



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:05 AM UTC

PDB ID : 4MAD / pdb_00004mad
Title : Crystal structure of beta-galactosidase C (BgaC) from *Bacillus circulans* ATCC 31382
Authors : Kamerke, C.; You, D.J.; Kanaya, S.; Elling, L.
Deposited on : 2013-08-16
Resolution : 1.80 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

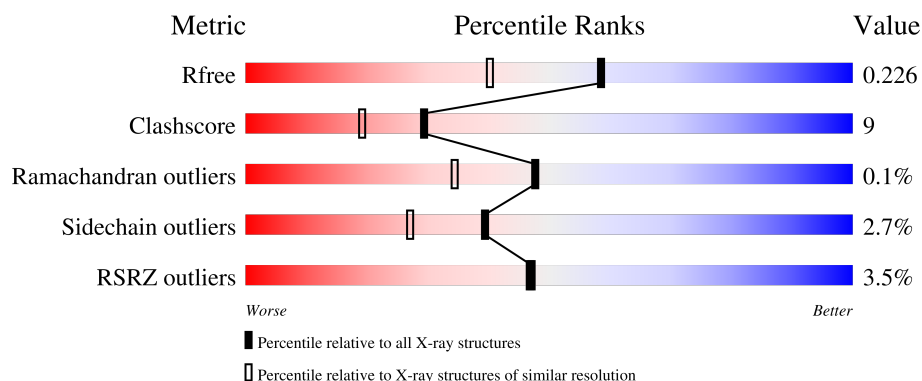
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	600	
1	B	600	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9884 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 Beta-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	581	Total	C	N	O	S	0	0	0
			4698	3040	770	874	14			
1	B	586	Total	C	N	O	S	0	0	0
			4737	3066	776	881	14			

There are 28 discrepancies between the modelled and reference sequences:

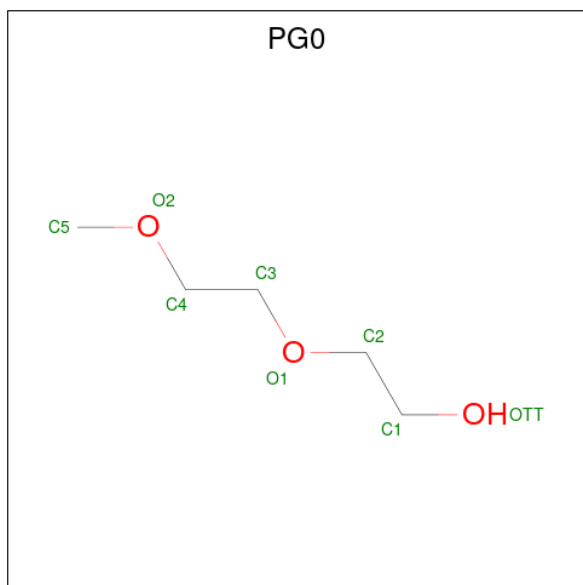
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP O31341
A	-12	GLY	-	expression tag	UNP O31341
A	-11	SER	-	expression tag	UNP O31341
A	-10	SER	-	expression tag	UNP O31341
A	-9	HIS	-	expression tag	UNP O31341
A	-8	HIS	-	expression tag	UNP O31341
A	-7	HIS	-	expression tag	UNP O31341
A	-6	HIS	-	expression tag	UNP O31341
A	-5	HIS	-	expression tag	UNP O31341
A	-4	HIS	-	expression tag	UNP O31341
A	-3	SER	-	expression tag	UNP O31341
A	-2	GLN	-	expression tag	UNP O31341
A	-1	ASP	-	expression tag	UNP O31341
A	0	PRO	-	expression tag	UNP O31341
B	-13	MET	-	expression tag	UNP O31341
B	-12	GLY	-	expression tag	UNP O31341
B	-11	SER	-	expression tag	UNP O31341
B	-10	SER	-	expression tag	UNP O31341
B	-9	HIS	-	expression tag	UNP O31341
B	-8	HIS	-	expression tag	UNP O31341
B	-7	HIS	-	expression tag	UNP O31341
B	-6	HIS	-	expression tag	UNP O31341
B	-5	HIS	-	expression tag	UNP O31341
B	-4	HIS	-	expression tag	UNP O31341
B	-3	SER	-	expression tag	UNP O31341

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLN	-	expression tag	UNP O31341
B	-1	ASP	-	expression tag	UNP O31341
B	0	PRO	-	expression tag	UNP O31341

- Molecule 2 is 2-(2-METHOXYETHOXY)ETHANOL (CCD ID: PG0) (formula: C₅H₁₂O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	5	3		
2	A	1	Total	C	O	0	0
			8	5	3		
2	B	1	Total	C	O	0	0
			8	5	3		

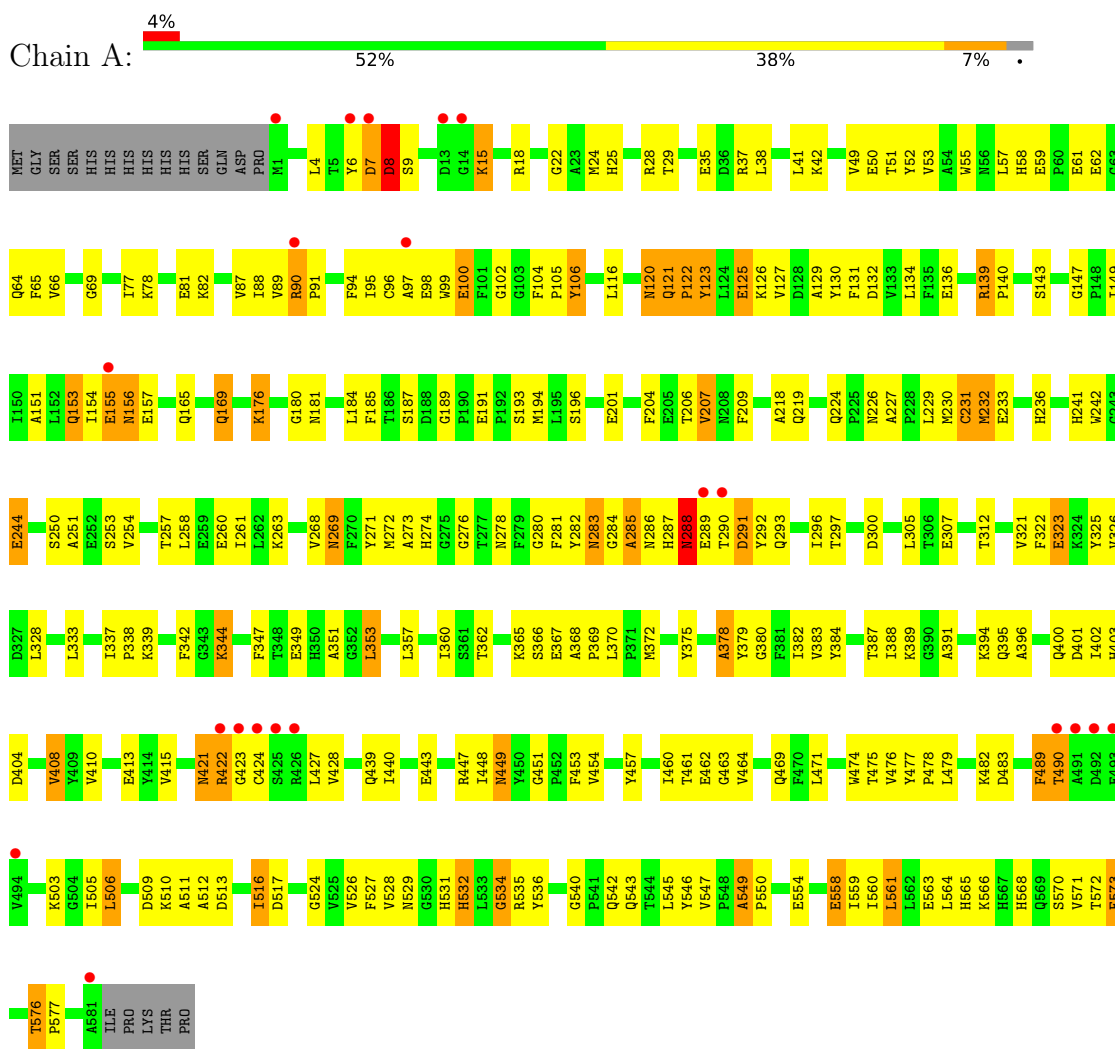
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	208	Total	O	0	0
			208	208		
3	B	217	Total	O	0	0
			217	217		

