



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 11:51 PM UTC

PDB ID : 2ZU8 / pdb_00002zu8
Title : Crystal structure of mannosyl-3-phosphoglycerate synthase from *Pyrococcus horikoshii*
Authors : Kawamura, T.; Watanabe, N.; Tanaka, I.
Deposited on : 2008-10-14
Resolution : 2.40 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

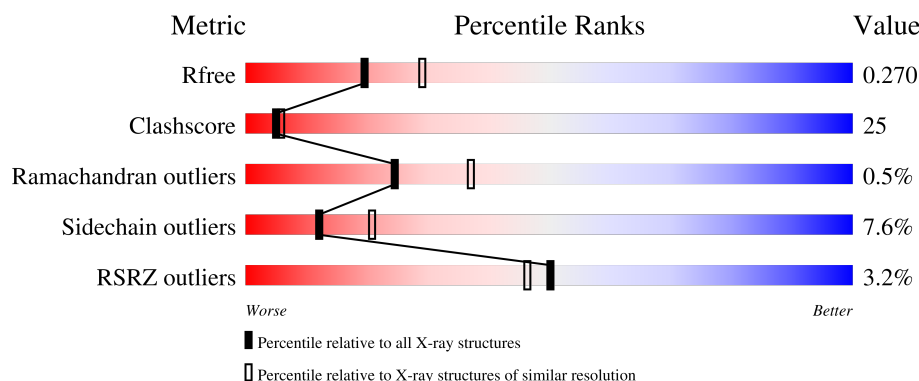
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	394	
1	B	394	

2 Entry composition [i](#)

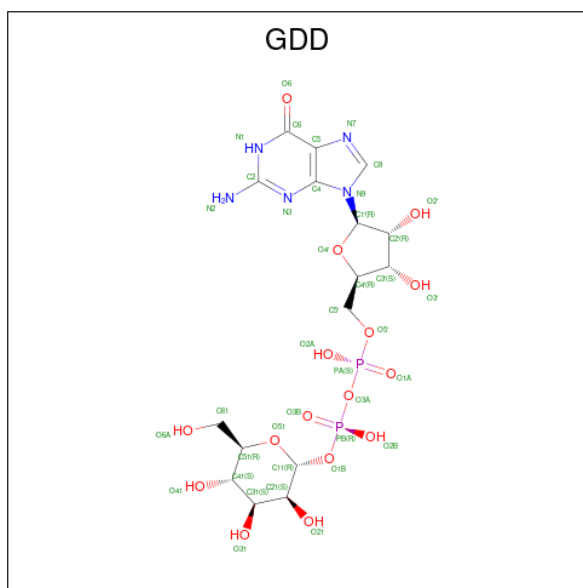
There are 2 unique types of molecules in this entry. The entry contains 6050 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Mannosyl-3-phosphoglycerate synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	Se	0	0	0
			3003	1944	496	547	1	15			
1	B	369	Total	C	N	O	S	Se	0	0	0
			2969	1916	491	546	1	15			

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE-ALPHA-D-MANNOSE (CCD ID: GDD) (formula: $C_{16}H_{25}N_5O_{16}P_2$).

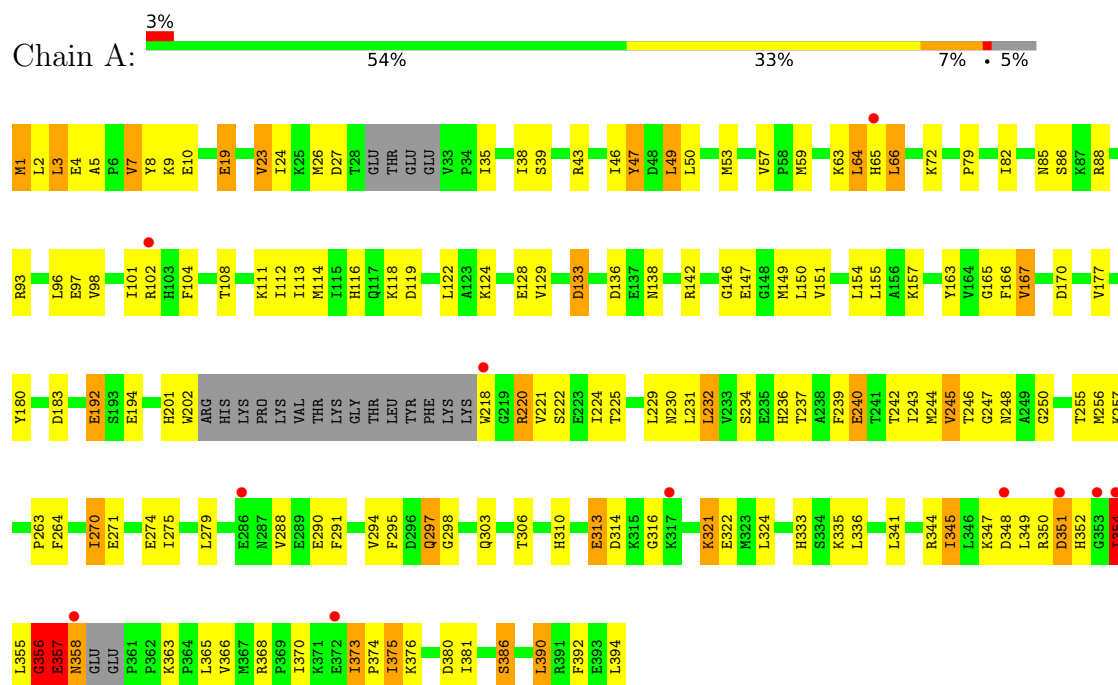


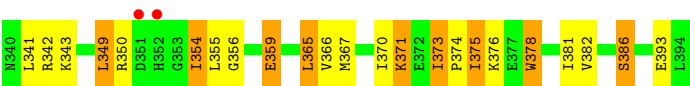
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			39	16	5	16	2		
2	B	1	Total	C	N	O	P	0	0
			39	16	5	16	2		

