



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 08:34 AM UTC

PDB ID : 3VVG / pdb_00003vvg
Title : The Crystal Structure of Cellulase-Inhibitor Complex.
Authors : Ishikawa, K.; Maeno, Y.; Kataoka, M.
Deposited on : 2012-07-24
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

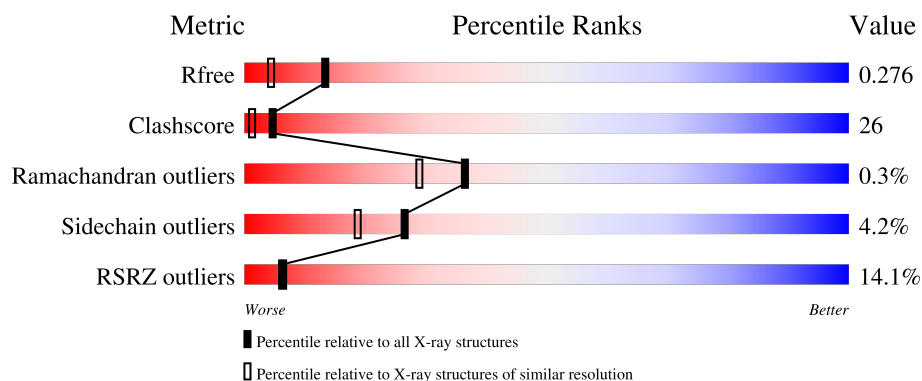
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	377	3% 77% 20% .
1	B	377	34% 49% 44% 6% .
1	C	377	6% 68% 29% .

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
2	ZGB	A	501	-	-	X	-
2	ZGB	C	501	-	-	X	-
3	PO4	A	502	-	-	X	-
3	PO4	B	502	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9943 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.

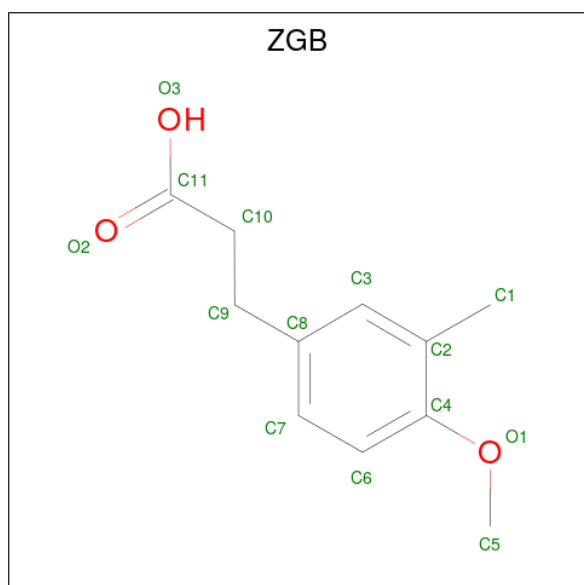
- Molecule 1 is a protein called 458aa long hypothetical endo-1,4-beta-glucanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	0	0
			3069	2002	500	557	10			
1	B	377	Total	C	N	O	S	0	0	0
			3069	2002	500	557	10			
1	C	377	Total	C	N	O	S	0	0	0
			3069	2002	500	557	10			

There are 3 discrepancies between the modelled and reference sequences:

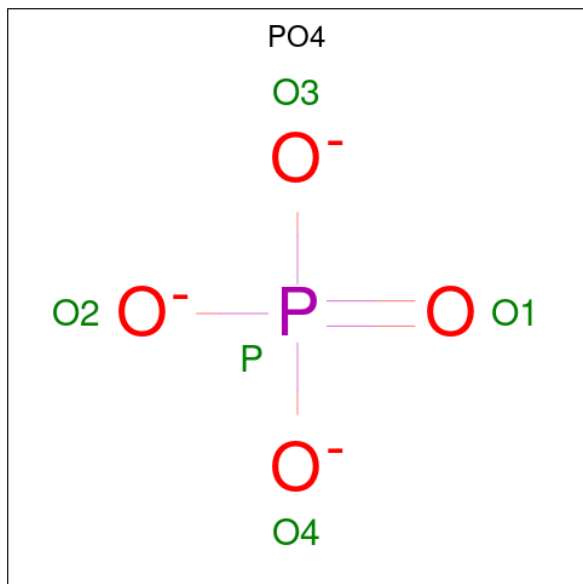
Chain	Residue	Modelled	Actual	Comment	Reference
A	289	LYS	ARG	conflict	UNP O58925
B	289	LYS	ARG	conflict	UNP O58925
C	289	LYS	ARG	conflict	UNP O58925

- Molecule 2 is 3-(4-methoxy-3-methylphenyl)propanoic acid (CCD ID: ZGB) (formula: $C_{11}H_{14}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	10	2		
2	A	1	Total	C	O	0	0
			12	10	2		
2	C	1	Total	C	O	0	0
			12	10	2		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

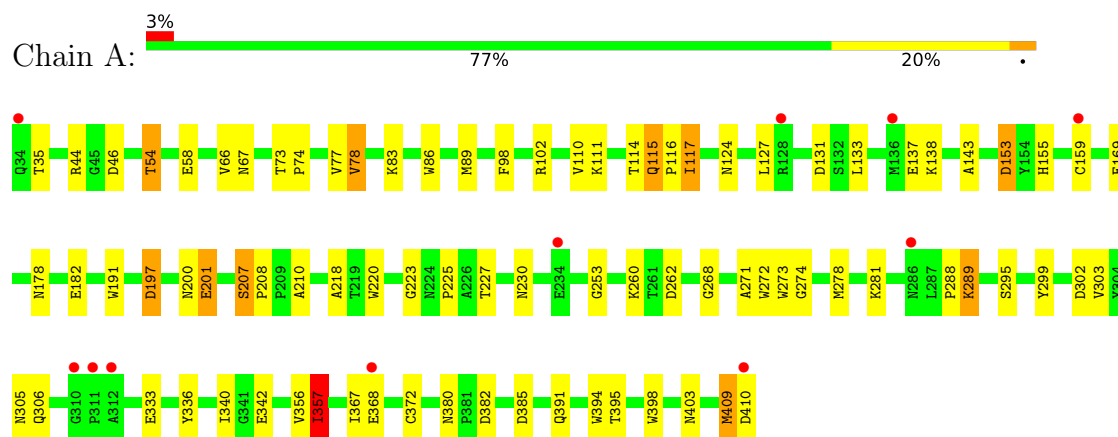
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	304	Total	O	0	0
			304	304		
4	B	146	Total	O	0	0
			146	146		
4	C	230	Total	O	0	0
			230	230		

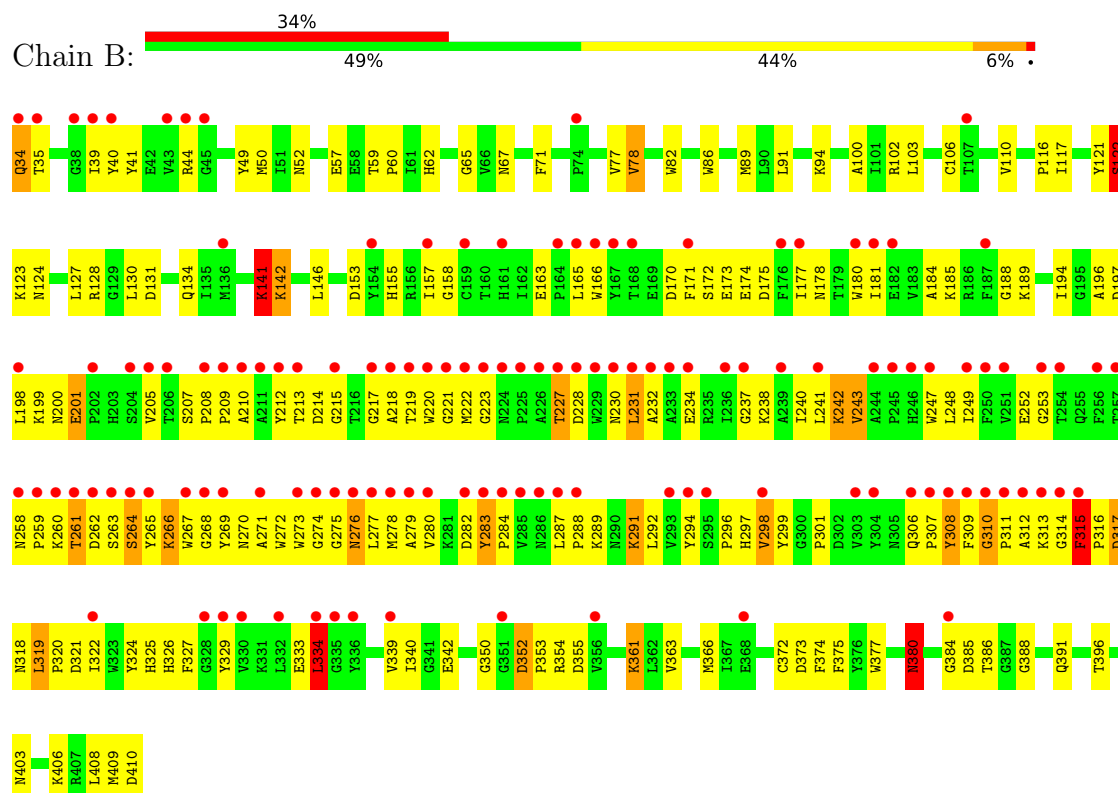
3 Residue-property plots

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.