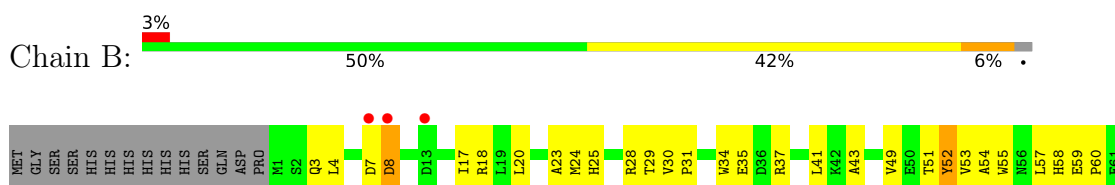
3 Residue-property plots

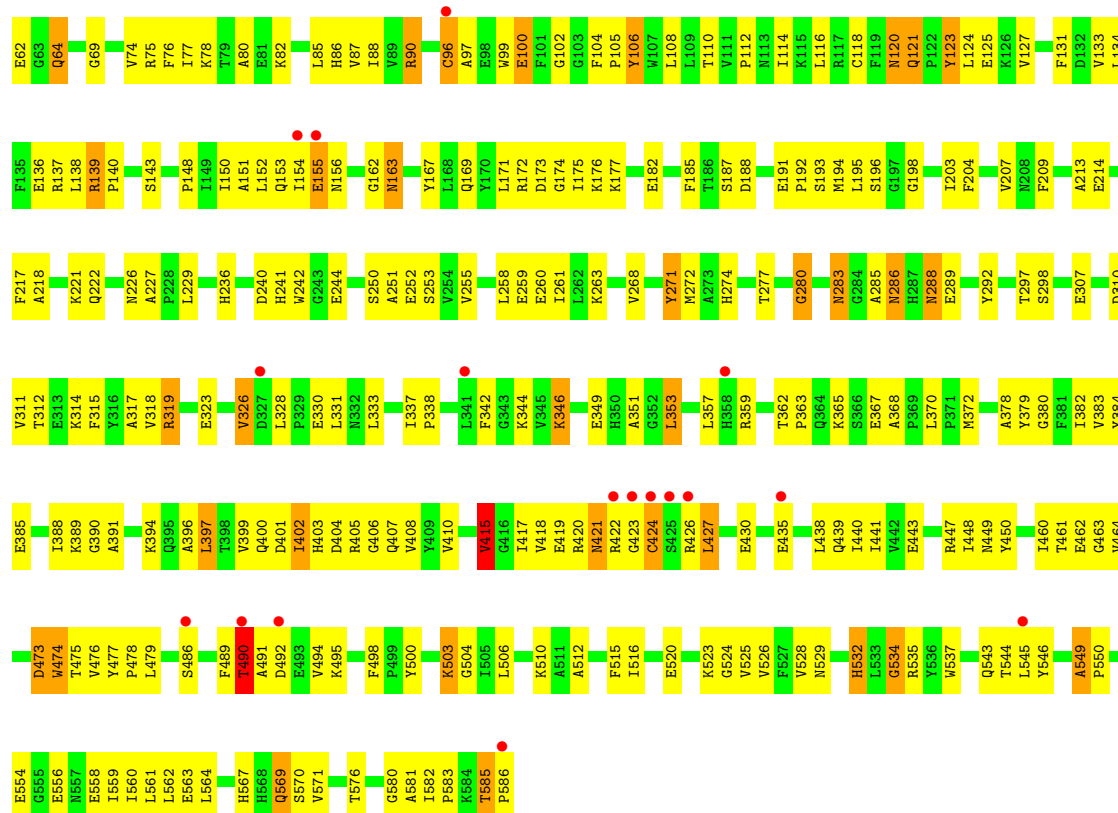
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Beta-galactosidase



• Molecule 1: Beta-galactosidase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	143.27Å 93.12Å 119.57Å 90.00° 125.67° 90.00°	Depositor
Resolution (Å)	41.66 – 1.80 41.66 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (41.66-1.80) 99.5 (41.66-1.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 1.79Å)	Xtriage
Refinement program	REFMAC refmac _5.5.0109	Depositor
R, R_{free}	0.181 , 0.216 0.193 , 0.226	Depositor DCC
R_{free} test set	5897 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.715	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9884	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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: PG0

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	2.14	206/4831 (4.3%)	1.15	28/6558 (0.4%)
1	B	2.13	223/4872 (4.6%)	1.13	27/6614 (0.4%)
All	All	2.14	429/9703 (4.4%)	1.14	55/13172 (0.4%)