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: Mannosyl-3-phosphoglycerate synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.24Å 84.99Å 83.59Å 90.00° 101.91° 90.00°	Depositor
Resolution (Å)	42.72 – 2.40 42.72 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.3 (42.72-2.40) 95.4 (42.72-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.90 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.272 0.226 , 0.270	Depositor DCC
R_{free} test set	1401 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	26.9	Xtriage
Anisotropy	0.951	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 33.3	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	0.92	EDS
Total number of atoms	6050	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% 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: GDD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.73	2/3054 (0.1%)	1.26	36/4099 (0.9%)
1	B	0.64	0/3017	1.19	29/4048 (0.7%)
All	All	0.69	2/6071 (0.0%)	1.23	65/8147 (0.8%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	357	GLU	CA-C	6.11	1.60	1.52
1	A	356	GLY	N-CA	5.16	1.52	1.45

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	354	ILE	N-CA-C	12.66	122.58	110.30
1	A	26	MSE	N-CA-C	12.13	126.61	111.69
1	B	270	ILE	N-CA-C	11.59	122.44	110.62
1	A	349	LEU	N-CA-C	-10.05	101.15	113.41
1	A	316	GLY	N-CA-C	9.55	121.02	111.95
1	A	322	GLU	N-CA-C	-9.21	101.20	111.14
1	B	237	THR	N-CA-C	-8.88	97.98	110.50
1	A	355	LEU	N-CA-C	8.87	123.56	110.17
1	A	138	ASN	N-CA-C	8.40	121.87	112.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	242	THR	N-CA-C	-8.21	101.28	112.03
1	A	23	VAL	N-CA-C	-7.92	99.41	109.30
1	A	7	VAL	N-CA-C	7.26	117.36	110.53
1	B	27	ASP	N-CA-C	7.25	119.96	107.28
1	B	88	ARG	N-CA-C	7.07	120.78	112.72
1	B	4	GLU	N-CA-C	-7.05	100.56	110.50
1	A	373	ILE	N-CA-C	-6.87	94.05	108.88
1	B	386	SER	N-CA-C	6.70	119.65	108.20
1	A	88	ARG	N-CA-C	6.61	121.56	112.90
1	A	47	TYR	N-CA-C	6.52	118.47	111.36
1	A	381	ILE	N-CA-C	-6.46	103.96	111.00
1	A	255	THR	N-CA-C	-6.34	100.19	110.20
1	A	354	ILE	CB-CA-C	-6.21	104.04	111.81
1	B	74	ILE	CA-C-N	-6.15	113.43	119.76
1	B	74	ILE	C-N-CA	-6.15	113.43	119.76
1	B	342	ARG	N-CA-C	6.13	118.04	111.36
1	B	381	ILE	N-CA-C	-6.13	104.77	110.53
1	A	85	ASN	N-CA-C	-6.12	103.24	111.87
1	B	266	THR	N-CA-C	6.06	119.24	110.28
1	A	357	GLU	O-C-N	6.05	130.64	122.59
1	A	386	SER	N-CA-C	6.00	118.50	108.96
1	B	255	THR	N-CA-C	-5.94	100.31	109.76
1	A	345	ILE	N-CA-C	-5.85	104.81	110.72
1	B	112	ILE	N-CA-C	5.84	117.09	108.45
1	B	373	ILE	N-CA-C	5.83	114.66	108.95
1	A	155	LEU	N-CA-C	-5.81	105.03	111.36
1	A	9	LYS	N-CA-C	5.74	116.12	108.38
1	B	11	ILE	N-CA-C	5.70	116.20	107.77
1	A	357	GLU	CA-C-N	5.68	131.92	121.70
1	A	357	GLU	C-N-CA	5.68	131.92	121.70
1	B	49	LEU	N-CA-C	-5.64	105.12	112.23
1	A	232	LEU	N-CA-C	-5.60	105.26	111.36
1	A	264	PHE	N-CA-C	5.60	118.36	109.24
1	B	26	MSE	N-CA-C	5.55	119.67	113.01
1	B	85	ASN	N-CA-C	-5.48	104.37	111.71
1	B	79	PRO	N-CA-C	-5.47	102.61	111.19
1	B	359	GLU	N-CA-C	-5.46	100.86	109.50
1	A	356	GLY	O-C-N	5.46	129.79	122.70
1	B	317	LYS	N-CA-C	5.34	117.18	111.36
1	A	49	LEU	CD1-CG-CD2	5.32	122.50	110.80
1	A	357	GLU	CA-CB-CG	-5.27	103.57	114.10
1	A	270	ILE	N-CA-C	5.24	115.86	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	378	TRP	N-CA-C	-5.18	105.81	111.82
1	B	335	LYS	N-CA-C	-5.17	106.23	113.37
1	A	64	LEU	N-CA-C	5.16	116.90	111.28
1	A	313	GLU	N-CA-C	-5.15	102.23	109.96
1	A	146	GLY	N-CA-C	-5.12	106.58	112.83
1	A	19	GLU	N-CA-C	-5.10	103.31	110.50
1	B	236	HIS	N-CA-C	-5.09	104.70	112.04
1	B	371	LYS	N-CA-C	5.09	119.72	111.37
1	B	327	SER	N-CA-C	-5.09	105.82	112.23
1	B	119	ASP	CA-C-N	5.05	124.84	119.28
1	B	119	ASP	C-N-CA	5.05	124.84	119.28
1	A	298	GLY	N-CA-C	-5.05	106.32	112.68
1	A	358	ASN	N-CA-C	-5.02	96.95	111.00
1	B	257	LYS	N-CA-C	5.02	116.75	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	356	GLY	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3003	0	3052	144	0
1	B	2969	0	3015	164	0
2	A	39	0	23	0	0
2	B	39	0	23	3	0
All	All	6050	0	6113	303	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 25.