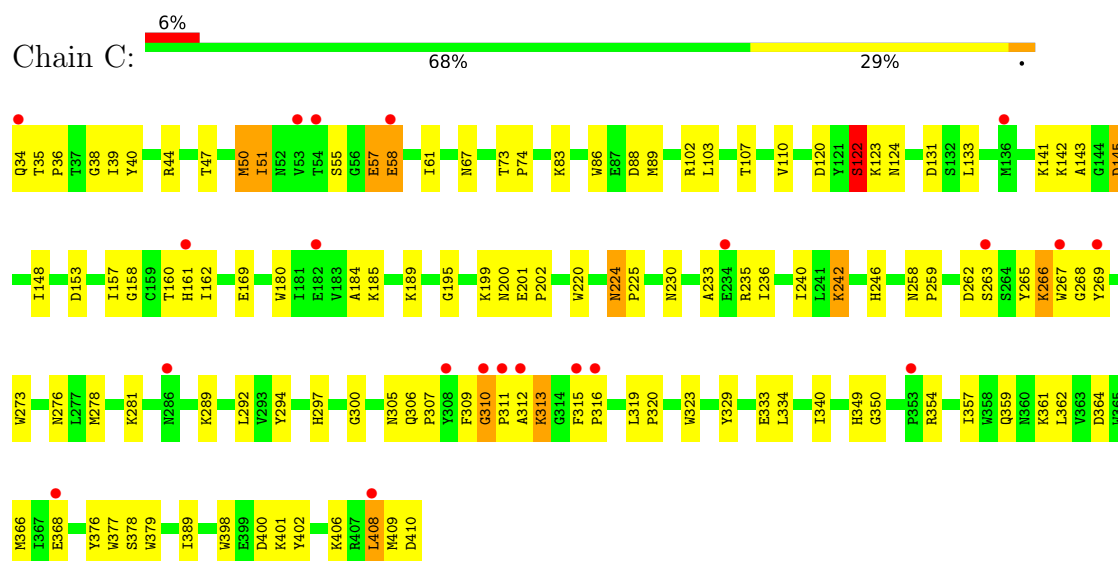
- Molecule 1: 458aa long hypothetical endo-1,4-beta-glucanase



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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	163.57Å 58.43Å 138.01Å 90.00° 109.01° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 50.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-1.90) 99.1 (50.00-1.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.220 , 0.286 0.216 , 0.276	Depositor DCC
R_{free} test set	4906 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9943	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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: PO4, ZGB

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	1.50	16/3180 (0.5%)	1.28	11/4341 (0.3%)
1	B	1.22	9/3180 (0.3%)	1.28	25/4341 (0.6%)
1	C	1.24	6/3180 (0.2%)	1.21	15/4341 (0.3%)
All	All	1.33	31/9540 (0.3%)	1.26	51/13023 (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	B	0	1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	356	VAL	CA-CB	8.95	1.64	1.54
1	B	197	ASP	CA-C	6.65	1.61	1.52
1	A	197	ASP	C-O	6.57	1.31	1.24
1	A	342	GLU	N-CA	6.52	1.53	1.46
1	A	288	PRO	CA-C	6.38	1.60	1.52
1	A	271	ALA	CA-CB	6.35	1.63	1.53
1	B	89	MET	CA-C	6.34	1.60	1.52
1	B	77	VAL	CA-CB	6.23	1.62	1.55
1	C	142	LYS	N-CA	6.21	1.53	1.46
1	C	233	ALA	N-CA	6.12	1.53	1.46
1	B	377	TRP	N-CA	6.10	1.54	1.46
1	A	201	GLU	CA-CB	6.00	1.57	1.52
1	A	201	GLU	C-O	5.83	1.26	1.23
1	C	157	ILE	CA-CB	5.80	1.62	1.54
1	A	278	MET	SD-CE	-5.75	1.65	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	298	VAL	CA-CB	5.74	1.61	1.55
1	C	145	ASP	C-O	5.73	1.30	1.24
1	B	380	ASN	N-CA	5.71	1.54	1.46
1	B	201	GLU	CA-CB	5.34	1.56	1.52
1	A	340	ILE	CA-CB	-5.34	1.47	1.53
1	C	107	THR	CA-CB	5.32	1.61	1.53
1	A	218	ALA	CA-CB	5.29	1.61	1.53
1	A	262	ASP	N-CA	5.25	1.52	1.46
1	A	367	ILE	N-CA	-5.15	1.40	1.46
1	B	375	PHE	N-CA	5.12	1.52	1.46
1	A	143	ALA	CA-CB	5.08	1.61	1.53
1	B	78	VAL	CA-CB	5.02	1.59	1.54
1	A	295	SER	CA-C	5.01	1.58	1.52
1	A	305	ASN	CA-CB	5.01	1.59	1.52
1	C	103	LEU	N-CA	-5.01	1.41	1.46
1	A	357	ILE	CA-CB	5.01	1.60	1.54

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	287	LEU	CA-C-N	-8.15	111.39	119.78
1	B	287	LEU	C-N-CA	-8.15	111.39	119.78
1	B	283	TYR	CA-C-N	7.84	127.77	119.85
1	B	283	TYR	C-N-CA	7.84	127.77	119.85
1	B	82	TRP	N-CA-C	-7.83	103.53	113.23
1	C	158	GLY	N-CA-C	-7.65	100.94	112.41
1	C	306	GLN	CA-C-N	7.64	126.92	118.97
1	C	306	GLN	C-N-CA	7.64	126.92	118.97
1	B	141	LYS	N-CA-C	7.09	119.01	111.28
1	A	207	SER	CA-C-N	6.92	127.50	120.38
1	A	207	SER	C-N-CA	6.92	127.50	120.38
1	C	195	GLY	N-CA-C	6.78	119.05	110.38
1	B	110	VAL	CB-CA-C	-6.48	104.74	112.19
1	C	350	GLY	N-CA-C	-6.45	106.33	115.43
1	B	222	MET	N-CA-C	-6.36	105.66	113.41
1	B	352	ASP	CA-C-N	-6.25	113.24	119.56
1	B	352	ASP	C-N-CA	-6.25	113.24	119.56
1	C	38	GLY	N-CA-C	-6.24	106.81	114.92
1	B	334	LEU	N-CA-C	6.23	120.74	113.20
1	B	297	HIS	CA-C-N	-6.11	112.60	121.95
1	B	297	HIS	C-N-CA	-6.11	112.60	121.95
1	A	268	GLY	N-CA-C	6.08	121.20	113.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	LYS	CA-C-N	-6.07	113.53	119.78
1	A	111	LYS	C-N-CA	-6.07	113.53	119.78
1	C	236	ILE	N-CA-C	-6.00	105.00	110.82
1	A	227	THR	N-CA-C	-5.93	106.66	114.31
1	B	361	LYS	N-CA-C	5.93	117.74	111.28
1	C	224	ASN	CA-C-N	5.93	126.04	119.87
1	C	224	ASN	C-N-CA	5.93	126.04	119.87
1	C	122	SER	N-CA-C	-5.87	104.96	111.36
1	A	115	GLN	CA-C-N	-5.86	114.57	120.31
1	A	115	GLN	C-N-CA	-5.86	114.57	120.31
1	B	261	THR	N-CA-C	-5.78	104.62	111.03
1	B	122	SER	N-CA-C	-5.67	106.07	112.87
1	B	237	GLY	N-CA-C	5.55	119.60	112.83
1	A	357	ILE	CB-CA-C	-5.54	104.88	111.97
1	C	50	MET	N-CA-C	-5.49	99.96	108.90
1	C	162	ILE	CB-CA-C	-5.43	104.72	111.08
1	B	384	GLY	N-CA-C	5.42	119.23	112.73
1	A	409	MET	N-CA-C	-5.38	106.56	113.23
1	B	291	LYS	N-CA-C	-5.30	108.58	114.62
1	B	317	ASP	N-CA-C	-5.28	105.48	112.34
1	C	184	ALA	N-CA-C	5.25	117.00	111.28
1	A	138	LYS	N-CA-C	-5.24	105.65	111.36
1	B	103	LEU	CA-C-N	5.20	124.96	119.76
1	B	103	LEU	C-N-CA	5.20	124.96	119.76
1	B	319	LEU	N-CA-C	5.13	121.15	109.81
1	C	310	GLY	CA-C-N	-5.12	113.44	119.84
1	C	310	GLY	C-N-CA	-5.12	113.44	119.84
1	B	252	GLU	N-CA-C	5.07	117.07	110.53
1	B	315	PHE	N-CA-C	-5.06	103.78	109.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	310	GLY	Peptide

5.2 Too-close contacts [i](#)

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	3069	0	2910	86	2
1	B	3069	0	2907	267	0
1	C	3069	0	2908	112	0
2	A	24	0	20	12	2
2	C	12	0	10	8	0
3	A	5	0	0	3	0
3	B	15	0	0	3	0
4	A	304	0	0	25	0
4	B	146	0	0	37	0
4	C	230	0	0	17	0
All	All	9943	0	8755	467	2

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 26.