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	1
1	B	0	1
All	All	0	2

All (429) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	293	GLN	C-O	-9.68	1.17	1.25
1	A	288	ASN	C-N	-9.64	1.20	1.33
1	B	546	TYR	C-O	-9.26	1.12	1.24
1	B	139	ARG	C-O	-8.81	1.16	1.24
1	A	284	GLY	C-O	-8.37	1.16	1.23
1	B	123	TYR	C-O	-8.35	1.14	1.24
1	A	300	ASP	C-O	-8.30	1.14	1.24
1	B	549	ALA	C-O	-8.20	1.17	1.24
1	A	528	VAL	C-O	-8.00	1.15	1.24
1	B	35	GLU	C-N	-7.83	1.24	1.33
1	B	121	GLN	C-O	-7.79	1.17	1.24
1	B	477	TYR	C-O	-7.74	1.17	1.24
1	B	88	ILE	C-O	-7.72	1.15	1.24
1	A	155	GLU	C-O	-7.69	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	566	LYS	C-O	-7.68	1.15	1.24
1	A	477	TYR	C-O	-7.67	1.17	1.24
1	B	380	GLY	C-O	-7.67	1.18	1.24
1	A	370	LEU	C-O	-7.63	1.16	1.24
1	B	31	PRO	C-O	-7.60	1.14	1.24
1	A	96	CYS	C-O	-7.58	1.17	1.24
1	B	258	LEU	C-O	-7.50	1.15	1.24
1	A	545	LEU	C-O	-7.49	1.15	1.24
1	A	273	ALA	C-O	-7.48	1.15	1.24
1	A	402	ILE	C-O	-7.47	1.16	1.24
1	B	125	GLU	C-O	-7.46	1.15	1.24
1	B	222	GLN	C-O	-7.43	1.15	1.24
1	A	536	TYR	C-O	-7.43	1.14	1.23
1	A	408	VAL	C-O	-7.41	1.16	1.24
1	B	43	ALA	CA-CB	-7.41	1.41	1.53
1	A	448	ILE	C-O	-7.37	1.16	1.24
1	A	104	PHE	C-O	-7.34	1.14	1.24
1	B	528	VAL	C-O	-7.32	1.16	1.24
1	A	53	VAL	C-O	-7.29	1.16	1.24
1	B	396	ALA	CA-CB	-7.29	1.43	1.53
1	B	24	MET	C-O	-7.28	1.15	1.23
1	A	120	ASN	C-O	-7.22	1.15	1.24
1	B	370	LEU	C-O	-7.22	1.16	1.24
1	B	448	ILE	C-O	-7.17	1.16	1.24
1	A	55	TRP	C-O	-7.16	1.15	1.24
1	B	34	TRP	C-N	-7.15	1.24	1.34
1	A	105	PRO	C-O	-7.14	1.15	1.23
1	A	449	ASN	C-O	-7.13	1.14	1.24
1	A	362	THR	C-O	-7.04	1.16	1.25
1	A	29	THR	C-O	-7.04	1.15	1.23
1	B	525	VAL	C-O	-7.04	1.16	1.23
1	A	439	GLN	C-O	-7.02	1.16	1.24
1	B	150	ILE	C-O	-7.01	1.17	1.24
1	B	131	PHE	C-O	-6.98	1.16	1.24
1	B	564	LEU	C-O	-6.97	1.15	1.24
1	B	54	ALA	CA-CB	-6.93	1.44	1.52
1	A	185	PHE	C-O	-6.93	1.15	1.23
1	A	38	LEU	C-O	-6.93	1.16	1.24
1	B	17	ILE	C-O	-6.92	1.16	1.23
1	A	251	ALA	CA-CB	-6.90	1.42	1.53
1	B	382	ILE	C-O	-6.88	1.17	1.24
1	B	315	PHE	C-O	-6.86	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	87	VAL	C-O	-6.85	1.17	1.24
1	B	317	ALA	C-O	-6.79	1.16	1.24
1	A	81	GLU	C-O	-6.77	1.16	1.24
1	A	440	ILE	C-O	-6.75	1.16	1.24
1	B	59	GLU	C-O	-6.75	1.16	1.24
1	B	75	ARG	C-O	-6.72	1.16	1.24
1	B	479	LEU	C-O	-6.70	1.16	1.24
1	B	297	THR	C-O	-6.69	1.16	1.24
1	B	118	CYS	C-O	-6.68	1.15	1.23
1	A	513	ASP	C-O	-6.66	1.15	1.23
1	A	134	LEU	C-O	-6.64	1.16	1.24
1	B	156	ASN	C-O	-6.63	1.16	1.24
1	A	287	HIS	C-O	-6.63	1.16	1.23
1	A	130	TYR	C-O	-6.61	1.16	1.24
1	A	42	LYS	C-O	-6.61	1.16	1.24
1	A	125	GLU	C-O	-6.60	1.16	1.24
1	B	351	ALA	CA-CB	-6.58	1.42	1.53
1	B	74	VAL	C-O	-6.57	1.16	1.24
1	B	251	ALA	CA-CB	-6.56	1.43	1.53
1	B	318	VAL	C-O	-6.56	1.16	1.24
1	A	464	VAL	C-O	-6.55	1.17	1.24
1	A	242	TRP	C-O	-6.55	1.16	1.23
1	A	269	ASN	C-O	-6.54	1.16	1.24
1	B	512	ALA	C-O	-6.54	1.16	1.23
1	A	388	ILE	C-O	-6.53	1.16	1.24
1	B	274	HIS	C-O	-6.53	1.16	1.24
1	B	90	ARG	C-O	-6.51	1.16	1.24
1	A	479	LEU	C-O	-6.50	1.16	1.24
1	B	209	PHE	C-O	-6.50	1.16	1.23
1	B	560	ILE	C-O	-6.49	1.17	1.24
1	B	498	PHE	C-O	-6.49	1.16	1.24
1	B	280	GLY	C-O	-6.49	1.15	1.24
1	A	121	GLN	C-O	-6.48	1.18	1.24
1	B	563	GLU	C-O	-6.48	1.16	1.24
1	A	230	MET	C-O	-6.47	1.16	1.24
1	A	576	THR	C-O	-6.44	1.17	1.24
1	B	476	VAL	C-O	-6.44	1.17	1.24
1	A	365	LYS	C-O	-6.41	1.15	1.24
1	B	108	LEU	C-O	-6.41	1.16	1.24
1	B	185	PHE	C-O	-6.41	1.16	1.23
1	A	224	GLN	C-O	-6.39	1.17	1.24
1	A	511	ALA	CA-CB	-6.38	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	413	GLU	C-O	-6.36	1.16	1.24
1	B	384	TYR	C-O	-6.35	1.16	1.24
1	A	154	ILE	C-O	-6.35	1.16	1.24
1	A	22	GLY	C-O	-6.34	1.15	1.23
1	A	428	VAL	C-O	-6.34	1.17	1.24
1	B	439	GLN	C-O	-6.34	1.16	1.24
1	A	353	LEU	C-O	-6.32	1.16	1.24
1	B	102	GLY	C-O	-6.31	1.15	1.24
1	A	561	LEU	C-O	-6.31	1.16	1.24
1	B	37	ARG	C-O	-6.30	1.16	1.24
1	B	240	ASP	C-O	-6.29	1.16	1.23
1	B	379	TYR	C-O	-6.28	1.16	1.23
1	A	274	HIS	C-O	-6.27	1.16	1.24
1	A	136	GLU	C-O	-6.26	1.16	1.24
1	A	471	LEU	C-O	-6.25	1.16	1.23
1	B	580	GLY	C-O	-6.24	1.15	1.23
1	A	503	LYS	C-O	-6.22	1.16	1.24
1	A	375	TYR	C-O	-6.21	1.15	1.24
1	B	55	TRP	C-O	-6.20	1.16	1.24
1	B	523	LYS	C-O	-6.19	1.16	1.23
1	A	558	GLU	C-O	-6.18	1.16	1.24
1	B	298	SER	C-O	-6.17	1.16	1.23
1	A	326	VAL	C-O	-6.16	1.17	1.23
1	B	399	VAL	C-O	-6.16	1.17	1.24
1	B	151	ALA	CA-CB	-6.16	1.43	1.53
1	A	233	GLU	C-O	-6.15	1.17	1.24
1	B	51	THR	C-O	-6.15	1.16	1.23
1	A	57	LEU	C-O	-6.14	1.17	1.24
1	B	188	ASP	C-O	-6.14	1.16	1.23
1	B	18	ARG	C-O	-6.13	1.16	1.24
1	A	372	MET	C-O	-6.13	1.16	1.24
1	B	114	ILE	C-O	-6.13	1.16	1.24
1	B	408	VAL	C-O	-6.12	1.17	1.24
1	B	167	TYR	C-O	-6.11	1.17	1.24
1	A	253	SER	C-O	-6.10	1.17	1.24
1	A	564	LEU	C-O	-6.09	1.16	1.24
1	B	163	ASN	C-O	-6.09	1.15	1.24
1	B	138	LEU	C-O	-6.08	1.16	1.24
1	A	396	ALA	CA-CB	-6.07	1.45	1.53
1	B	82	LYS	C-O	-6.07	1.17	1.24
1	B	143	SER	C-O	-6.07	1.16	1.24