All (303) 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:350:ARG:HH11	1:A:357:GLU:HG3	1.14	1.12
1:B:197:MSE:HE3	1:B:199:ARG:HD2	1.27	1.12
1:B:147:GLU:HG3	1:B:367:MSE:HE1	1.23	1.10
1:B:323:MSE:HE1	2:B:395:GDD:H31	1.30	1.08
1:A:102:ARG:HH21	1:A:390:LEU:HD21	1.20	1.06
1:B:26:MSE:HE3	1:B:307:LEU:HD23	1.39	1.03
1:B:52:LYS:HD3	1:B:162:GLU:OE1	1.55	1.03
1:B:349:LEU:O	1:B:354:ILE:HG23	1.62	0.99
1:A:24:ILE:O	1:B:72:LYS:HG2	1.64	0.97
1:A:350:ARG:NH1	1:A:357:GLU:HG3	1.78	0.96
1:B:142:ARG:HH12	1:B:367:MSE:HE2	1.32	0.94
1:B:61:ASN:HD21	1:B:87:LYS:H	1.13	0.94
1:A:104:PHE:O	1:A:108:THR:HG22	1.69	0.92
1:A:221:VAL:HG22	1:A:324:LEU:HD13	1.50	0.91
1:A:350:ARG:NH1	1:A:357:GLU:HA	1.86	0.89
1:B:194:GLU:HG2	1:B:257:LYS:HD2	1.54	0.88
1:A:119:ASP:OD2	1:A:386:SER:HB2	1.74	0.88
1:A:1:MSE:HE2	1:A:3:LEU:HD11	1.55	0.85
1:B:142:ARG:NH1	1:B:367:MSE:HE2	1.93	0.83
1:A:116:HIS:HD2	1:A:118:LYS:H	1.27	0.83
1:A:245:VAL:H	1:A:303:GLN:HE22	1.22	0.83
1:B:256:MSE:HE3	1:B:256:MSE:O	1.78	0.82
1:B:171:ASN:HD22	1:B:173:ILE:H	1.28	0.81
1:A:244:MSE:HE3	1:A:247:GLY:N	1.96	0.81
1:A:232:LEU:HG	1:A:336:LEU:HD22	1.63	0.80
1:A:113:ILE:HG13	1:A:394:LEU:HD23	1.63	0.80
1:A:321:LYS:HB2	1:A:354:ILE:HD13	1.63	0.79
1:A:49:LEU:HD11	1:A:163:TYR:CE2	2.18	0.79
1:B:256:MSE:HE2	1:B:260:GLU:HB3	1.63	0.79
1:A:350:ARG:CZ	1:A:357:GLU:HA	2.13	0.78
1:B:197:MSE:CE	1:B:199:ARG:HD2	2.12	0.78
1:B:271:GLU:HG2	1:B:272:PRO:HD3	1.63	0.78
1:A:244:MSE:HE2	1:A:275:ILE:HG13	1.64	0.77
1:A:324:LEU:HD23	1:A:354:ILE:HD11	1.64	0.77
1:A:237:THR:HG22	1:A:239:PHE:HB2	1.65	0.77
1:B:321:LYS:HG2	1:B:354:ILE:HD13	1.66	0.77
1:A:1:MSE:HE3	1:A:23:VAL:HG22	1.67	0.77
1:B:105:TYR:HE1	1:B:393:GLU:OE2	1.66	0.77
1:B:323:MSE:HE1	2:B:395:GDD:C31	2.13	0.76
1:A:116:HIS:CD2	1:A:118:LYS:H	2.03	0.76
1:A:244:MSE:HE3	1:A:247:GLY:HA2	1.67	0.76
1:A:347:LYS:HE2	1:A:351:ASP:OD2	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:TYR:CE1	1:B:393:GLU:OE2	2.38	0.76
1:A:244:MSE:HE3	1:A:247:GLY:CA	2.15	0.75
1:A:86:SER:O	1:A:116:HIS:HE1	1.68	0.74
1:A:194:GLU:HB2	1:A:297:GLN:HE21	1.52	0.74
1:B:5:ALA:HA	1:B:39:SER:OG	1.88	0.73
1:B:2:LEU:HD13	1:B:28:THR:HG21	1.70	0.73
1:B:68:ASP:CG	1:B:72:LYS:HE3	2.13	0.73
1:A:220:ARG:HE	1:A:220:ARG:HA	1.54	0.72
1:B:2:LEU:HB2	1:B:25:LYS:HB3	1.70	0.72
1:A:218:TRP:CZ2	1:A:224:ILE:HD11	2.24	0.72
1:A:63:LYS:HE3	1:A:313:GLU:OE2	1.90	0.71
1:A:102:ARG:NH2	1:A:390:LEU:HD21	2.02	0.71
1:B:171:ASN:ND2	1:B:173:ILE:H	1.87	0.71
1:B:147:GLU:CG	1:B:367:MSE:HE1	2.12	0.71
1:A:1:MSE:CE	1:A:23:VAL:HG22	2.22	0.70
1:B:116:HIS:HD2	1:B:118:LYS:H	1.40	0.69
1:A:356:GLY:O	1:A:357:GLU:HB2	1.92	0.69
1:B:365:LEU:HD12	1:B:366:VAL:N	2.07	0.69
1:A:47:TYR:CE1	1:B:43:ARG:NH2	2.61	0.69
1:B:116:HIS:CD2	1:B:118:LYS:H	2.11	0.69
1:A:230:ASN:HD21	1:A:244:MSE:H	1.40	0.68
1:B:315:LYS:HB2	1:B:319:HIS:CD2	2.27	0.68
1:B:375:ILE:HG23	1:B:376:LYS:N	2.08	0.68
1:B:9:LYS:HD2	1:B:16:THR:CG2	2.25	0.67
1:B:197:MSE:HE2	1:B:301:ILE:HG12	1.77	0.67
1:B:268:TYR:HB2	1:B:326:LEU:HD11	1.77	0.67
1:B:24:ILE:HD12	1:B:38:ILE:CD1	2.25	0.66
1:A:244:MSE:CE	1:A:247:GLY:HA2	2.26	0.66
1:B:142:ARG:NH1	1:B:367:MSE:CE	2.58	0.66
1:A:234:SER:CB	1:A:240:GLU:HA	2.26	0.66
1:A:244:MSE:CE	1:A:275:ILE:HG13	2.25	0.66
1:B:235:GLU:HG2	1:B:338:THR:HG21	1.77	0.65
1:B:61:ASN:HD22	1:B:93:ARG:HG2	1.61	0.64
1:B:50:LEU:CD2	1:B:78:CYS:SG	2.84	0.64