All (467) 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:191:TRP:CD1	3:A:502:PO4:O3	1.73	1.40
1:B:234:GLU:HB3	4:B:713:HOH:O	1.16	1.34
1:B:217:GLY:O	1:B:227:THR:CG2	1.85	1.25
1:B:34:GLN:HG3	1:B:40:TYR:CD1	1.72	1.25
1:A:159:CYS:HB3	4:A:887:HOH:O	1.07	1.25
1:A:191:TRP:HD1	3:A:502:PO4:O3	0.92	1.25
1:B:34:GLN:HG3	1:B:40:TYR:CE1	1.72	1.24
1:A:372:CYS:SG	4:A:833:HOH:O	1.96	1.23
1:A:410:ASP:HA	4:A:811:HOH:O	1.35	1.21
1:B:122:SER:OG	3:B:502:PO4:O2	1.56	1.20
1:B:220:TRP:HA	4:B:677:HOH:O	1.43	1.19
1:B:122:SER:O	1:C:123:LYS:NZ	1.76	1.19
1:B:220:TRP:NE1	1:B:230:ASN:HB3	1.57	1.18
1:B:315:PHE:HA	1:B:318:ASN:OD1	1.43	1.17
2:A:503:ZGB:C11	2:A:503:ZGB:H7	1.74	1.16
1:B:220:TRP:CE2	1:B:230:ASN:HB3	1.79	1.16
1:B:234:GLU:O	1:B:238:LYS:HG3	1.43	1.15
1:B:228:ASP:OD2	1:B:231:LEU:CD1	1.95	1.15
1:C:266:LYS:HD2	1:C:266:LYS:N	1.58	1.15
1:B:217:GLY:O	1:B:227:THR:HG21	1.43	1.14
1:C:266:LYS:CD	1:C:266:LYS:H	1.57	1.14
1:B:260:LYS:O	1:B:264:SER:HB3	1.48	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:LYS:HD2	1:C:266:LYS:H	0.96	1.09
1:B:312:ALA:HA	4:B:683:HOH:O	1.53	1.07
1:B:220:TRP:NE1	1:B:230:ASN:CB	2.17	1.07
1:B:306:GLN:CG	1:B:309:PHE:HE2	1.68	1.07
1:B:34:GLN:CG	1:B:40:TYR:CD1	2.37	1.06
1:B:306:GLN:CG	1:B:309:PHE:CE2	2.39	1.06
1:B:311:PRO:HA	4:B:683:HOH:O	1.54	1.05
1:B:141:LYS:HE3	4:B:714:HOH:O	1.56	1.05
1:B:403:ASN:HA	1:B:406:LYS:HD2	1.41	1.03
1:B:141:LYS:CE	4:B:714:HOH:O	2.03	1.03
1:C:406:LYS:HA	1:C:409:MET:CE	1.90	1.02
1:B:306:GLN:HB2	1:B:309:PHE:CD2	1.95	1.01
1:C:268:GLY:HA2	1:C:278:MET:HE1	1.43	1.00
1:B:174:GLU:O	1:B:178:ASN:ND2	1.96	0.97
1:B:260:LYS:O	1:B:264:SER:CB	2.12	0.97
1:B:306:GLN:HG3	1:B:309:PHE:CE2	1.99	0.96
1:C:364:ASP:O	1:C:368:GLU:HG3	1.65	0.95
1:B:128:ARG:HD3	4:C:747:HOH:O	1.64	0.95
1:C:67:ASN:HD21	1:C:102:ARG:HD3	1.31	0.94
1:C:309:PHE:O	1:C:354:ARG:NH1	1.99	0.94
1:C:406:LYS:HA	1:C:409:MET:HE3	1.48	0.94
1:B:242:LYS:HD2	1:B:242:LYS:O	1.67	0.93
1:B:234:GLU:O	1:B:238:LYS:CG	2.16	0.93
1:C:281:LYS:HE2	4:C:791:HOH:O	1.68	0.93
1:B:243:VAL:HA	4:B:706:HOH:O	1.68	0.92
1:A:368:GLU:OE2	4:A:831:HOH:O	1.88	0.92
1:B:270:ASN:O	1:B:308:TYR:OH	1.86	0.91
1:B:34:GLN:CG	1:B:40:TYR:CE1	2.53	0.91
1:B:228:ASP:OD2	1:B:231:LEU:HD12	1.69	0.91
1:B:242:LYS:HD2	1:B:242:LYS:C	1.94	0.91
1:B:217:GLY:O	1:B:227:THR:HG23	1.72	0.88
1:B:218:ALA:HA	1:B:227:THR:HG22	1.54	0.88
1:C:50:MET:HE1	2:C:501:ZGB:H10A	1.55	0.88
1:A:372:CYS:CB	4:A:833:HOH:O	2.13	0.86
1:B:234:GLU:OE2	4:B:628:HOH:O	1.93	0.86
1:B:270:ASN:ND2	1:B:307:PRO:CD	2.39	0.85
1:C:259:PRO:HG2	4:C:776:HOH:O	1.75	0.85
1:B:177:ILE:HG22	1:B:181:ILE:CD1	2.06	0.85
1:B:199:LYS:HE2	4:B:670:HOH:O	1.75	0.85
1:B:220:TRP:CE2	1:B:230:ASN:CB	2.59	0.85
1:A:67:ASN:HD21	1:A:102:ARG:HD3	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:ILE:O	1:B:181:ILE:HD12	1.77	0.84
1:A:403:ASN:OD1	4:A:669:HOH:O	1.96	0.83
1:B:220:TRP:CD1	1:B:230:ASN:OD1	2.31	0.83
1:B:270:ASN:HD22	1:B:307:PRO:CD	1.92	0.82
1:B:228:ASP:OD2	1:B:231:LEU:HD13	1.77	0.82
1:B:306:GLN:HG2	1:B:309:PHE:HE2	1.43	0.82
2:A:503:ZGB:C11	2:A:503:ZGB:C7	2.48	0.82
1:B:260:LYS:HE2	4:B:660:HOH:O	1.79	0.82
1:A:54:THR:O	4:A:848:HOH:O	1.98	0.81
1:A:67:ASN:HD21	1:A:102:ARG:HH11	1.25	0.81
1:B:228:ASP:HB3	1:B:231:LEU:HB2	1.62	0.81
1:B:270:ASN:ND2	1:B:307:PRO:CG	2.45	0.80
1:B:209:PRO:HA	1:B:212:TYR:CD2	2.16	0.80
1:B:306:GLN:HB2	1:B:309:PHE:CE2	2.16	0.80
1:B:288:PRO:CB	4:B:658:HOH:O	2.29	0.80
1:B:321:ASP:O	1:B:325:HIS:N	2.15	0.80
1:C:406:LYS:HA	1:C:409:MET:HE2	1.62	0.80
1:C:67:ASN:HD21	1:C:102:ARG:HH11	1.30	0.79
1:A:372:CYS:SG	4:A:872:HOH:O	2.35	0.79
1:B:340:ILE:HD12	1:B:366:MET:HE3	1.64	0.78
1:A:273:TRP:H	2:A:501:ZGB:H1	1.49	0.78
1:B:306:GLN:HG3	1:B:309:PHE:HE2	1.41	0.78
1:B:220:TRP:CD1	1:B:230:ASN:HB3	2.18	0.77
1:B:288:PRO:CG	4:B:658:HOH:O	2.33	0.76
1:B:253:GLY:O	1:B:274:GLY:HA2	1.86	0.76
1:B:306:GLN:CB	1:B:309:PHE:CE2	2.69	0.75
1:C:313:LYS:HA	4:C:744:HOH:O	1.85	0.75
1:B:270:ASN:HD22	1:B:307:PRO:HD2	1.51	0.74
1:B:313:LYS:CG	1:B:313:LYS:O	2.35	0.74
1:C:51:ILE:HG13	1:C:58:GLU:HB2	1.70	0.74
1:A:272:TRP:HA	2:A:501:ZGB:H3	1.70	0.73
1:B:34:GLN:HG3	1:B:40:TYR:HD1	1.51	0.73
1:B:223:GLY:N	4:B:655:HOH:O	2.20	0.73
1:A:410:ASP:CA	4:A:811:HOH:O	2.07	0.73
1:B:299:TYR:OH	1:B:342:GLU:OE1	2.06	0.73
1:B:317:ASP:O	4:B:644:HOH:O	2.08	0.72
1:B:128:ARG:CD	4:C:747:HOH:O	2.30	0.72
1:A:409:MET:O	1:A:410:ASP:HB2	1.88	0.72
1:B:189:LYS:NZ	4:B:745:HOH:O	2.19	0.72
1:A:368:GLU:CD	4:A:831:HOH:O	2.28	0.71
1:B:184:ALA:O	4:B:712:HOH:O	2.07	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:PHE:CE1	1:B:175:ASP:HB3	2.25	0.71
1:A:102:ARG:HH22	1:A:200:ASN:HD22	1.39	0.71
1:C:50:MET:CE	1:C:61:ILE:HG21	2.21	0.71
1:A:67:ASN:ND2	1:A:102:ARG:HH11	1.88	0.70
1:B:34:GLN:HG2	1:B:40:TYR:CD1	2.22	0.70
1:B:230:ASN:OD1	4:B:677:HOH:O	2.09	0.70
1:C:406:LYS:CA	1:C:409:MET:CE	2.68	0.70
1:A:409:MET:O	1:A:410:ASP:CB	2.39	0.70
1:C:50:MET:HE2	1:C:61:ILE:HG21	1.72	0.70
1:C:263:SER:HB3	1:C:269:TYR:OH	1.90	0.70
1:A:116:PRO:C	1:A:117:ILE:HD13	2.17	0.69
1:A:210:ALA:CB	4:A:714:HOH:O	2.40	0.69
1:B:292:LEU:HD21	1:B:294:TYR:CZ	2.28	0.69