1	A	382	ILE	C-O	-6.06	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	534	GLY	C-O	-6.06	1.17	1.24
1	A	254	VAL	C-O	-6.05	1.17	1.24
1	A	378	ALA	C-O	-6.05	1.16	1.24
1	B	516	ILE	C-O	-6.04	1.17	1.24
1	A	189	GLY	C-O	-6.03	1.15	1.24
1	A	339	LYS	C-O	-6.03	1.16	1.24
1	A	59	GLU	C-O	-6.02	1.17	1.24
1	A	181	ASN	C-O	-6.02	1.16	1.24
1	A	289	GLU	C-N	-6.02	1.25	1.33
1	A	291	ASP	C-O	-6.02	1.16	1.23
1	A	457	TYR	C-O	-6.01	1.16	1.23
1	B	353	LEU	C-O	-6.01	1.17	1.24
1	B	174	GLY	C-O	-6.00	1.16	1.23
1	A	534	GLY	C-O	-6.00	1.17	1.23
1	A	151	ALA	C-O	-6.00	1.16	1.23
1	A	307	GLU	C-O	-5.99	1.17	1.24
1	A	95	ILE	C-O	-5.99	1.17	1.24
1	B	196	SER	C-O	-5.97	1.17	1.24
1	A	129	ALA	CA-CB	-5.96	1.43	1.53
1	B	76	PHE	C-O	-5.96	1.17	1.24
1	B	69	GLY	C-O	-5.96	1.15	1.24
1	B	134	LEU	C-O	-5.95	1.17	1.24
1	B	326	VAL	C-O	-5.95	1.17	1.23
1	A	526	VAL	C-O	-5.95	1.18	1.24
1	A	258	LEU	C-O	-5.94	1.17	1.24
1	B	271	TYR	C-O	-5.94	1.17	1.24
1	B	571	VAL	C-O	-5.93	1.17	1.23
1	B	415	VAL	C-O	-5.93	1.17	1.23
1	A	563	GLU	C-O	-5.93	1.16	1.24
1	A	532	HIS	C-O	-5.93	1.16	1.24
1	A	387	THR	C-O	-5.92	1.16	1.24
1	A	18	ARG	C-O	-5.92	1.16	1.24
1	A	64	GLN	C-O	-5.91	1.17	1.24
1	A	571	VAL	C-O	-5.91	1.16	1.23
1	B	390	GLY	C-O	-5.91	1.17	1.24
1	B	368	ALA	CA-CB	-5.91	1.45	1.53
1	A	260	GLU	C-O	-5.91	1.17	1.24
1	A	153	GLN	C-O	-5.90	1.16	1.23
1	B	253	SER	C-O	-5.90	1.17	1.24
1	B	567	HIS	C-O	-5.89	1.17	1.23
1	A	516	ILE	C-O	-5.88	1.17	1.24
1	A	184	LEU	C-O	-5.88	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	263	LYS	C-O	-5.88	1.16	1.24
1	B	64	GLN	C-O	-5.86	1.17	1.24
1	B	136	GLU	C-O	-5.85	1.17	1.24
1	B	562	LEU	C-O	-5.85	1.17	1.24
1	A	296	ILE	C-O	-5.84	1.17	1.24
1	B	447	ARG	C-O	-5.84	1.16	1.23
1	B	96	CYS	C-O	-5.84	1.19	1.24
1	A	88	ILE	C-O	-5.84	1.17	1.24
1	B	198	GLY	C-O	-5.84	1.16	1.23
1	B	259	GLU	C-O	-5.83	1.17	1.24
1	B	418	VAL	C-O	-5.83	1.18	1.24
1	A	447	ARG	C-O	-5.82	1.17	1.23
1	A	139	ARG	C-O	-5.81	1.19	1.24
1	B	127	VAL	C-O	-5.81	1.17	1.24
1	A	540	GLY	C-O	-5.80	1.16	1.24
1	B	49	VAL	C-O	-5.80	1.17	1.24
1	B	407	GLN	C-O	-5.80	1.17	1.24
1	A	106	TYR	C-O	-5.80	1.16	1.24
1	B	80	ALA	C-O	-5.80	1.17	1.24
1	B	41	LEU	C-O	-5.80	1.17	1.24
1	A	347	PHE	C-O	-5.79	1.17	1.24
1	B	283	ASN	C-O	-5.79	1.16	1.23
1	B	462	GLU	C-O	-5.79	1.16	1.24
1	B	213	ALA	C-O	-5.78	1.17	1.24
1	A	231	CYS	C-O	-5.77	1.16	1.23
1	B	162	GLY	C-O	-5.77	1.18	1.23
1	A	559	ILE	C-O	-5.77	1.18	1.24
1	B	182	GLU	C-O	-5.77	1.16	1.23
1	B	337	ILE	C-O	-5.77	1.17	1.24
1	B	385	GLU	C-O	-5.76	1.17	1.23
1	A	312	THR	C-O	-5.76	1.16	1.23
1	B	195	LEU	C-O	-5.75	1.17	1.24
1	A	65	PHE	C-O	-5.75	1.17	1.24
1	A	62	GLU	C-N	-5.74	1.25	1.33
1	A	49	VAL	C-O	-5.74	1.18	1.24
1	A	554	GLU	C-O	-5.74	1.17	1.23
1	B	410	VAL	C-O	-5.74	1.18	1.24
1	A	250	SER	C-O	-5.73	1.16	1.23
1	A	89	VAL	C-O	-5.72	1.18	1.24
1	B	406	GLY	C-O	-5.72	1.17	1.24
1	A	288	ASN	C-O	-5.71	1.18	1.23
1	B	154	ILE	C-O	-5.71	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	214	GLU	C-O	-5.71	1.17	1.24
1	B	120	ASN	C-O	-5.70	1.17	1.24
1	B	367	GLU	C-O	-5.70	1.17	1.24
1	A	244	GLU	C-O	-5.70	1.16	1.23
1	A	476	VAL	C-O	-5.69	1.18	1.24
1	B	137	ARG	C-O	-5.69	1.17	1.24
1	A	380	GLY	C-O	-5.69	1.16	1.23
1	B	532	HIS	C-O	-5.69	1.17	1.24
1	B	175	ILE	C-O	-5.68	1.17	1.24
1	A	531	HIS	C-O	-5.68	1.17	1.24
1	A	257	THR	C-O	-5.67	1.17	1.24
1	B	34	TRP	C-O	-5.66	1.17	1.24
1	A	333	LEU	C-O	-5.66	1.17	1.23
1	A	122	PRO	C-O	-5.66	1.17	1.24
1	B	218	ALA	CA-CB	-5.66	1.44	1.53
1	A	24	MET	C-O	-5.65	1.17	1.23
1	A	90	ARG	C-O	-5.65	1.17	1.24
1	B	152	LEU	C-O	-5.65	1.17	1.23
1	B	191	GLU	C-O	-5.65	1.18	1.24
1	B	207	VAL	C-O	-5.65	1.17	1.23
1	A	383	VAL	C-O	-5.64	1.18	1.24
1	B	87	VAL	C-O	-5.64	1.18	1.24
1	B	475	THR	C-O	-5.64	1.17	1.24
1	A	219	GLN	C-O	-5.64	1.17	1.24
1	B	405	ARG	C-O	-5.63	1.17	1.23
1	A	37	ARG	C-O	-5.62	1.17	1.24
1	A	78	LYS	C-O	-5.62	1.17	1.24
1	B	203	ILE	C-O	-5.62	1.18	1.24
1	B	397	LEU	C-O	-5.62	1.17	1.24
1	B	464	VAL	C-O	-5.61	1.18	1.24
1	A	510	LYS	C-O	-5.61	1.17	1.23
1	B	330	GLU	C-O	-5.61	1.17	1.23
1	B	85	LEU	C-O	-5.60	1.17	1.24
1	B	252	GLU	C-O	-5.60	1.17	1.24
1	B	187	SER	C-O	-5.60	1.17	1.23
1	A	151	ALA	CA-CB	-5.59	1.43	1.53
1	B	438	LEU	C-O	-5.58	1.17	1.24
1	B	116	LEU	C-O	-5.55	1.17	1.23
1	A	187	SER	C-O	-5.55	1.17	1.23
1	B	312	THR	C-O	-5.55	1.16	1.23
1	A	547	VAL	C-O	-5.55	1.17	1.24
1	A	193	SER	C-O	-5.54	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	410	VAL	C-O	-5.54	1.18	1.24
1	A	478	PRO	C-O	-5.54	1.17	1.23
1	A	194	MET	C-O	-5.53	1.17	1.24
1	A	506	LEU	C-O	-5.53	1.17	1.24
1	A	517	ASP	C-O	-5.52	1.17	1.24
1	B	440	ILE	C-O	-5.52	1.18	1.24
1	A	395	GLN	C-O	-5.52	1.17	1.23
1	A	204	PHE	C-O	-5.51	1.17	1.23
1	A	321	VAL	C-O	-5.51	1.17	1.24
1	A	560	ILE	C-O	-5.51	1.18	1.24
1	B	338	PRO	C-O	-5.50	1.17	1.23
1	A	451	GLY	C-O	-5.50	1.16	1.24
1	A	505	ILE	C-O	-5.50	1.18	1.24
1	B	515	PHE	C-O	-5.49	1.17	1.24
1	A	512	ALA	CA-CB	-5.49	1.44	1.53
1	B	112	PRO	C-O	-5.49	1.17	1.23
1	B	255	VAL	C-O	-5.49	1.17	1.24
1	A	546	TYR	C-O	-5.47	1.17	1.23