1:B:229:LEU:HD12	1:B:247:GLY:HA3	1.78	0.64
1:B:62:GLU:HA	1:B:62:GLU:OE1	1.97	0.64
1:B:194:GLU:HB2	1:B:297:GLN:HE22	1.61	0.64
1:A:236:HIS:HE1	1:A:336:LEU:O	1.81	0.63
1:A:234:SER:HB3	1:A:240:GLU:HA	1.81	0.63
1:A:245:VAL:H	1:A:303:GLN:NE2	1.95	0.63
1:B:82:ILE:HD12	1:B:112:ILE:HD11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:LYS:CG	1:B:354:ILE:HD13	2.29	0.62
1:A:218:TRP:CH2	1:A:348:ASP:O	2.53	0.62
1:A:225:THR:OG1	1:A:248:ASN:ND2	2.32	0.62
1:B:125:ALA:O	1:B:129:VAL:HG22	2.00	0.62
1:A:66:LEU:HD23	1:A:170:ASP:HA	1.81	0.62
1:A:324:LEU:HD23	1:A:354:ILE:CD1	2.29	0.62
1:A:53:MSE:HE2	1:A:165:GLY:HA3	1.82	0.61
1:B:375:ILE:HG23	1:B:376:LYS:H	1.65	0.61
1:A:49:LEU:HD12	1:A:49:LEU:O	1.99	0.61
1:A:98:VAL:HA	1:A:114:MSE:HE1	1.82	0.61
1:B:44:GLU:O	1:B:48:ASP:HB2	1.99	0.61
1:B:289:GLU:HA	1:B:292:LYS:HZ3	1.65	0.61
1:A:218:TRP:CZ2	1:A:224:ILE:CD1	2.83	0.61
1:B:229:LEU:CD1	1:B:247:GLY:HA3	2.31	0.61
1:A:1:MSE:HE2	1:A:3:LEU:CD1	2.28	0.60
1:A:375:ILE:HG23	1:A:376:LYS:N	2.16	0.60
1:B:325:LEU:HB2	1:B:354:ILE:HD11	1.84	0.60
1:B:61:ASN:ND2	1:B:87:LYS:H	1.93	0.60
1:A:4:GLU:HG2	1:A:24:ILE:HD11	1.83	0.60
1:A:237:THR:CG2	1:A:239:PHE:HB2	2.32	0.60
1:B:50:LEU:CD2	1:B:77:LYS:HG3	2.32	0.60
1:B:26:MSE:O	1:B:26:MSE:HG2	2.02	0.60
1:B:52:LYS:CD	1:B:162:GLU:OE1	2.41	0.59
1:B:337:ALA:HA	1:B:341:LEU:HD23	1.84	0.59
1:A:1:MSE:CE	1:A:3:LEU:HD11	2.31	0.59
1:B:334:SER:C	1:B:336:LEU:H	2.09	0.59
1:A:231:LEU:HD23	1:A:341:LEU:CD1	2.33	0.59
1:B:142:ARG:HH12	1:B:367:MSE:CE	2.10	0.59
1:B:27:ASP:OD1	1:B:43:ARG:NH2	2.36	0.58
1:A:2:LEU:C	1:A:3:LEU:HD22	2.28	0.58
1:A:288:VAL:HG13	1:A:295:PHE:CD2	2.38	0.58
1:A:290:GLU:HG2	1:A:291:PHE:CD2	2.39	0.58
1:A:375:ILE:CG2	1:A:376:LYS:N	2.67	0.58
1:B:294:VAL:HG13	1:B:299:ILE:HD11	1.84	0.58
1:A:221:VAL:O	1:A:224:ILE:HG22	2.04	0.57
1:A:65:HIS:CE1	1:A:66:LEU:HD12	2.39	0.57
1:A:243:ILE:HG23	1:A:244:MSE:N	2.20	0.57
1:A:244:MSE:HE3	1:A:246:THR:C	2.30	0.57
1:A:43:ARG:NH2	1:B:47:TYR:CE2	2.73	0.57
1:A:365:LEU:HD23	1:A:366:VAL:N	2.20	0.57
1:B:68:ASP:OD2	1:B:72:LYS:HE3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:GLU:HG2	1:B:257:LYS:CD	2.29	0.56
1:B:119:ASP:CG	1:B:386:SER:OG	2.49	0.56
1:A:35:ILE:HB	1:A:38:ILE:HB	1.87	0.56
1:B:194:GLU:H	1:B:297:GLN:NE2	2.04	0.56
1:A:150:LEU:C	1:A:150:LEU:HD23	2.30	0.56
1:A:234:SER:HB2	1:A:239:PHE:O	2.05	0.55
1:A:357:GLU:O	1:A:358:ASN:OD1	2.25	0.55
1:A:245:VAL:O	1:A:245:VAL:CG1	2.54	0.55
1:B:98:VAL:HA	1:B:114:MSE:HE1	1.88	0.55
1:B:335:LYS:O	1:B:335:LYS:HG2	2.05	0.55
1:A:150:LEU:HD23	1:A:150:LEU:O	2.07	0.54
1:A:350:ARG:C	1:A:352:HIS:N	2.64	0.54
1:B:232:LEU:HD23	1:B:341:LEU:CD2	2.36	0.54
1:B:245:VAL:H	1:B:303:GLN:HE22	1.55	0.54
1:B:269:SER:HB3	1:B:326:LEU:HD13	1.90	0.54
1:B:2:LEU:C	1:B:3:LEU:HD22	2.32	0.54
1:B:82:ILE:CD1	1:B:112:ILE:HD11	2.37	0.54
1:B:328:LEU:HD23	1:B:349:LEU:HD13	1.90	0.54
1:A:250:GLY:HA2	1:A:271:GLU:OE2	2.07	0.54
1:B:50:LEU:HD21	1:B:78:CYS:SG	2.47	0.54
1:A:157:LYS:HA	1:A:256:MSE:HE3	1.89	0.54
1:B:61:ASN:HD21	1:B:87:LYS:N	1.94	0.53
1:A:116:HIS:HD2	1:A:118:LYS:N	2.02	0.53
1:B:147:GLU:HG3	1:B:367:MSE:CE	2.16	0.53
1:B:378:TRP:O	1:B:382:VAL:HG23	2.08	0.53
1:B:24:ILE:CD1	1:B:38:ILE:CD1	2.86	0.53
1:A:194:GLU:HB2	1:A:297:GLN:NE2	2.23	0.52
1:A:231:LEU:HD23	1:A:341:LEU:HD12	1.91	0.52
1:B:269:SER:N	1:B:326:LEU:HD13	2.23	0.52
1:A:72:LYS:HG2	1:B:24:ILE:O	2.10	0.52