1:B:34:GLN:HG3	1:B:40:TYR:HE1	1.53	0.69
1:B:175:ASP:OD1	4:B:681:HOH:O	2.10	0.69
1:B:212:TYR:CD1	1:B:259:PRO:HD3	2.27	0.69
1:C:258:ASN:HB2	1:C:259:PRO:HD2	1.75	0.69
1:B:177:ILE:HG22	1:B:181:ILE:HD11	1.74	0.69
1:B:209:PRO:HA	1:B:212:TYR:CE2	2.28	0.68
3:B:502:PO4:O4	1:C:88:ASP:OD2	2.10	0.68
1:B:277:LEU:HB3	1:B:280:VAL:HG23	1.75	0.68
1:B:311:PRO:CA	4:B:683:HOH:O	2.25	0.68
1:C:67:ASN:ND2	1:C:102:ARG:HD3	2.07	0.68
1:C:39:ILE:HD11	2:C:501:ZGB:H1B	1.77	0.67
1:B:313:LYS:O	1:B:313:LYS:HG2	1.94	0.67
1:C:189:LYS:HD2	4:C:735:HOH:O	1.95	0.67
1:A:281:LYS:HD3	4:A:845:HOH:O	1.95	0.66
1:B:259:PRO:O	1:B:263:SER:OG	2.11	0.66
1:B:277:LEU:HB3	1:B:280:VAL:CG2	2.24	0.66
1:B:306:GLN:CB	1:B:309:PHE:CD2	2.77	0.66
1:B:184:ALA:HA	1:B:247:TRP:CH2	2.31	0.65
1:B:230:ASN:ND2	4:B:628:HOH:O	2.24	0.65
1:C:406:LYS:CA	1:C:409:MET:HE3	2.22	0.65
1:C:292:LEU:HD21	1:C:294:TYR:CE2	2.32	0.65
1:A:306:GLN:HE22	2:A:501:ZGB:H10A	1.61	0.65
1:B:188:GLY:HA3	4:B:712:HOH:O	1.95	0.64
1:B:316:PRO:CB	1:B:319:LEU:HD12	2.27	0.64
1:C:102:ARG:HH22	1:C:200:ASN:HD22	1.45	0.64
1:B:181:ILE:CG2	1:B:185:LYS:HE3	2.27	0.64
1:C:160:THR:OG1	1:C:161:HIS:HD2	1.80	0.64
1:B:228:ASP:CG	1:B:231:LEU:CD1	2.71	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:LYS:HE2	1:B:146:LEU:O	1.97	0.63
1:B:165:LEU:HD22	1:B:166:TRP:CZ3	2.33	0.63
1:B:270:ASN:HD21	1:B:307:PRO:HG3	1.63	0.63
1:B:301:PRO:HB3	1:B:354:ARG:HH21	1.64	0.63
1:B:219:THR:OG1	1:B:227:THR:HB	1.99	0.63
1:C:67:ASN:ND2	1:C:102:ARG:HH11	1.95	0.63
1:A:273:TRP:N	2:A:501:ZGB:H1	2.14	0.62
1:C:44:ARG:HH22	1:C:58:GLU:CD	2.07	0.62
1:B:220:TRP:NE1	1:B:230:ASN:CG	2.56	0.62
1:B:208:PRO:CB	1:B:212:TYR:HE2	2.12	0.62
1:C:161:HIS:HE1	4:C:812:HOH:O	1.83	0.62
1:B:238:LYS:HD2	4:B:633:HOH:O	2.00	0.61
1:B:260:LYS:O	1:B:264:SER:N	2.33	0.61
1:B:311:PRO:HB3	4:B:683:HOH:O	2.01	0.61
1:B:228:ASP:HB3	1:B:231:LEU:CD1	2.30	0.61
1:B:296:PRO:HG3	1:B:327:PHE:CD2	2.35	0.61
1:C:50:MET:CE	2:C:501:ZGB:H9A	2.29	0.61
1:B:228:ASP:CB	1:B:231:LEU:CD1	2.78	0.61
1:B:316:PRO:O	1:B:318:ASN:N	2.34	0.61
1:A:67:ASN:ND2	1:A:102:ARG:HD3	2.15	0.60
1:C:266:LYS:N	1:C:266:LYS:CD	2.31	0.60
1:B:141:LYS:NZ	4:B:714:HOH:O	2.28	0.60
1:B:353:PRO:C	1:B:355:ASP:H	2.10	0.60
1:C:305:ASN:O	1:C:305:ASN:ND2	2.34	0.60
1:B:210:ALA:O	1:B:214:ASP:HB3	2.01	0.60
1:C:266:LYS:H	1:C:266:LYS:HD3	1.63	0.60
1:C:292:LEU:HD21	1:C:294:TYR:CZ	2.37	0.60
1:B:181:ILE:O	1:B:185:LYS:HG3	2.01	0.59
1:B:141:LYS:HE2	4:B:606:HOH:O	2.02	0.59
1:B:316:PRO:C	1:B:318:ASN:N	2.57	0.59
1:C:316:PRO:HG3	1:C:357:ILE:HG21	1.84	0.59
1:B:172:SER:O	1:B:175:ASP:N	2.35	0.59
1:B:339:VAL:HG22	1:B:373:ASP:HB2	1.84	0.59
1:B:141:LYS:HG3	1:B:141:LYS:O	2.00	0.59
1:C:409:MET:O	1:C:410:ASP:HB2	2.02	0.59
1:B:228:ASP:CG	1:B:231:LEU:HD12	2.27	0.59
1:B:277:LEU:CD2	1:B:294:TYR:CD1	2.86	0.59
1:C:122:SER:OG	4:C:736:HOH:O	2.16	0.58
1:B:177:ILE:CG2	1:B:181:ILE:HD11	2.33	0.58
1:B:315:PHE:C	1:B:315:PHE:CD2	2.82	0.58
1:A:102:ARG:HH22	1:A:200:ASN:ND2	2.00	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:THR:OG1	1:C:39:ILE:O	2.10	0.58
1:B:241:LEU:HD21	1:B:291:LYS:HD3	1.85	0.58
1:A:191:TRP:CG	3:A:502:PO4:O3	2.49	0.58
1:A:86:TRP:HD1	1:A:124:ASN:HD22	1.52	0.58
1:B:180:TRP:CG	1:B:240:ILE:HD11	2.39	0.58
1:B:315:PHE:CA	1:B:318:ASN:OD1	2.35	0.58
1:A:210:ALA:HB3	4:A:714:HOH:O	2.03	0.57
1:A:210:ALA:HB2	4:A:714:HOH:O	2.04	0.57
1:B:333:GLU:HG2	1:B:334:LEU:HD23	1.86	0.57
1:B:282:ASP:O	1:B:283:TYR:CD1	2.58	0.57
1:A:357:ILE:N	1:A:357:ILE:CD1	2.67	0.57
1:B:177:ILE:HG22	1:B:181:ILE:HD12	1.85	0.57
1:B:228:ASP:CB	1:B:231:LEU:HD13	2.35	0.57
1:B:180:TRP:CH2	1:B:196:ALA:HB1	2.40	0.57
1:C:220:TRP:CE2	1:C:230:ASN:HB3	2.39	0.57
1:B:242:LYS:O	1:B:242:LYS:CD	2.48	0.57
1:B:234:GLU:CB	4:B:713:HOH:O	1.99	0.56
1:B:320:PRO:HD3	1:B:361:LYS:HE3	1.86	0.56
1:C:50:MET:HE2	1:C:61:ILE:CG2	2.35	0.56
1:B:67:ASN:HD21	1:B:102:ARG:HD3	1.70	0.56
1:B:185:LYS:HG3	1:B:243:VAL:HG21	1.87	0.56
1:B:220:TRP:CD1	1:B:230:ASN:CG	2.84	0.56
1:B:277:LEU:CD2	1:B:294:TYR:HD1	2.19	0.56
1:C:86:TRP:H	1:C:124:ASN:HD21	1.54	0.56
1:B:301:PRO:HB3	1:B:354:ARG:NH2	2.21	0.56
1:C:102:ARG:HH22	1:C:200:ASN:ND2	2.02	0.56
1:C:50:MET:CE	1:C:61:ILE:CG2	2.84	0.55
1:B:220:TRP:HE1	1:B:230:ASN:CB	2.12	0.55
1:B:271:ALA:CB	1:B:276:ASN:HB2	2.36	0.55
1:B:86:TRP:HD1	1:B:124:ASN:HD22	1.54	0.55
1:B:311:PRO:CB	4:B:683:HOH:O	2.47	0.55
1:C:120:ASP:OD1	1:C:120:ASP:C	2.50	0.55
1:C:389:ILE:HA	4:C:788:HOH:O	2.06	0.55
1:B:270:ASN:ND2	1:B:307:PRO:HG3	2.20	0.55
1:B:409:MET:O	1:B:410:ASP:HB2	2.07	0.55
1:B:208:PRO:HB3	1:B:212:TYR:HE2	1.72	0.55
1:C:36:PRO:HD2	1:C:246:HIS:CE1	2.41	0.55
1:B:288:PRO:HB2	4:B:658:HOH:O	1.98	0.54
1:B:268:GLY:HA2	1:B:278:MET:HE1	1.90	0.54
1:C:311:PRO:C	1:C:313:LYS:H	2.14	0.54
1:B:121:TYR:C	1:B:123:LYS:N	2.65	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:LEU:CD2	1:B:294:TYR:CE2	2.90	0.54
1:B:228:ASP:HB3	1:B:231:LEU:HD12	1.90	0.54
1:B:272:TRP:O	1:B:275:GLY:N	2.35	0.54
1:A:89:MET:HE1	1:A:394:TRP:CE3	2.43	0.54
1:A:306:GLN:NE2	2:A:501:ZGB:H10A	2.22	0.54
1:B:261:THR:HA	1:B:264:SER:OG	2.07	0.54
1:B:218:ALA:HA	1:B:227:THR:CG2	2.31	0.53