1	A	573	PHE	C-O	-5.47	1.17	1.24
1	B	307	GLU	C-O	-5.47	1.17	1.24
1	A	323	GLU	C-O	-5.46	1.17	1.24
1	B	556	GLU	C-O	-5.45	1.17	1.24
1	A	218	ALA	CA-CB	-5.45	1.44	1.53
1	B	450	TYR	C-O	-5.45	1.17	1.23
1	A	229	LEU	C-O	-5.45	1.17	1.24
1	A	543	GLN	C-O	-5.45	1.16	1.24
1	B	372	MET	C-O	-5.45	1.17	1.24
1	A	127	VAL	C-O	-5.44	1.17	1.24
1	B	204	PHE	C-O	-5.44	1.17	1.23
1	B	357	LEU	C-O	-5.44	1.17	1.24
1	B	473	ASP	C-O	-5.44	1.17	1.24
1	B	286	ASN	C-O	-5.44	1.16	1.23
1	B	430	GLU	C-O	-5.43	1.17	1.23
1	A	102	GLY	C-O	-5.43	1.17	1.24
1	B	260	GLU	C-O	-5.42	1.17	1.24
1	A	116	LEU	C-O	-5.42	1.17	1.23
1	B	104	PHE	C-O	-5.42	1.16	1.24
1	B	537	TRP	C-O	-5.42	1.17	1.23
1	A	227	ALA	CA-CB	-5.42	1.44	1.53
1	A	51	THR	C-O	-5.41	1.17	1.23
1	A	460	ILE	C-O	-5.41	1.18	1.24
1	B	194	MET	C-O	-5.39	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	VAL	C-O	-5.38	1.18	1.24
1	A	524	GLY	C-O	-5.38	1.16	1.23
1	B	110	THR	C-O	-5.38	1.16	1.24
1	B	362	THR	C-O	-5.38	1.18	1.25
1	A	206	THR	C-O	-5.37	1.17	1.23
1	A	389	LYS	C-O	-5.37	1.17	1.24
1	A	475	THR	C-O	-5.37	1.17	1.24
1	A	123	TYR	C-O	-5.37	1.18	1.24
1	B	544	THR	C-O	-5.37	1.17	1.23
1	B	268	VAL	C-O	-5.36	1.17	1.23
1	B	365	LYS	C-O	-5.36	1.17	1.24
1	B	3	GLN	C-O	-5.36	1.17	1.23
1	B	443	GLU	C-O	-5.35	1.17	1.24
1	A	305	LEU	C-O	-5.33	1.17	1.23
1	B	227	ALA	C-O	-5.33	1.16	1.23
1	A	338	PRO	C-O	-5.33	1.17	1.23
1	A	41	LEU	C-O	-5.31	1.18	1.24
1	B	171	LEU	C-O	-5.29	1.18	1.24
1	A	549	ALA	CA-CB	-5.29	1.46	1.54
1	B	251	ALA	C-O	-5.29	1.18	1.24
1	B	288	ASN	C-O	-5.29	1.17	1.24
1	A	360	ILE	C-O	-5.28	1.17	1.24
1	A	366	SER	C-O	-5.28	1.17	1.23
1	A	570	SER	C-O	-5.27	1.17	1.23
1	B	62	GLU	C-O	-5.27	1.17	1.23
1	B	526	VAL	C-O	-5.27	1.18	1.24
1	A	474	TRP	C-O	-5.26	1.17	1.23
1	B	148	PRO	C-O	-5.26	1.18	1.24
1	A	283	ASN	C-O	-5.26	1.17	1.23
1	B	427	LEU	C-O	-5.26	1.17	1.23
1	B	510	LYS	C-O	-5.25	1.17	1.23
1	A	368	ALA	CA-CB	-5.24	1.46	1.53
1	B	226	ASN	C-O	-5.24	1.17	1.24
1	B	29	THR	C-O	-5.24	1.17	1.23
1	B	176	LYS	C-O	-5.24	1.18	1.24
1	B	242	TRP	C-O	-5.24	1.17	1.23
1	A	261	ILE	C-O	-5.23	1.18	1.24
1	A	191	GLU	C-O	-5.22	1.18	1.24
1	B	495	LYS	C-O	-5.22	1.17	1.24
1	A	285	ALA	C-O	-5.21	1.17	1.23
1	A	94	PHE	C-O	-5.21	1.17	1.24
1	A	572	THR	C-O	-5.21	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	LEU	C-O	-5.21	1.17	1.24
1	A	196	SER	C-O	-5.21	1.18	1.24
1	B	52	TYR	C-O	-5.21	1.16	1.23
1	A	443	GLU	C-O	-5.20	1.17	1.24
1	A	131	PHE	C-O	-5.20	1.18	1.24
1	B	4	LEU	C-O	-5.20	1.17	1.24
1	B	35	GLU	C-O	-5.20	1.17	1.24
1	B	394	LYS	C-O	-5.20	1.17	1.23
1	B	383	VAL	C-O	-5.19	1.18	1.24
1	B	20	LEU	C-O	-5.18	1.18	1.24
1	B	317	ALA	CA-CB	-5.18	1.45	1.53
1	A	367	GLU	C-O	-5.18	1.18	1.24
1	A	379	TYR	C-O	-5.18	1.17	1.23
1	B	105	PRO	C-O	-5.18	1.17	1.23
1	B	151	ALA	C-O	-5.18	1.17	1.23
1	B	250	SER	C-O	-5.17	1.17	1.23
1	B	77	ILE	C-O	-5.16	1.18	1.24
1	B	460	ILE	C-O	-5.16	1.18	1.24
1	B	346	LYS	C-O	-5.16	1.17	1.24
1	A	276	GLY	C-O	-5.16	1.17	1.24
1	B	53	VAL	C-O	-5.16	1.18	1.24
1	B	218	ALA	C-O	-5.16	1.18	1.24
1	A	209	PHE	C-O	-5.14	1.17	1.23
1	B	490	THR	C-O	-5.14	1.17	1.23
1	B	23	ALA	C-O	-5.14	1.17	1.24
1	B	559	ILE	C-O	-5.14	1.18	1.24
1	A	132	ASP	C-O	-5.14	1.18	1.24
1	A	169	GLN	C-O	-5.14	1.18	1.24
1	B	106	TYR	C-O	-5.14	1.17	1.24
1	B	227	ALA	CA-CB	-5.14	1.45	1.53
1	A	322	PHE	C-O	-5.14	1.18	1.24
1	A	344	LYS	C-O	-5.13	1.17	1.23
1	A	427	LEU	C-O	-5.12	1.17	1.23
1	B	420	ARG	C-O	-5.12	1.18	1.24
1	B	124	LEU	C-O	-5.12	1.17	1.24
1	B	229	LEU	C-O	-5.11	1.17	1.24
1	B	78	LYS	C-O	-5.11	1.18	1.24
1	B	333	LEU	C-O	-5.11	1.18	1.23
1	A	219	GLN	CD-NE2	-5.11	1.22	1.33
1	B	543	GLN	C-O	-5.11	1.17	1.24
1	A	384	TYR	C-O	-5.10	1.17	1.24
1	B	368	ALA	C-O	-5.10	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	391	ALA	C-O	-5.10	1.17	1.24
1	A	453	PHE	C-O	-5.09	1.17	1.23
1	A	571	VAL	C-N	-5.09	1.25	1.33
1	B	30	VAL	C-O	-5.09	1.18	1.24
1	A	542	GLN	C-O	-5.09	1.17	1.23
1	A	527	PHE	C-O	-5.08	1.17	1.24
1	B	311	VAL	C-O	-5.08	1.17	1.24
1	A	282	TYR	C-O	-5.08	1.17	1.24
1	B	396	ALA	C-O	-5.08	1.17	1.24
1	B	461	THR	C-O	-5.08	1.18	1.24
1	A	126	LYS	C-O	-5.08	1.18	1.24
1	B	581	ALA	C-O	-5.08	1.17	1.23
1	B	402	ILE	C-O	-5.07	1.18	1.24
1	A	351	ALA	CA-CB	-5.07	1.45	1.53
1	A	391	ALA	CA-CB	-5.07	1.46	1.52
1	B	86	HIS	C-O	-5.06	1.17	1.23
1	B	155	GLU	C-O	-5.06	1.17	1.24
1	B	363	PRO	C-O	-5.05	1.18	1.23
1	B	389	LYS	C-O	-5.05	1.17	1.24
1	A	489	PHE	C-O	-5.05	1.17	1.23
1	A	278	ASN	C-O	-5.04	1.16	1.23
1	B	570	SER	C-O	-5.03	1.17	1.23
1	B	388	ILE	C-O	-5.03	1.18	1.24
1	B	478	PRO	C-O	-5.03	1.18	1.23
1	B	193	SER	C-O	-5.03	1.18	1.24
1	A	77	ILE	C-O	-5.02	1.18	1.24
1	B	192	PRO	C-O	-5.02	1.17	1.24
1	B	463	GLY	C-O	-5.02	1.18	1.23
1	A	337	ILE	C-O	-5.02	1.18	1.24
1	B	292	TYR	C-O	-5.01	1.18	1.23
1	B	310	ASP	C-O	-5.01	1.17	1.23
1	A	297	THR	C-O	-5.01	1.18	1.24
1	B	277	THR	C-O	-5.01	1.17	1.23
1	A	69	GLY	C-O	-5.01	1.17	1.24
1	B	441	ILE	C-O	-5.01	1.18	1.24
1	A	325	TYR	C-O	-5.00	1.17	1.24
1	A	268	VAL	C-O	-5.00	1.18	1.23