1:A:201:HIS:ND1	1:A:245:VAL:HG13	2.25	0.52
1:B:197:MSE:HE3	1:B:199:ARG:CD	2.19	0.52
1:A:5:ALA:HA	1:A:39:SER:OG	2.10	0.52
1:B:339:ASP:OD1	1:B:343:LYS:HE3	2.10	0.52
1:A:27:ASP:O	1:B:76:HIS:HB2	2.10	0.51
1:A:133:ASP:OD1	1:A:368:ARG:NH1	2.41	0.51
1:B:118:LYS:NZ	1:B:141:ILE:O	2.43	0.51
1:B:289:GLU:HG3	1:B:292:LYS:HZ1	1.75	0.51
1:B:50:LEU:HD22	1:B:77:LYS:HG3	1.91	0.51
1:B:197:MSE:HE2	1:B:301:ILE:CG1	2.41	0.51
1:A:46:ILE:O	1:A:50:LEU:HG	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:MSE:HE3	1:A:166:PHE:CG	2.46	0.51
1:B:235:GLU:HG2	1:B:338:THR:CG2	2.39	0.51
1:A:93:ARG:HG3	1:A:96:LEU:HD12	1.93	0.51
1:A:333:HIS:CG	1:A:363:LYS:HG2	2.45	0.51
1:B:271:GLU:HA	1:B:274:GLU:OE1	2.11	0.51
1:B:256:MSE:CE	1:B:260:GLU:HB3	2.39	0.50
1:A:237:THR:CG2	1:A:237:THR:O	2.60	0.50
1:A:234:SER:HB2	1:A:240:GLU:HA	1.94	0.50
1:B:41:ILE:N	1:B:41:ILE:HD12	2.26	0.50
1:A:8:TYR:HD2	1:A:19:GLU:HB2	1.75	0.50
1:A:237:THR:HG22	1:A:237:THR:O	2.11	0.50
1:B:123:ALA:HB2	1:B:141:ILE:HD12	1.93	0.50
1:A:57:VAL:HG22	1:A:167:VAL:HG22	1.94	0.50
1:B:323:MSE:CE	2:B:395:GDD:H31	2.22	0.50
1:A:245:VAL:O	1:A:245:VAL:HG13	2.11	0.50
1:B:108:THR:O	1:B:109:HIS:HB2	2.11	0.50
1:B:234:SER:HA	1:B:237:THR:OG1	2.12	0.49
1:A:111:LYS:C	1:A:112:ILE:HG13	2.37	0.49
1:A:394:LEU:HG	1:A:394:LEU:OXT	2.12	0.49
1:B:294:VAL:CG1	1:B:299:ILE:HD11	2.42	0.49
1:B:334:SER:C	1:B:336:LEU:N	2.70	0.49
1:A:1:MSE:HE1	1:A:183:ASP:OD1	2.12	0.49
1:A:350:ARG:O	1:A:352:HIS:N	2.45	0.49
1:B:234:SER:O	1:B:237:THR:O	2.29	0.49
1:A:350:ARG:C	1:A:352:HIS:H	2.19	0.49
1:A:183:ASP:OD2	1:A:306:THR:HG22	2.12	0.48
1:A:348:ASP:O	1:A:352:HIS:CD2	2.66	0.48
1:B:41:ILE:HG22	1:B:46:ILE:HG13	1.95	0.48
1:B:45:LYS:O	1:B:48:ASP:HB3	2.13	0.48
1:B:271:GLU:N	1:B:272:PRO:CD	2.76	0.48
1:A:53:MSE:HE2	1:A:165:GLY:CA	2.44	0.48
1:A:97:GLU:O	1:A:101:ILE:HG12	2.12	0.48
1:A:221:VAL:C	1:A:224:ILE:HG22	2.39	0.48
1:A:290:GLU:HG2	1:A:291:PHE:CE2	2.49	0.48
1:B:269:SER:O	1:B:272:PRO:HD2	2.14	0.48
1:A:221:VAL:HA	1:A:224:ILE:HG22	1.95	0.48
1:B:197:MSE:CE	1:B:301:ILE:HG23	2.44	0.48
1:B:375:ILE:CG2	1:B:376:LYS:N	2.77	0.48
1:A:59:MSE:HE3	1:A:82:ILE:HG23	1.96	0.47
1:B:350:ARG:HG2	1:B:356:GLY:O	2.14	0.47
1:B:373:ILE:HA	1:B:374:PRO:HD3	1.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:LEU:HD23	1:B:78:CYS:SG	2.54	0.47
1:B:231:LEU:HD23	1:B:341:LEU:CD1	2.45	0.47
1:B:260:GLU:O	1:B:371:LYS:HB2	2.13	0.47
1:A:129:VAL:HG13	1:A:374:PRO:HD2	1.97	0.47
1:B:281:ARG:NH1	1:B:287:ASN:HB3	2.30	0.47
1:A:270:ILE:O	1:A:274:GLU:HG3	2.14	0.47
1:A:201:HIS:CE1	1:A:245:VAL:HG13	2.49	0.47
1:A:348:ASP:O	1:A:352:HIS:HD2	1.98	0.47
1:B:50:LEU:HD23	1:B:77:LYS:HG3	1.96	0.47
1:A:202:TRP:CG	1:A:310:HIS:HB2	2.50	0.46
1:B:370:ILE:C	1:B:370:ILE:HD12	2.40	0.46
1:A:133:ASP:OD2	1:A:133:ASP:N	2.48	0.46
1:A:270:ILE:HG23	1:A:271:GLU:N	2.30	0.46
1:B:59:MSE:O	1:B:84:SER:HA	2.16	0.46
1:B:61:ASN:ND2	1:B:93:ARG:HG2	2.28	0.46
1:B:281:ARG:HH12	1:B:287:ASN:HB3	1.79	0.46
1:B:26:MSE:HE3	1:B:307:LEU:CD2	2.26	0.46
1:B:124:LYS:O	1:B:128:GLU:HG2	2.14	0.46
1:B:89:GLU:OE1	1:B:89:GLU:C	2.59	0.46
1:B:256:MSE:O	1:B:256:MSE:CE	2.55	0.46
1:B:8:TYR:O	1:B:9:LYS:HB3	2.16	0.46
1:B:27:ASP:OD1	1:B:27:ASP:C	2.58	0.46
1:B:50:LEU:HD21	1:B:75:PRO:HG2	1.98	0.46
1:B:171:ASN:HD22	1:B:172:TYR:N	2.13	0.46
1:B:59:MSE:HE3	1:B:59:MSE:HB2	1.82	0.46
