.14	12 (2%) 56 60	5, 11, 25, 90	0
All	All	1838/1940 (94%)	-0.17	51 (2%) 53 57	5, 11, 25, 90	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	350	TRP	9.7
1	D	312	ASP	8.4
1	D	329	THR	7.5
1	C	313	GLY	7.2
1	D	313	GLY	6.8
1	C	312	ASP	6.6
1	D	311	PRO	6.6
1	B	350[A]	TRP	6.0
1	C	352	TRP	5.6
1	C	314	VAL	5.4
1	C	311	PRO	5.4
1	D	314	VAL	5.4
1	D	350	TRP	5.4
1	D	352	TRP	5.1
1	A	352	TRP	5.1
1	A	313	GLY	4.9
1	B	312	ASP	4.9
1	D	310	PRO	4.8
1	C	329	THR	4.7
1	B	352	TRP	4.6
1	A	312	ASP	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	5	HIS	4.3
1	B	313	GLY	4.1
1	B	311	PRO	4.0
1	B	314	VAL	3.9
1	A	311	PRO	3.8
1	B	5	HIS	3.6
1	B	351[A]	ASP	3.5
1	A	389	PRO	3.3
1	D	5	HIS	3.3
1	C	310	PRO	3.2
1	A	348	THR	3.1
1	D	351	ASP	3.0
1	A	314	VAL	3.0
1	A	477	GLU	3.0
1	A	478	LEU	2.9
1	D	330	SER	2.9
1	C	350	TRP	2.9
1	A	347	THR	2.8
1	A	5	HIS	2.8
1	B	389	PRO	2.6
1	C	330	SER	2.6
1	A	346	ASP	2.6
1	A	351	ASP	2.5
1	A	349	ASN	2.4
1	B	310	PRO	2.3
1	B	392	ILE	2.3
1	B	348	THR	2.2
1	A	384	PHE	2.2
1	D	91	ASP	2.1
1	A	310	PRO	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 carbohydrates 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(\AA^2)	Q<0.9
3	IMD	D	502	5/5	0.69	0.16	19,25,31,32	5
2	GOL	B	503	6/6	0.85	0.19	29,34,35,35	0
2	GOL	D	501	6/6	0.85	0.17	34,35,37,40	0
3	IMD	A	505	5/5	0.87	0.10	33,38,42,45	0
2	GOL	A	503	6/6	0.87	0.16	31,32,35,35	0
3	IMD	C	503	5/5	0.88	0.21	22,26,31,35	0
2	GOL	A	504	6/6	0.90	0.18	38,40,43,47	0
2	GOL	C	502	6/6	0.92	0.17	30,31,32,33	0
2	GOL	C	501	6/6	0.92	0.20	17,26,33,44	0
2	GOL	B	501	6/6	0.95	0.11	13,17,22,25	0
2	GOL	A	501	6/6	0.96	0.11	13,15,20,22	0
2	GOL	B	502	6/6	0.96	0.10	13,15,21,23	0
2	GOL	A	502	6/6	0.97	0.10	13,17,20,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.