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	474	TRP	N-CA-C	14.58	132.06	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	ASP	N-CA-C	-11.02	100.33	113.88
1	A	156	ASN	N-CA-C	9.80	124.41	108.34
1	B	474	TRP	N-CA-CB	-9.03	96.57	110.29
1	A	154	ILE	CA-C-N	-8.99	105.29	123.99
1	A	154	ILE	C-N-CA	-8.99	105.29	123.99
1	A	7	ASP	N-CA-C	8.70	123.86	112.72
1	A	7	ASP	CB-CA-C	-8.69	96.11	110.37
1	B	424	CYS	N-CA-C	8.32	123.05	111.56
1	A	155	GLU	N-CA-C	-7.91	98.14	109.29
1	A	61	GLU	CA-C-N	-7.81	109.81	120.82
1	A	61	GLU	C-N-CA	-7.81	109.81	120.82
1	B	156	ASN	N-CA-C	7.61	120.83	108.34
1	B	380	GLY	N-CA-C	7.56	119.19	111.56
1	B	435	GLU	O-C-N	7.53	132.50	123.24
1	B	154	ILE	CA-C-N	-7.44	107.32	121.54
1	B	154	ILE	C-N-CA	-7.44	107.32	121.54
1	A	58	HIS	N-CA-C	7.42	120.43	111.82
1	A	156	ASN	N-CA-CB	-7.29	99.32	110.77
1	A	474	TRP	N-CA-C	7.09	121.58	110.17
1	B	461	THR	N-CA-C	6.98	118.97	111.36
1	A	423	GLY	N-CA-C	-6.98	106.19	115.40
1	B	423	GLY	CA-C-N	-6.90	109.94	122.50
1	B	423	GLY	C-N-CA	-6.90	109.94	122.50
1	B	155	GLU	N-CA-C	-6.75	96.41	110.80
1	A	288	ASN	CA-C-N	-6.74	107.84	121.18
1	A	288	ASN	C-N-CA	-6.74	107.84	121.18
1	A	207	VAL	O-C-N	6.66	130.10	122.97
1	B	546	TYR	CA-C-N	6.66	134.45	122.13
1	B	546	TYR	C-N-CA	6.66	134.45	122.13
1	A	461	THR	N-CA-C	6.65	118.33	111.14
1	A	149	ILE	CB-CA-C	-6.42	105.00	111.80
1	B	8	ASP	N-CA-C	-6.34	106.08	113.88
1	A	474	TRP	N-CA-CB	-6.16	100.60	110.63
1	A	564	LEU	N-CA-C	6.09	117.99	111.36
1	A	6	TYR	N-CA-C	5.85	118.03	108.55
1	B	150	ILE	N-CA-C	5.71	121.78	113.39
1	A	6	TYR	CB-CA-C	-5.67	99.66	109.86
1	B	415	VAL	N-CA-C	5.65	116.47	111.90
1	B	96	CYS	N-CA-C	-5.57	99.36	108.67
1	B	154	ILE	O-C-N	-5.51	115.68	122.57
1	B	524	GLY	N-CA-C	5.51	118.29	110.74
1	A	226	ASN	N-CA-C	5.46	120.08	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	490	THR	CB-CA-C	-5.34	99.73	110.30
1	B	58	HIS	N-CA-C	5.32	119.82	113.23
1	B	545	LEU	O-C-N	5.32	130.14	123.12
1	A	232	MET	N-CA-C	5.31	117.98	111.82
1	A	565	HIS	N-CA-C	5.30	119.22	112.12
1	A	87	VAL	N-CA-C	5.27	115.71	108.12
1	B	133	VAL	N-CA-C	5.20	115.42	110.53
1	B	59	GLU	CA-C-N	5.18	124.98	119.28
1	B	59	GLU	C-N-CA	5.18	124.98	119.28
1	B	268	VAL	N-CA-C	5.18	115.83	108.42
1	B	261	ILE	CB-CA-C	-5.17	105.35	111.97
1	A	357	LEU	N-CA-C	5.04	116.47	111.07