1:A:224:ILE:HD13	1:A:324:LEU:HD11	1.98	0.46
1:A:350:ARG:O	1:A:352:HIS:O	2.34	0.46
1:B:5:ALA:O	1:B:7:VAL:HG23	2.15	0.46
1:B:289:GLU:HG3	1:B:292:LYS:NZ	2.30	0.46
1:A:124:LYS:O	1:A:128:GLU:HB2	2.15	0.45
1:B:24:ILE:HD12	1:B:38:ILE:HD11	1.95	0.45
1:A:63:LYS:CE	1:A:313:GLU:OE2	2.62	0.45
1:B:349:LEU:HD12	1:B:349:LEU:HA	1.72	0.45
1:B:3:LEU:HD23	1:B:41:ILE:HD13	1.99	0.45
1:B:87:LYS:O	1:B:93:ARG:HB3	2.16	0.45
1:B:371:LYS:HD2	1:B:371:LYS:O	2.16	0.45
1:A:8:TYR:CD2	1:A:19:GLU:HB2	2.51	0.45
1:B:47:TYR:O	1:B:77:LYS:HD2	2.17	0.44
1:A:3:LEU:HD13	1:A:23:VAL:HA	2.00	0.44
1:A:220:ARG:HG3	1:A:222:SER:H	1.82	0.44
1:B:68:ASP:OD2	1:B:72:LYS:CE	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:PHE:CZ	1:A:108:THR:HG21	2.52	0.44
1:B:76:HIS:HE1	1:B:108:THR:O	2.01	0.44
1:A:53:MSE:O	1:A:79:PRO:HD2	2.16	0.44
1:A:218:TRP:HZ2	1:A:348:ASP:OD1	2.01	0.44
1:A:225:THR:O	1:A:229:LEU:HG	2.18	0.43
1:B:154:LEU:HD21	1:B:370:ILE:HB	2.00	0.43
1:B:245:VAL:H	1:B:303:GLN:NE2	2.16	0.43
1:A:234:SER:CB	1:A:239:PHE:O	2.66	0.43
1:B:105:TYR:CE1	1:B:109:HIS:HA	2.53	0.43
1:B:197:MSE:HE2	1:B:301:ILE:HG23	1.99	0.43
1:A:201:HIS:ND1	1:A:245:VAL:CG1	2.82	0.43
1:A:136:ASP:C	1:A:136:ASP:OD1	2.61	0.43
1:B:335:LYS:HB3	1:B:335:LYS:HE2	1.62	0.43
1:B:356:GLY:HA3	1:B:359:GLU:HB2	2.01	0.43
1:A:129:VAL:HG11	1:A:373:ILE:HG23	2.01	0.43
1:A:154:LEU:HD21	1:A:370:ILE:HB	2.01	0.43
1:B:3:LEU:O	1:B:38:ILE:HD12	2.19	0.43
1:A:147:GLU:OE1	1:A:147:GLU:N	2.51	0.42
1:A:192:GLU:C	1:A:192:GLU:OE1	2.62	0.42
1:B:4:GLU:HG2	1:B:24:ILE:HD11	2.00	0.42
1:A:390:LEU:HD12	1:A:392:PHE:CE2	2.54	0.42
1:A:392:PHE:C	1:A:394:LEU:N	2.75	0.42
1:B:46:ILE:C	1:B:48:ASP:H	2.28	0.42
1:A:380:ASP:C	1:A:380:ASP:OD1	2.62	0.42
1:B:113:ILE:HD11	1:B:159:ILE:HG21	2.02	0.42
1:B:350:ARG:HG3	1:B:355:LEU:HB3	2.00	0.42
1:A:129:VAL:CG1	1:A:374:PRO:HD2	2.50	0.42
1:A:218:TRP:CE2	1:A:224:ILE:HD12	2.55	0.42
1:B:354:ILE:O	1:B:354:ILE:HG13	2.20	0.42
1:A:177:VAL:HA	1:A:180:TYR:CD2	2.54	0.42
1:A:291:PHE:HB3	1:A:294:VAL:HB	2.02	0.42
1:B:3:LEU:HD22	1:B:3:LEU:N	2.35	0.42
1:B:9:LYS:HD2	1:B:16:THR:HG21	2.01	0.42
1:B:105:TYR:OH	1:B:393:GLU:OE2	2.38	0.42
1:B:243:ILE:HG23	1:B:244:MSE:N	2.35	0.42
1:B:9:LYS:HD2	1:B:16:THR:HG23	2.01	0.41
1:B:105:TYR:CZ	1:B:393:GLU:OE2	2.73	0.41
1:B:7:VAL:HG12	1:B:8:TYR:CE1	2.55	0.41
1:B:220:ARG:O	1:B:221:VAL:C	2.63	0.41
1:A:129:VAL:HG12	1:A:129:VAL:O	2.19	0.41
1:A:1:MSE:HE2	1:A:3:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ARG:HA	1:A:220:ARG:NE	2.30	0.41
1:B:20:VAL:HA	1:B:303:GLN:O	2.20	0.41
1:B:68:ASP:OD2	1:B:72:LYS:NZ	2.53	0.41
1:B:199:ARG:HH22	1:B:271:GLU:HB2	1.86	0.41
1:A:263:PRO:O	1:A:263:PRO:HG2	2.21	0.41
1:B:46:ILE:C	1:B:48:ASP:N	2.76	0.41
1:B:62:GLU:HG3	1:B:169:ALA:HB3	2.02	0.41
1:B:173:ILE:O	1:B:174:PRO:C	2.62	0.41
1:B:119:ASP:OD2	1:B:386:SER:OG	2.39	0.41
1:A:122:LEU:HD21	1:A:151:VAL:HG11	2.02	0.40
1:B:134:ILE:HA	1:B:367:MSE:HE2	2.02	0.40
1:A:142:ARG:HH11	1:A:142:ARG:HD2	1.75	0.40
1:B:197:MSE:HE2	1:B:301:ILE:CG2	2.52	0.40
1:A:122:LEU:HD12	1:A:122:LEU:HA	1.98	0.40
1:B:87:LYS:O	1:B:93:ARG:CB	2.69	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	365/394 (93%)	348 (95%)	14 (4%)	3 (1%)	16	25
1	B	363/394 (92%)	337 (93%)	25 (7%)	1 (0%)	36	50
All	All	728/788 (92%)	685 (94%)	39 (5%)	4 (0%)	24	37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	357	GLU
1	B	375	ILE
1	A	351	ASP