1:B:248:LEU:C	1:B:249:ILE:HD13	2.33	0.53
1:B:299:TYR:OH	1:B:342:GLU:HB3	2.08	0.53
1:B:272:TRP:O	1:B:273:TRP:C	2.51	0.53
1:B:181:ILE:HG23	1:B:243:VAL:HG11	1.89	0.53
1:C:400:ASP:OD1	1:C:401:LYS:N	2.42	0.53
1:C:267:TRP:CH2	1:C:307:PRO:HB2	2.43	0.53
1:B:121:TYR:C	1:B:123:LYS:H	2.16	0.53
1:B:131:ASP:C	1:B:131:ASP:OD1	2.52	0.53
1:B:270:ASN:HD21	1:B:307:PRO:CG	2.17	0.53
1:B:353:PRO:C	1:B:355:ASP:N	2.67	0.53
1:A:44:ARG:NH2	4:A:757:HOH:O	2.41	0.53
1:B:34:GLN:CG	1:B:40:TYR:HD1	2.08	0.53
1:B:59:THR:HB	1:B:60:PRO:HD2	1.91	0.53
1:C:86:TRP:H	1:C:124:ASN:ND2	2.06	0.53
1:B:271:ALA:HB1	1:B:276:ASN:HB2	1.89	0.53
1:C:50:MET:CE	2:C:501:ZGB:H10A	2.35	0.53
1:B:380:ASN:OD1	1:B:380:ASN:N	2.42	0.53
1:C:310:GLY:O	1:C:313:LYS:N	2.30	0.53
1:B:306:GLN:HG2	1:B:309:PHE:CE2	2.29	0.53
1:B:130:LEU:HD13	1:B:134:GLN:HB3	1.92	0.52
1:B:262:ASP:O	1:B:268:GLY:HA3	2.09	0.52
1:B:198:LEU:HD21	1:B:249:ILE:HG23	1.91	0.52
1:B:52:ASN:OD1	1:B:52:ASN:C	2.52	0.52
1:B:230:ASN:O	1:B:234:GLU:HG3	2.10	0.52
1:C:406:LYS:CB	1:C:409:MET:HE3	2.40	0.52
1:A:114:THR:O	1:A:131:ASP:HB2	2.10	0.52
1:A:289:LYS:HD3	4:A:671:HOH:O	2.09	0.52
1:B:209:PRO:HA	1:B:212:TYR:HD2	1.73	0.52
1:C:185:LYS:O	1:C:189:LYS:HE2	2.10	0.52
1:A:357:ILE:N	1:A:357:ILE:HD12	2.25	0.52
1:B:86:TRP:H	1:B:124:ASN:HD21	1.57	0.52
1:B:218:ALA:CA	1:B:227:THR:HG22	2.34	0.52
1:B:62:HIS:HD2	1:B:372:CYS:HB3	1.75	0.52
1:C:39:ILE:HD11	2:C:501:ZGB:C1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:PRO:O	1:B:317:ASP:C	2.51	0.52
1:B:292:LEU:HD21	1:B:294:TYR:CE2	2.45	0.51
1:A:110:VAL:HA	1:A:133:LEU:HD13	1.92	0.51
1:C:300:GLY:HA2	1:C:309:PHE:CZ	2.45	0.51
1:A:86:TRP:H	1:A:124:ASN:ND2	2.08	0.51
1:A:372:CYS:CA	4:A:833:HOH:O	2.52	0.51
1:A:273:TRP:H	2:A:501:ZGB:H3	1.75	0.51
1:B:166:TRP:CZ2	1:B:232:ALA:HB2	2.45	0.51
1:B:153:ASP:OD1	1:B:153:ASP:C	2.52	0.51
1:B:258:ASN:OD1	1:B:260:LYS:HG2	2.11	0.51
1:B:324:TYR:CE2	1:B:329:TYR:HB3	2.46	0.51
1:A:73:THR:HB	1:A:74:PRO:HD2	1.93	0.51
1:B:181:ILE:HG22	1:B:185:LYS:HE3	1.93	0.51
1:C:276:ASN:OD1	1:C:278:MET:HG3	2.11	0.50
1:B:106:CYS:HB2	1:B:158:GLY:O	2.12	0.50
1:B:165:LEU:CD2	1:B:166:TRP:CZ3	2.94	0.50
1:C:311:PRO:O	1:C:313:LYS:N	2.45	0.50
1:C:359:GLN:NE2	1:C:376:TYR:OH	2.43	0.50
1:A:223:GLY:O	1:A:225:PRO:HD3	2.11	0.50
1:B:221:GLY:O	1:B:258:ASN:HB3	2.12	0.50
1:C:311:PRO:C	1:C:313:LYS:N	2.70	0.50
1:B:214:ASP:OD1	1:B:215:GLY:N	2.45	0.50
1:C:281:LYS:CE	4:C:791:HOH:O	2.42	0.50
1:A:159:CYS:CB	4:A:887:HOH:O	1.94	0.49
1:B:314:GLY:O	1:B:315:PHE:C	2.53	0.49
1:A:73:THR:HB	1:A:74:PRO:CD	2.42	0.49
1:A:289:LYS:HE2	1:A:336:TYR:CE2	2.47	0.49
1:B:102:ARG:HH22	1:B:200:ASN:HD22	1.60	0.49
1:C:268:GLY:CA	1:C:278:MET:HE1	2.31	0.49
1:A:395:THR:HG23	4:A:774:HOH:O	2.12	0.49
1:B:380:ASN:O	1:B:388:GLY:HA3	2.13	0.49
1:B:265:TYR:CE2	1:B:267:TRP:HB2	2.47	0.49
1:C:89:MET:CG	1:C:379:TRP:HE1	2.25	0.49
1:B:263:SER:C	1:B:265:TYR:H	2.21	0.49
1:B:163:GLU:O	1:B:199:LYS:CE	2.61	0.48
1:C:319:LEU:HB2	1:C:320:PRO:HD3	1.95	0.48
1:B:163:GLU:O	1:B:199:LYS:HE3	2.12	0.48
1:C:141:LYS:NZ	1:C:145:ASP:OD1	2.41	0.48
1:B:155:HIS:HA	1:B:200:ASN:HB2	1.94	0.48
1:B:374:PHE:CD1	1:B:408:LEU:HD13	2.48	0.48
1:C:220:TRP:NE1	1:C:230:ASN:HB3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:LYS:CA	4:C:744:HOH:O	2.55	0.48
1:B:67:ASN:ND2	1:B:102:ARG:HG2	2.28	0.48
1:A:220:TRP:CE2	1:A:230:ASN:HB3	2.49	0.48
1:B:165:LEU:HD21	1:B:227:THR:HG23	1.96	0.48
1:A:86:TRP:N	1:A:124:ASN:HD21	2.11	0.48
1:A:357:ILE:CD1	1:A:357:ILE:H	2.26	0.47
2:A:501:ZGB:C1	4:A:748:HOH:O	2.62	0.47
1:B:71:PHE:CE2	1:B:78:VAL:HG13	2.49	0.47
1:A:86:TRP:H	1:A:124:ASN:HD21	1.61	0.47
1:A:155:HIS:HA	1:A:200:ASN:CB	2.44	0.47
1:B:313:LYS:HB2	1:B:313:LYS:HE3	1.52	0.47
1:C:406:LYS:CA	1:C:409:MET:HE2	2.35	0.47
1:B:320:PRO:O	1:B:324:TYR:N	2.41	0.47
1:B:350:GLY:HA2	4:B:709:HOH:O	2.14	0.47
3:B:502:PO4:P	1:C:88:ASP:OD2	2.72	0.47
1:C:143:ALA:HB1	1:C:148:ILE:HB	1.96	0.47
1:A:357:ILE:H	1:A:357:ILE:HD13	1.79	0.47
1:B:228:ASP:CG	1:B:231:LEU:HD13	2.34	0.47
1:B:228:ASP:CB	1:B:231:LEU:HD12	2.44	0.47
1:A:306:GLN:HE22	2:A:501:ZGB:C11	2.27	0.47
1:B:313:LYS:O	1:B:313:LYS:HG3	2.13	0.47
1:B:391:GLN:NE2	1:B:396:THR:CG2	2.77	0.47
1:B:174:GLU:HG2	4:B:681:HOH:O	2.14	0.47
1:B:209:PRO:CA	1:B:212:TYR:CD2	2.95	0.47
1:B:44:ARG:HB2	1:B:49:TYR:CD2	2.49	0.47
1:B:127:LEU:O	1:B:128:ARG:C	2.58	0.47
1:B:142:LYS:HB2	1:B:142:LYS:HE2	1.60	0.47
1:B:242:LYS:C	1:B:242:LYS:CD	2.78	0.47
1:B:266:LYS:NZ	4:B:629:HOH:O	2.47	0.47
1:B:316:PRO:HB2	1:B:319:LEU:HD12	1.97	0.47
1:A:410:ASP:CB	4:A:811:HOH:O	2.54	0.47
1:B:316:PRO:C	1:B:318:ASN:H	2.22	0.47
1:A:115:GLN:NE2	4:A:814:HOH:O	2.46	0.47
1:B:219:THR:O	1:B:228:ASP:HA	2.15	0.47
1:B:298:VAL:HG22	4:B:605:HOH:O	2.15	0.47
1:A:117:ILE:HD13	1:A:117:ILE:N	2.28	0.46
1:A:201:GLU:HB3	1:A:273:TRP:HB3	1.97	0.46
1:A:333:GLU:O	2:C:501:ZGB:H10	2.15	0.46
1:C:110:VAL:HA	1:C:133:LEU:HD13	1.98	0.46
1:B:157:ILE:HG23	1:B:171:PHE:CD2	2.49	0.46
1:B:276:ASN:C	1:B:276:ASN:OD1	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:GLU:HA	4:C:680:HOH:O	2.15	0.46
1:A:302:ASP:HB3	1:A:385:ASP:O	2.16	0.46