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	421	ASN	Peptide
1	B	421	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	4698	0	4542	74	0
1	B	4737	0	4587	86	0
2	A	16	0	24	3	0
2	B	8	0	12	0	0
3	A	208	0	0	3	0
3	B	217	0	0	2	0
All	All	9884	0	9165	160	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 9.

All (160) 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:B:490:THR:HG22	1:B:492:ASP:H	1.08	1.15
1:A:15:LYS:HB2	1:A:15:LYS:NZ	1.48	1.14
1:B:319:ARG:HH11	1:B:319:ARG:CG	1.64	1.06
1:B:319:ARG:HH11	1:B:319:ARG:HG3	1.23	1.01
1:B:585:THR:HG22	1:B:585:THR:O	1.64	0.97
1:A:15:LYS:NZ	1:A:15:LYS:CB	2.29	0.93
1:A:15:LYS:HB2	1:A:15:LYS:HZ2	1.15	0.92
1:A:15:LYS:HB2	1:A:15:LYS:HZ3	1.32	0.90
1:B:490:THR:CG2	1:B:492:ASP:H	1.84	0.90
1:B:490:THR:HG22	1:B:492:ASP:N	1.91	0.85
1:A:25:HIS:HD2	1:A:28:ARG:HH11	1.23	0.84
1:B:25:HIS:HD2	1:B:28:ARG:HH11	1.26	0.84
1:A:241:HIS:HE1	1:A:286:ASN:HD22	1.30	0.79
1:B:319:ARG:HG3	1:B:319:ARG:NH1	1.96	0.79
1:A:288:ASN:ND2	1:A:291:ASP:H	1.82	0.78
1:B:585:THR:O	1:B:585:THR:CG2	2.29	0.78
1:A:7:ASP:OD1	1:A:8:ASP:N	2.16	0.77
1:B:241:HIS:HE1	1:B:286:ASN:HD22	1.33	0.77
1:A:288:ASN:HD21	1:A:291:ASP:H	1.33	0.76
1:A:483:ASP:H	2:A:901:PG0:H53	1.50	0.76
1:A:165:GLN:HE21	1:A:169:GLN:HE21	1.35	0.74
1:A:283:ASN:HD21	1:A:535:ARG:HH21	1.35	0.74
1:A:97:ALA:O	1:A:98:GLU:HB2	1.87	0.73
1:B:490:THR:HG21	1:B:492:ASP:CG	2.15	0.72
1:B:319:ARG:HH11	1:B:319:ARG:HG2	1.55	0.72
1:A:292:TYR:H	1:A:421:ASN:HD21	1.38	0.71
1:A:50:GLU:OE2	1:A:90:ARG:HD3	1.93	0.68
1:B:349:GLU:HB3	1:B:489:PHE:HB3	1.75	0.68
1:A:15:LYS:CB	1:A:15:LYS:HZ3	1.97	0.68
2:A:901:PG0:H52	3:A:1069:HOH:O	1.94	0.68
1:A:236:HIS:HE1	1:A:272:MET:O	1.77	0.67
1:A:25:HIS:CD2	1:A:28:ARG:HH11	2.10	0.67
1:B:319:ARG:NH1	1:B:323:GLU:OE2	2.27	0.67
1:B:344:LYS:NZ	1:B:346:LYS:HZ2	1.93	0.66
1:B:421:ASN:O	1:B:424:CYS:HB2	1.95	0.66
1:B:490:THR:CG2	1:B:492:ASP:CG	2.70	0.64
1:B:319:ARG:NE	1:B:331:LEU:HD13	2.13	0.63
1:B:344:LYS:NZ	1:B:346:LYS:NZ	2.47	0.62
1:B:25:HIS:CD2	1:B:28:ARG:HH11	2.12	0.62
1:B:96:CYS:O	1:B:97:ALA:HB3	1.97	0.62
1:B:236:HIS:HE1	1:B:272:MET:O	1.83	0.62
1:B:319:ARG:CD	1:B:331:LEU:HD13	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ASN:HD22	1:A:123:TYR:H	1.49	0.60
1:A:532:HIS:HD2	1:A:534:GLY:H	1.47	0.60
1:B:173:ASP:OD2	1:B:177:LYS:CE	2.50	0.60
1:B:283:ASN:HD21	1:B:535:ARG:HH21	1.50	0.60
1:A:280:GLY:HA2	1:A:532:HIS:CG	2.37	0.59
1:A:353:LEU:C	1:A:353:LEU:HD23	2.27	0.59
1:B:532:HIS:HD2	1:B:534:GLY:H	1.48	0.59
1:B:319:ARG:HD3	1:B:331:LEU:HD13	1.84	0.59
1:B:7:ASP:CG	1:B:8:ASP:H	2.10	0.59
1:B:7:ASP:OD1	1:B:8:ASP:N	2.36	0.59
1:A:482:LYS:H	2:A:901:PG0:H51	1.68	0.58
1:A:283:ASN:HD21	1:A:535:ARG:NH2	2.01	0.58
1:A:241:HIS:HD2	1:A:244:GLU:OE2	1.86	0.58
1:A:176:LYS:HE3	1:A:180:GLY:O	2.03	0.58
1:B:236:HIS:HD2	1:B:314:LYS:HD3	1.69	0.57
1:B:353:LEU:C	1:B:353:LEU:HD23	2.30	0.57
1:B:106:TYR:CD2	1:B:378:ALA:HB2	2.39	0.56
1:B:326:VAL:HG23	1:B:328:LEU:HG	1.86	0.56
1:B:319:ARG:CG	1:B:319:ARG:NH1	2.39	0.56
1:B:576:THR:HG23	3:B:1109:HOH:O	2.06	0.56
1:B:25:HIS:HE1	3:B:1055:HOH:O	1.87	0.56
1:B:90:ARG:HH11	1:B:153:GLN:HE22	1.54	0.56
1:A:532:HIS:CD2	1:A:534:GLY:H	2.22	0.56
1:B:169:GLN:HE22	1:B:172:ARG:HH11	1.52	0.56
1:A:283:ASN:ND2	1:A:535:ARG:HH21	2.02	0.55
1:A:408:VAL:O	1:A:415:VAL:HG22	2.06	0.55
1:A:288:ASN:C	1:A:288:ASN:HD22	2.14	0.55
1:B:397:LEU:O	1:B:426:ARG:HA	2.07	0.54
1:B:532:HIS:CD2	1:B:534:GLY:H	2.25	0.54
1:B:280:GLY:HA2	1:B:532:HIS:CG	2.44	0.53
1:A:106:TYR:CD2	1:A:378:ALA:HB2	2.44	0.53
1:B:241:HIS:CE1	1:B:286:ASN:HD22	2.20	0.53
1:A:201:GLU:HA	1:A:201:GLU:OE1	2.09	0.53
1:A:120:ASN:ND2	1:A:123:TYR:H	2.07	0.52
1:A:35:GLU:OE2	1:A:82:LYS:HE2	2.09	0.52
1:B:139:ARG:HB3	1:B:140:PRO:HD3	1.92	0.52
1:A:241:HIS:CE1	1:A:286:ASN:HD22	2.19	0.51
1:A:568:HIS:HE1	3:A:1190:HOH:O	1.92	0.51
1:B:359:ARG:HD3	1:B:486:SER:O	2.10	0.51
1:B:585:THR:N	1:B:586:PRO:CD	2.73	0.51
1:A:349:GLU:HB3	1:A:489:PHE:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:ARG:HE	1:B:331:LEU:HD13	1.74	0.51
1:A:285:ALA:H	1:A:449:ASN:HD22	1.59	0.51
1:A:121:GLN:O	1:A:125:GLU:HG3	2.11	0.50
1:A:422:ARG:C	1:A:424:CYS:H	2.18	0.50
1:B:474:TRP:CD1	1:B:474:TRP:H	2.27	0.50
1:A:25:HIS:HE1	3:A:1043:HOH:O	1.94	0.50
1:B:490:THR:CG2	1:B:491:ALA:N	2.74	0.50
1:A:576:THR:OG1	1:A:577:PRO:HD2	2.12	0.49
1:B:241:HIS:HD2	1:B:244:GLU:OE2	1.96	0.49
1:B:576:THR:HG23	1:B:576:THR:O	2.12	0.49
1:B:415:VAL:HG22	1:B:427:LEU:HD13	1.95	0.48
1:B:120:ASN:HD22	1:B:123:TYR:H	1.60	0.48
1:B:60:PRO:HD2	1:B:64:GLN:O	2.14	0.48
1:B:474:TRP:CD1	1:B:474:TRP:N	2.78	0.48
1:B:288:ASN:O	1:B:289:GLU:HB2	2.13	0.48
1:A:232:MET:O	1:A:269:ASN:HB3	2.14	0.48
1:A:120:ASN:ND2	1:A:122:PRO:HD2	2.29	0.47
1:B:139:ARG:N	1:B:140:PRO:CD	2.76	0.47
1:B:569:GLN:CD	1:B:569:GLN:N	2.72	0.47
1:A:288:ASN:ND2	1:A:290:THR:H	2.12	0.47
1:A:454:VAL:HG22	1:A:454:VAL:O	2.15	0.47
1:A:292:TYR:H	1:A:421:ASN:ND2	2.11	0.46
1:B:283:ASN:ND2	1:B:535:ARG:HE	2.13	0.46
1:A:549:ALA:N	1:A:550:PRO:CD	2.78	0.46
1:B:285:ALA:H	1:B:449:ASN:HD22	1.63	0.46
1:A:52:TYR:CE2	1:A:97:ALA:HB2	2.50	0.46
1:A:236:HIS:CE1	1:A:272:MET:O	2.64	0.46
1:B:549:ALA:N	1:B:550:PRO:CD	2.78	0.46
1:A:139:ARG:N	1:A:140:PRO:CD	2.79	0.46
1:B:173:ASP:OD2	1:B:177:LYS:NZ	2.49	0.45
1:A:561:LEU:C	1:A:561:LEU:HD23	2.40	0.45
1:B:520:GLU:O	1:B:520:GLU:HG2	2.16	0.45
1:B:283:ASN:HD21	1:B:535:ARG:NH2	2.13	0.45
1:A:283:ASN:ND2	1:A:535:ARG:HE	2.15	0.45
1:A:516:ILE:HG12	1:A:573:PHE:CE1	2.52	0.45
1:A:349:GLU:HB3	1:A:489:PHE:CB	2.47	0.45
1:A:400:GLN:O	1:A:462:GLU:HB2	2.17	0.45
1:A:176:LYS:HA	1:A:176:LYS:HD2	1.67	0.44
1:A:529:ASN:ND2	1:A:558:GLU:H	2.14	0.44
1:B:283:ASN:ND2	1:B:535:ARG:HH21	2.16	0.44
1:A:271:TYR:HA	1:A:272:MET:HA	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:PHE:O	1:B:221:LYS:HG3	2.17	0.44
1:B:529:ASN:ND2	1:B:558:GLU:H	2.16	0.44
1:B:532:HIS:CD2	1:B:532:HIS:C	2.95	0.44
1:A:143:SER:HA	1:A:147:GLY:O	2.18	0.44
1:A:342:PHE:HB3	1:A:506:LEU:HD11	2.00	0.44
1:B:402:ILE:O	1:B:402:ILE:HG23	2.18	0.44
1:B:582:ILE:HA	1:B:583:PRO:HD3	1.84	0.43
1:B:283:ASN:HD21	1:B:535:ARG:HE	1.66	0.43
1:B:344:LYS:HZ1	1:B:346:LYS:NZ	2.16	0.43
1:B:52:TYR:CE2	1:B:97:ALA:HB2	2.53	0.43
1:B:236:HIS:CE1	1:B:272:MET:O	2.69	0.43
1:B:561:LEU:C	1:B:561:LEU:HD23	2.43	0.43
1:A:99:TRP:O	1:A:100:GLU:C	2.62	0.43
1:B:120:ASN:ND2	1:B:123:TYR:H	2.16	0.43
1:A:400:GLN:HA	1:A:401:ASP:HA	1.84	0.42
1:B:494:VAL:HG12	1:B:500:TYR:CD1	2.54	0.42
1:A:241:HIS:HE1	1:A:286:ASN:ND2	2.08	0.42
1:B:319:ARG:HE	1:B:331:LEU:CD1	2.33	0.42
1:B:342:PHE:HB3	1:B:506:LEU:HD11	2.01	0.42
1:A:281:PHE:CZ	1:A:532:HIS:HE1	2.37	0.42
1:A:207:VAL:O	1:A:231:CYS:HA	2.20	0.42
1:B:90:ARG:HH11	1:B:153:GLN:NE2	2.15	0.41
1:A:369:PRO:HG2	1:A:463:GLY:HA2	2.02	0.41
1:B:503:LYS:HG2	1:B:504:GLY:N	2.34	0.41
1:B:271:TYR:HA	1:B:272:MET:HA	1.86	0.41
1:B:549:ALA:HB3	1:B:550:PRO:HD3	2.03	0.41
1:A:241:HIS:CD2	1:A:244:GLU:OE2	2.72	0.41
1:B:400:GLN:HA	1:B:401:ASP:HA	1.88	0.41
1:A:91:PRO:HD2	1:A:153:GLN:O	2.21	0.41
1:A:156:ASN:O	1:A:157:GLU:C	2.63	0.41
1:A:403:HIS:HA	1:A:404:ASP:HA	1.80	0.41
1:A:549:ALA:HB3	1:A:550:PRO:HD3	2.03	0.41
1:A:469:GLN:NE2	1:B:163:ASN:HB3	2.36	0.40
1:B:99:TRP:O	1:B:100:GLU:C	2.62	0.40
1:A:323:GLU:HG2	1:A:328:LEU:HD12	2.03	0.40
1:B:403:HIS:HA	1:B:404:ASP:HA	1.77	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	579/600 (96%)	565 (98%)	14 (2%)	0	100	100
1	B	584/600 (97%)	568 (97%)	15 (3%)	1 (0%)	43	31
All	All	1163/1200 (97%)	1133 (97%)	29 (2%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	473	ASP