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Mol	Chain	Res	Type
1	A	375	ILE

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	329/334 (98%)	306 (93%)	23 (7%)	14	24
1	B	326/334 (98%)	299 (92%)	27 (8%)	10	17
All	All	655/668 (98%)	605 (92%)	50 (8%)	12	21

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	3	LEU
1	A	7	VAL
1	A	10	GLU
1	A	64	LEU
1	A	66	LEU
1	A	133	ASP
1	A	167	VAL
1	A	192	GLU
1	A	220	ARG
1	A	240	GLU
1	A	245	VAL
1	A	257	LYS
1	A	279	LEU
1	A	297	GLN
1	A	314	ASP
1	A	321	LYS
1	A	335	LYS
1	A	344	ARG
1	A	345	ILE
1	A	354	ILE
1	A	357	GLU

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Mol	Chain	Res	Type
1	A	390	LEU
1	B	3	LEU
1	B	50	LEU
1	B	64	LEU
1	B	71	LEU
1	B	72	LYS
1	B	91	PRO
1	B	96	LEU
1	B	100	LEU
1	B	102	ARG
1	B	164	VAL
1	B	171	ASN
1	B	174	PRO
1	B	194	GLU
1	B	223	GLU
1	B	232	LEU
1	B	242	THR
1	B	271	GLU
1	B	279	LEU
1	B	287	ASN
1	B	290	GLU
1	B	305	GLU
1	B	327	SER
1	B	328	LEU
1	B	339	ASP
1	B	349	LEU
1	B	354	ILE
1	B	365	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	65	HIS
1	A	116	HIS
1	A	138	ASN
1	A	230	ASN
1	A	236	HIS
1	A	248	ASN
1	A	287	ASN
1	A	297	GLN
1	A	303	GLN

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Mol	Chain	Res	Type
1	A	352	HIS
1	B	21	GLN
1	B	40	ASN
1	B	61	ASN
1	B	76	HIS
1	B	116	HIS
1	B	171	ASN
1	B	252	HIS
1	B	297	GLN
1	B	303	GLN
1	B	319	HIS
1	B	333	HIS
1	B	340	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	GDD	B	395	-	41,42,42	0.95	1 (2%)	62,65,65	1.44	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GDD	A	395	-	41,42,42	0.88	1 (2%)	62,65,65	1.65	12 (19%)