1:B:292:LEU:HD23	1:B:294:TYR:CE2	2.51	0.46
1:B:177:ILE:CG2	1:B:181:ILE:CD1	2.86	0.46
1:A:66:VAL:HG13	1:A:98:PHE:CD1	2.51	0.46
1:C:315:PHE:CD1	1:C:316:PRO:HA	2.50	0.46
1:B:220:TRP:CD1	1:B:230:ASN:CB	2.87	0.46
1:B:270:ASN:ND2	1:B:307:PRO:HD3	2.27	0.46
1:C:86:TRP:N	1:C:124:ASN:HD21	2.13	0.46
1:B:91:LEU:HD23	1:B:146:LEU:HD21	1.98	0.46
1:B:44:ARG:HB2	1:B:49:TYR:CE2	2.51	0.46
1:B:34:GLN:CD	1:B:40:TYR:CE1	2.94	0.46
1:B:260:LYS:CE	4:B:660:HOH:O	2.51	0.46
1:A:133:LEU:O	1:A:137:GLU:HG3	2.15	0.46
1:A:155:HIS:HA	1:A:200:ASN:HB2	1.98	0.46
1:B:86:TRP:H	1:B:124:ASN:ND2	2.14	0.45
1:C:262:ASP:O	1:C:268:GLY:HA3	2.17	0.45
1:A:260:LYS:HB2	4:A:809:HOH:O	2.16	0.45
1:B:200:ASN:ND2	1:B:201:GLU:HG3	2.32	0.45
1:B:283:TYR:HA	1:B:284:PRO:HD2	1.67	0.45
1:A:153:ASP:HA	1:A:197:ASP:HB3	1.98	0.45
1:A:299:TYR:CD1	1:A:303:VAL:HG21	2.52	0.45
1:B:116:PRO:O	1:B:117:ILE:HD13	2.16	0.45
1:B:185:LYS:CG	1:B:243:VAL:HG21	2.47	0.45
1:A:409:MET:O	1:A:410:ASP:CG	2.59	0.45
1:C:366:MET:HE2	1:C:408:LEU:HD11	1.99	0.45
1:C:329:TYR:C	1:C:329:TYR:CD2	2.94	0.45
1:A:368:GLU:HG3	4:A:737:HOH:O	2.15	0.45
1:B:266:LYS:HD3	1:B:267:TRP:CD1	2.52	0.45
1:C:349:HIS:ND1	1:C:398:TRP:CZ3	2.85	0.45
1:A:44:ARG:NH2	1:A:58:GLU:OE2	2.43	0.45
1:B:163:GLU:O	1:B:199:LYS:NZ	2.48	0.45
1:B:128:ARG:HE	1:B:128:ARG:HB2	1.39	0.44
1:B:324:TYR:OH	1:B:333:GLU:HB2	2.17	0.44
1:B:310:GLY:HA3	4:B:675:HOH:O	2.17	0.44
2:A:503:ZGB:O1	4:A:817:HOH:O	2.20	0.44
1:B:41:TYR:CZ	1:B:194:ILE:HG22	2.52	0.44
1:B:320:PRO:CD	1:B:361:LYS:HE3	2.48	0.44
1:C:55:SER:OG	1:C:57:GLU:HG3	2.16	0.44
1:B:67:ASN:HD21	1:B:102:ARG:CD	2.30	0.44
1:B:352:ASP:OD1	1:B:353:PRO:HD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ILE:HD12	1:B:50:MET:HE3	1.99	0.44
1:B:277:LEU:O	1:B:280:VAL:HG23	2.18	0.44
1:B:316:PRO:CA	1:B:319:LEU:HD12	2.47	0.44
1:C:50:MET:HE1	1:C:61:ILE:HG21	1.96	0.44
1:C:73:THR:HB	1:C:74:PRO:CD	2.48	0.44
1:C:240:ILE:C	1:C:242:LYS:H	2.26	0.44
1:C:316:PRO:O	1:C:319:LEU:HG	2.18	0.44
1:B:155:HIS:HA	1:B:200:ASN:CB	2.47	0.44
1:B:363:VAL:HG13	1:B:408:LEU:HG	1.99	0.43
1:B:172:SER:O	1:B:173:GLU:C	2.61	0.43
1:B:228:ASP:CB	1:B:231:LEU:HB2	2.42	0.43
1:C:34:GLN:O	1:C:40:TYR:HD1	2.01	0.43
1:C:57:GLU:HG2	4:C:698:HOH:O	2.18	0.43
1:B:268:GLY:CA	1:B:278:MET:HE1	2.48	0.43
1:C:36:PRO:CD	1:C:246:HIS:CE1	3.01	0.43
1:A:391:GLN:HG2	1:A:398:TRP:CE2	2.53	0.43
1:B:207:SER:HB3	1:B:208:PRO:HD2	2.00	0.43
1:B:208:PRO:HB3	1:B:212:TYR:CE2	2.52	0.43
1:B:277:LEU:C	1:B:279:ALA:N	2.74	0.43
1:B:65:GLY:HA2	1:B:100:ALA:O	2.19	0.43
1:B:301:PRO:HB2	1:B:352:ASP:OD2	2.18	0.43
1:C:200:ASN:HD21	1:C:297:HIS:HE1	1.66	0.43
1:B:262:ASP:HB3	1:B:269:TYR:CE1	2.54	0.43
1:A:306:GLN:HE22	2:A:501:ZGB:C10	2.30	0.43
1:B:277:LEU:C	1:B:279:ALA:H	2.26	0.43
1:B:391:GLN:NE2	1:B:396:THR:HG21	2.33	0.43
1:C:377:TRP:HA	1:C:378:SER:HA	1.87	0.43
1:A:207:SER:HB3	1:A:208:PRO:HD2	2.01	0.43
1:C:268:GLY:HA2	1:C:278:MET:CE	2.32	0.43
1:C:50:MET:SD	2:C:501:ZGB:H9A	2.59	0.42
1:B:189:LYS:CE	4:B:745:HOH:O	2.62	0.42
1:A:102:ARG:NH2	1:A:200:ASN:HD22	2.12	0.42
1:B:308:TYR:HA	1:B:313:LYS:HD2	2.02	0.42
1:B:324:TYR:CZ	1:B:329:TYR:HB3	2.54	0.42
1:A:44:ARG:HH21	1:A:58:GLU:CD	2.27	0.42
1:C:201:GLU:HB3	1:C:273:TRP:HB3	2.02	0.42
1:C:319:LEU:HB3	1:C:323:TRP:CZ2	2.54	0.42
1:A:178:ASN:O	1:A:182:GLU:HG3	2.19	0.42
1:B:385:ASP:OD2	1:B:386:THR:HG23	2.19	0.42
1:C:289:LYS:HE3	4:C:820:HOH:O	2.19	0.42
1:A:46:ASP:OD2	1:C:57:GLU:OE2	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:VAL:HG13	1:A:98:PHE:CE1	2.54	0.42
1:A:89:MET:HE1	1:A:394:TRP:HE3	1.85	0.42
1:B:67:ASN:ND2	1:B:102:ARG:CG	2.83	0.42
1:B:198:LEU:N	4:B:672:HOH:O	2.52	0.42
1:C:199:LYS:HE3	1:C:202:PRO:HA	2.02	0.42
1:B:321:ASP:OD2	1:B:325:HIS:ND1	2.52	0.41
1:C:319:LEU:O	1:C:320:PRO:C	2.62	0.41
1:C:34:GLN:NE2	4:C:622:HOH:O	2.33	0.41
1:B:67:ASN:HD21	1:B:102:ARG:CG	2.33	0.41
1:B:214:ASP:OD1	1:B:214:ASP:C	2.63	0.41
1:C:83:LYS:O	1:C:123:LYS:HE3	2.20	0.41
1:B:322:ILE:O	1:B:326:HIS:N	2.38	0.41
1:A:253:GLY:O	1:A:274:GLY:HA2	2.20	0.41
1:B:121:TYR:CD1	1:B:128:ARG:HG3	2.56	0.41
1:B:220:TRP:HD1	1:B:230:ASN:OD1	1.95	0.41
1:C:361:LYS:O	1:C:364:ASP:HB2	2.20	0.41
1:B:223:GLY:CA	4:B:655:HOH:O	2.64	0.41
1:C:131:ASP:OD1	1:C:131:ASP:C	2.63	0.41
1:C:50:MET:HE3	2:C:501:ZGB:H9A	2.01	0.41
1:A:116:PRO:O	1:A:117:ILE:CD1	2.69	0.41
1:A:281:LYS:HE3	4:C:664:HOH:O	2.21	0.41
1:A:380:ASN:HB3	1:A:382:ASP:OD1	2.21	0.41
1:B:62:HIS:HD2	1:B:372:CYS:CB	2.34	0.41
1:B:155:HIS:CE1	1:B:200:ASN:CG	2.99	0.41
1:C:235:ARG:HD3	4:C:683:HOH:O	2.21	0.41
1:C:333:GLU:HG2	1:C:334:LEU:HG	2.02	0.41
1:C:224:ASN:HA	1:C:225:PRO:HD2	1.83	0.41
1:A:77:VAL:O	1:A:78:VAL:C	2.64	0.40
1:C:305:ASN:OD1	1:C:354:ARG:NH2	2.49	0.40
1:A:86:TRP:CD1	1:A:127:LEU:HD11	2.56	0.40
1:B:320:PRO:CG	1:B:361:LYS:HE3	2.51	0.40
1:C:265:TYR:CE2	1:C:267:TRP:HB2	2.56	0.40
1:C:323:TRP:CH2	1:C:362:LEU:HA	2.56	0.40
1:A:116:PRO:O	1:A:117:ILE:HD13	2.20	0.40
1:C:402:TYR:OH	1:C:406:LYS:HD2	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:ASN:ND2	2:A:503:ZGB:C1[4_546]	1.19	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:ASN:ND2	2:A:503:ZGB:C2[4_546]	1.96	0.24