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	503/521 (96%)	491 (98%)	12 (2%)	43	31
1	B	508/521 (98%)	493 (97%)	15 (3%)	36	24
All	All	1011/1042 (97%)	984 (97%)	27 (3%)	39	27

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASP
1	A	9	SER
1	A	15	LYS
1	A	100	GLU
1	A	155	GLU

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Mol	Chain	Res	Type
1	A	176	LYS
1	A	288	ASN
1	A	344	LYS
1	A	394	LYS
1	A	422	ARG
1	A	490	THR
1	A	509	ASP
1	B	57	LEU
1	B	100	GLU
1	B	121	GLN
1	B	155	GLU
1	B	263	LYS
1	B	319	ARG
1	B	415	VAL
1	B	417	ILE
1	B	419	GLU
1	B	422	ARG
1	B	490	THR
1	B	503	LYS
1	B	554	GLU
1	B	569	GLN
1	B	585	THR

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

Mol	Chain	Res	Type
1	A	25	HIS
1	A	64	GLN
1	A	120	ASN
1	A	165	GLN
1	A	236	HIS
1	A	241	HIS
1	A	264	GLN
1	A	283	ASN
1	A	286	ASN
1	A	288	ASN
1	A	293	GLN
1	A	358	HIS
1	A	421	ASN
1	A	449	ASN
1	A	469	GLN
1	A	529	ASN

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Mol	Chain	Res	Type
1	A	532	HIS
1	A	568	HIS
1	B	25	HIS
1	B	120	ASN
1	B	121	GLN
1	B	153	GLN
1	B	165	GLN
1	B	169	GLN
1	B	219	GLN
1	B	222	GLN
1	B	226	ASN
1	B	236	HIS
1	B	241	HIS
1	B	283	ASN
1	B	286	ASN
1	B	293	GLN
1	B	449	ASN
1	B	469	GLN
1	B	529	ASN
1	B	532	HIS
1	B	568	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	PG0	B	900	-	7,7,7	0.66	0	6,6,6	0.46	0
2	PG0	A	900	-	7,7,7	0.60	0	6,6,6	0.56	0
2	PG0	A	901	-	7,7,7	0.67	0	6,6,6	0.72	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	PG0	B	900	-	-	3/5/5/5	-
2	PG0	A	900	-	-	2/5/5/5	-
2	PG0	A	901	-	-	1/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	900	PG0	C4-C3-O1-C2
2	A	900	PG0	O1-C3-C4-O2
2	A	900	PG0	C3-C4-O2-C5
2	B	900	PG0	OTT-C1-C2-O1
2	B	900	PG0	C3-C4-O2-C5
2	A	901	PG0	O1-C3-C4-O2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	PG0	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	581/600 (96%)	0.27	21 (3%) 46 46	13, 20, 36, 54	0
1	B	586/600 (97%)	0.31	20 (3%) 48 48	14, 20, 37, 57	0
All	All	1167/1200 (97%)	0.29	41 (3%) 47 47	13, 20, 36, 57	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	424	CYS	6.6
1	A	289	GLU	5.8
1	A	491	ALA	4.9
1	A	423	GLY	4.6
1	A	97	ALA	4.6
1	A	424	CYS	4.6
1	B	422	ARG	4.4
1	B	7	ASP	4.0
1	A	581	ALA	4.0
1	A	492	ASP	3.8
1	A	7	ASP	3.5
1	A	422	ARG	3.3
1	A	14	GLY	3.3
1	B	358	HIS	3.2
1	B	545	LEU	3.2
1	B	425	SER	3.1
1	B	423	GLY	2.9
1	B	327	ASP	2.8
1	A	490	THR	2.7
1	A	6	TYR	2.7
1	B	492	ASP	2.7
1	B	586	PRO	2.7
1	A	1	MET	2.6
1	A	425	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	435	GLU	2.6
1	B	8	ASP	2.6
1	A	155	GLU	2.5
1	A	494	VAL	2.4
1	B	13	ASP	2.4
1	A	90	ARG	2.4
1	B	154	ILE	2.3
1	B	341	LEU	2.3
1	A	13	ASP	2.3
1	B	490	THR	2.3
1	B	155	GLU	2.2
1	A	290	THR	2.2
1	B	426	ARG	2.1
1	A	493	GLU	2.1
1	B	96	CYS	2.1
1	B	486	SER	2.0
1	A	426	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PG0	A	900	8/8	0.72	0.20	18,29,33,39	0
2	PG0	B	900	8/8	0.84	0.21	24,29,34,42	0
2	PG0	A	901	8/8	0.92	0.14	11,28,33,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.