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	375/377 (100%)	364 (97%)	11 (3%)	0	100	100
1	B	375/377 (100%)	341 (91%)	32 (8%)	2 (0%)	24	16
1	C	375/377 (100%)	358 (96%)	16 (4%)	1 (0%)	36	29
All	All	1125/1131 (100%)	1063 (94%)	59 (5%)	3 (0%)	36	29

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	264	SER
1	B	308	TYR
1	C	312	ALA

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	324/324 (100%)	315 (97%)	9 (3%)	38	32
1	B	324/324 (100%)	305 (94%)	19 (6%)	18	10
1	C	324/324 (100%)	311 (96%)	13 (4%)	28	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	972/972 (100%)	931 (96%)	41 (4%)	26	19

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	THR
1	A	54	THR
1	A	78	VAL
1	A	83	LYS
1	A	117	ILE
1	A	153	ASP
1	A	169	GLU
1	A	289	LYS
1	A	357	ILE
1	B	34	GLN
1	B	35	THR
1	B	57	GLU
1	B	122	SER
1	B	141	LYS
1	B	142	LYS
1	B	170	ASP
1	B	205	VAL
1	B	213	THR
1	B	227	THR
1	B	231	LEU
1	B	242	LYS
1	B	243	VAL
1	B	266	LYS
1	B	276	ASN
1	B	289	LYS
1	B	315	PHE
1	B	334	LEU
1	B	380	ASN
1	C	47	THR
1	C	51	ILE
1	C	57	GLU
1	C	58	GLU
1	C	122	SER
1	C	153	ASP
1	C	169	GLU
1	C	180	TRP
1	C	242	LYS

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Mol	Chain	Res	Type
1	C	266	LYS
1	C	313	LYS
1	C	340	ILE
1	C	408	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	67	ASN
1	A	124	ASN
1	A	200	ASN
1	A	270	ASN
1	A	306	GLN
1	A	359	GLN
1	A	403	ASN
1	B	62	HIS
1	B	67	ASN
1	B	124	ASN
1	B	161	HIS
1	B	200	ASN
1	B	230	ASN
1	B	270	ASN
1	B	359	GLN
1	C	67	ASN
1	C	124	ASN
1	C	161	HIS
1	C	200	ASN
1	C	359	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

7 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	ZGB	A	501	-	11,12,14	1.51	2 (18%)	15,15,18	2.02	6 (40%)
2	ZGB	C	501	-	12,12,14	1.60	2 (16%)	15,15,18	2.11	5 (33%)
3	PO4	B	502	-	4,4,4	0.86	0	6,6,6	0.67	0
2	ZGB	A	503	-	11,12,14	1.46	2 (18%)	15,15,18	1.88	4 (26%)
3	PO4	A	502	-	4,4,4	0.98	0	6,6,6	0.51	0
3	PO4	B	501	-	4,4,4	1.16	0	6,6,6	1.04	1 (16%)
3	PO4	B	503	-	4,4,4	0.86	0	6,6,6	0.58	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	ZGB	A	501	-	-	0/4/4/7	0/1/1/1
2	ZGB	A	503	-	-	4/4/4/7	0/1/1/1
2	ZGB	C	501	-	-	2/4/4/7	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	ZGB	C9-C10	-3.66	1.34	1.52
2	C	501	ZGB	C10-C9	-3.64	1.35	1.52
2	A	503	ZGB	C9-C10	-3.51	1.35	1.52
2	C	501	ZGB	O3-C11	-3.29	1.25	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	503	ZGB	C3-C2	2.63	1.43	1.39
2	A	501	ZGB	C7-C8	2.08	1.43	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	ZGB	C10-C9-C8	4.68	131.12	113.67
2	C	501	ZGB	C9-C10-C11	4.01	134.83	113.45
2	A	503	ZGB	C1-C2-C4	-3.65	116.94	120.69
2	A	501	ZGB	C7-C6-C4	-3.32	117.18	120.50
2	A	501	ZGB	C1-C2-C4	3.20	123.98	120.69
2	A	503	ZGB	C3-C2-C4	3.18	120.98	117.64
2	A	503	ZGB	C10-C9-C8	3.02	120.51	113.21
2	A	501	ZGB	C9-C8-C3	-2.97	115.55	120.54
2	A	501	ZGB	C3-C2-C4	2.86	120.64	117.64
2	C	501	ZGB	C2-C3-C8	-2.78	119.09	122.22
2	A	501	ZGB	C9-C10-C11	2.69	125.30	112.03
2	A	503	ZGB	C2-C3-C8	-2.63	119.25	122.22
2	C	501	ZGB	C3-C2-C4	2.47	120.24	117.64
2	A	501	ZGB	C1-C2-C3	-2.42	115.30	119.57
2	C	501	ZGB	O1-C4-C2	2.36	122.14	117.60
3	B	501	PO4	O4-P-O2	2.07	114.35	107.91

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	503	ZGB	C11-C10-C9-C8
2	A	503	ZGB	C9-C10-C11-O2
2	C	501	ZGB	C11-C10-C9-C8
2	A	503	ZGB	C3-C8-C9-C10
2	A	503	ZGB	C7-C8-C9-C10
2	C	501	ZGB	C3-C8-C9-C10

There are no ring outliers.

5 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	ZGB	9	0
2	C	501	ZGB	8	0
3	B	502	PO4	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	503	ZGB	3	2
3	A	502	PO4	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

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	377/377 (100%)	-0.16	11 (2%) 53 57	3, 16, 31, 40	8 (2%)
1	B	377/377 (100%)	1.61	128 (33%) 1 1	10, 34, 56, 64	10 (2%)
1	C	377/377 (100%)	0.44	21 (5%) 30 32	5, 26, 42, 54	9 (2%)
All	All	1131/1131 (100%)	0.63	160 (14%) 6 6	3, 25, 48, 64	27 (2%)

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	312	ALA	10.3
1	B	310	GLY	9.8
1	C	311	PRO	9.5
1	C	310	GLY	8.0
1	B	311	PRO	7.6
1	B	312	ALA	6.7
1	B	161	HIS	6.7
1	A	311	PRO	6.6
1	A	312	ALA	6.5
1	A	310	GLY	6.2
1	B	34	GLN	5.5
1	B	218	ALA	5.1
1	B	226	ALA	5.0
1	A	34	GLN	5.0
1	B	286	ASN	4.9
1	B	234	GLU	4.8
1	C	286	ASN	4.8
1	B	182	GLU	4.8
1	C	161	HIS	4.8
1	B	271	ALA	4.7
1	B	368	GLU	4.7
1	B	265	TYR	4.6
1	B	283	TYR	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	267	TRP	4.6
1	A	159	CYS	4.3
1	C	136	MET	4.2
1	B	213	THR	4.2
1	B	273	TRP	4.1
1	A	136	MET	4.1
1	B	212	TYR	4.1
1	B	314	GLY	4.0
1	C	182	GLU	4.0
1	B	268	GLY	4.0
1	B	220	TRP	3.8
1	B	166	TRP	3.8
1	B	275	GLY	3.7
1	B	225	PRO	3.7
1	B	229	TRP	3.7
1	A	286	ASN	3.7
1	B	176	PHE	3.7
1	B	211	ALA	3.6
1	B	259	PRO	3.6
1	C	368	GLU	3.6
1	B	136	MET	3.6
1	B	280	VAL	3.5
1	C	234	GLU	3.4
1	B	293	VAL	3.4
1	B	274	GLY	3.4
1	B	223	GLY	3.4
1	B	263	SER	3.4
1	B	304	TYR	3.3
1	B	159	CYS	3.3
1	B	244	ALA	3.2
1	B	279	ALA	3.2
1	B	202	PRO	3.2
1	B	278	MET	3.2
1	B	221	GLY	3.2
1	B	257	THR	3.1
1	B	284	PRO	3.1
1	B	308	TYR	3.1
1	B	165	LEU	3.1
1	B	208	PRO	3.1
1	B	210	ALA	3.1
1	B	231	LEU	3.0
1	B	40	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	269	TYR	3.0
1	C	58	GLU	3.0
1	B	309	PHE	3.0
1	B	254	THR	3.0
1	B	251	VAL	3.0
1	B	329	TYR	3.0
1	B	209	PRO	2.9
1	B	334	LEU	2.9
1	C	53	VAL	2.9
1	A	234	GLU	2.9
1	A	368	GLU	2.9
1	B	180	TRP	2.9
1	B	287	LEU	2.9
1	B	167	TYR	2.9
1	A	410	ASP	2.9
1	B	204	SER	2.9
1	B	236	ILE	2.9
1	B	227	THR	2.8
1	B	294	TYR	2.8
1	B	232	ALA	2.8
1	B	276	ASN	2.8
1	B	322	ILE	2.8
1	B	336	TYR	2.8
1	B	168	THR	2.8
1	B	261	THR	2.8
1	B	239	ALA	2.8
1	B	256	PHE	2.8
1	B	219	THR	2.7
1	B	282	ASP	2.7
1	B	241	LEU	2.7
1	B	264	SER	2.7
1	B	187	PHE	2.7
1	B	277	LEU	2.7
1	B	260	LYS	2.6
1	B	295	SER	2.6
1	B	224	ASN	2.6
1	C	54	THR	2.5
1	B	215	GLY	2.5
1	B	38	GLY	2.5
1	B	351	GLY	2.5
1	B	177	ILE	2.5
1	B	247	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	205	VAL	2.5
1	B	298	VAL	2.5
1	B	303	VAL	2.5
1	B	306	GLN	2.4
1	B	43	VAL	2.4
1	B	245	PRO	2.4
1	B	285	VAL	2.4
1	B	335	GLY	2.4
1	C	269	TYR	2.4
1	B	171	PHE	2.4
1	B	230	ASN	2.4
1	B	45	GLY	2.4
1	B	253	GLY	2.4
1	B	313	LYS	2.4
1	C	408	LEU	2.4
1	B	39	ILE	2.4
1	B	157	ILE	2.4
1	B	217	GLY	2.4
1	B	315	PHE	2.3
1	C	263	SER	2.3
1	B	328	GLY	2.3
1	B	258	ASN	2.3
1	B	74	PRO	2.2
1	C	308	TYR	2.2
1	B	181	ILE	2.2
1	B	339	VAL	2.2
1	B	356	VAL	2.2
1	C	34	GLN	2.2
1	B	250	PHE	2.2
1	B	107	THR	2.2
1	B	288	PRO	2.2
1	B	307	PRO	2.2
1	B	233	ALA	2.2
1	C	315	PHE	2.2
1	C	267	TRP	2.2
1	B	35	THR	2.2
1	B	206	THR	2.2
1	B	222	MET	2.1
1	B	198	LEU	2.1
1	B	332	LEU	2.1
1	B	262	ASP	2.1
1	B	237	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	384	GLY	2.1
1	B	164	PRO	2.1
1	A	128	ARG	2.1
1	B	330	VAL	2.1
1	B	228	ASP	2.1
1	B	246	HIS	2.0
1	C	316	PRO	2.0
1	C	353	PRO	2.0
1	B	249	ILE	2.0
1	B	154	TYR	2.0
1	B	44	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PO4	A	502	5/5	0.70	0.20	69,72,72,72	0
2	ZGB	C	501	12/14	0.79	0.18	34,39,41,45	0
3	PO4	B	503	5/5	0.80	0.12	49,49,51,53	0
2	ZGB	A	501	12/14	0.81	0.14	18,35,40,44	0
2	ZGB	A	503	12/14	0.82	0.13	35,39,41,44	0
3	PO4	B	502	5/5	0.85	0.15	43,46,51,52	0
3	PO4	B	501	5/5	0.91	0.11	30,33,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.