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	GDD	B	395	-	-	4/23/59/59	0/4/4/4
2	GDD	A	395	-	-	5/23/59/59	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	395	GDD	C5-N7	-2.80	1.33	1.39
2	B	395	GDD	C5-N7	-2.79	1.33	1.39

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	395	GDD	C2-N3-C4	5.57	121.89	112.30
2	B	395	GDD	C2-N3-C4	5.17	121.20	112.30
2	B	395	GDD	C5-C4-N3	-4.69	120.93	128.39
2	A	395	GDD	C5-C4-N3	-4.68	120.94	128.39
2	A	395	GDD	O3A-PA-O1A	-4.06	98.49	110.70
2	B	395	GDD	C2-N1-C6	-3.34	119.05	125.11
2	A	395	GDD	O2A-PA-O3A	-3.17	98.71	107.27
2	B	395	GDD	N9-C4-N3	3.16	132.28	125.95
2	A	395	GDD	N9-C4-N3	3.15	132.25	125.95
2	A	395	GDD	C2-N1-C6	-3.15	119.40	125.11
2	A	395	GDD	O2A-PA-O1A	2.60	124.53	112.44
2	B	395	GDD	O6-C6-C5	-2.35	120.32	126.53
2	B	395	GDD	C5-C6-N1	2.22	118.91	113.25
2	A	395	GDD	C8-N7-C5	2.21	108.19	104.26
2	A	395	GDD	O2A-PA-O5'	2.19	117.50	107.57
2	A	395	GDD	C4-C5-N7	-2.15	107.26	110.67
2	B	395	GDD	C4-C5-N7	-2.11	107.33	110.67
2	B	395	GDD	C8-N7-C5	2.07	107.95	104.26
2	A	395	GDD	C5-C6-N1	2.06	118.50	113.25
2	A	395	GDD	O4'-C1'-N9	2.03	112.95	108.36

There are no chirality outliers.

All (9) torsion outliers are listed below:

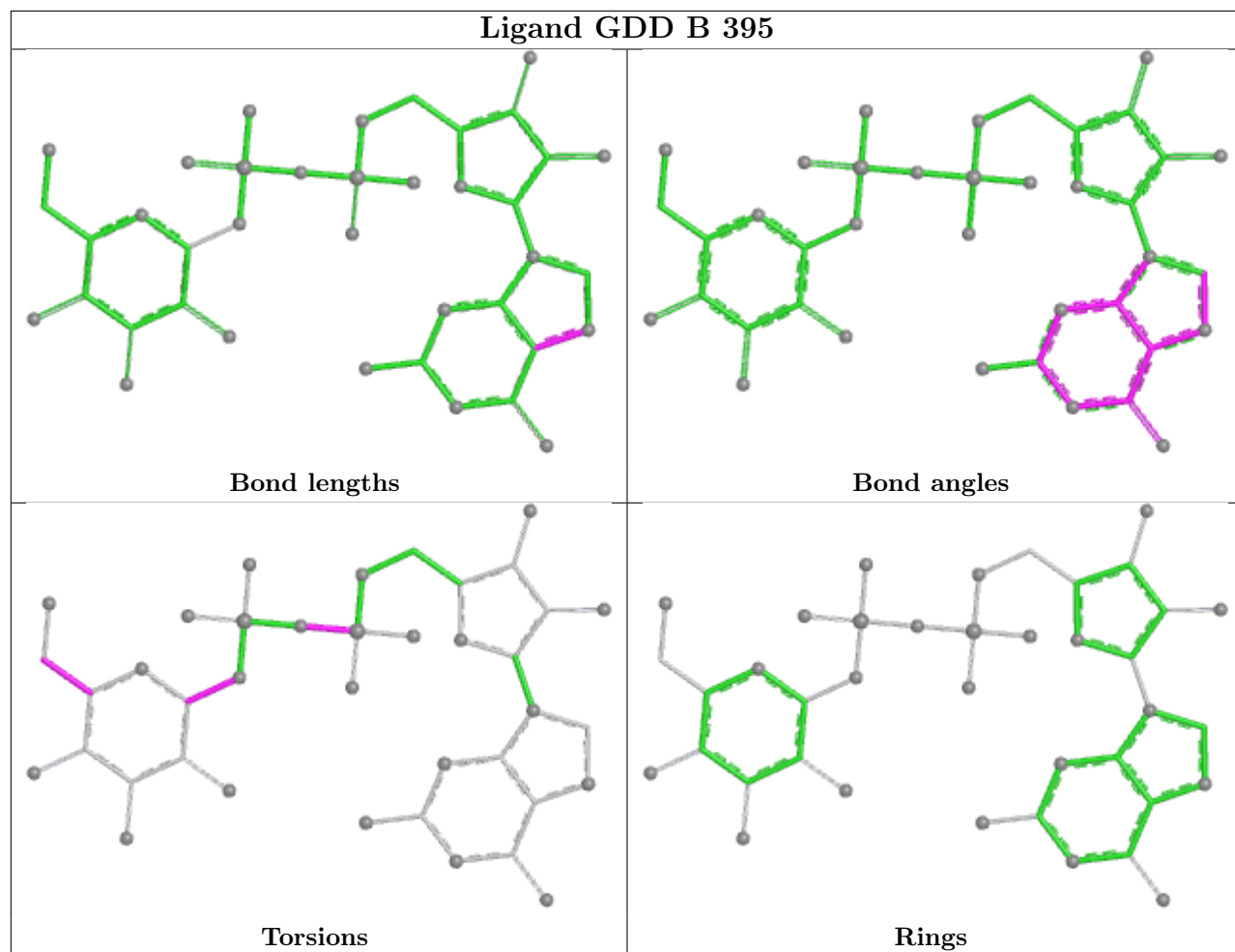
Mol	Chain	Res	Type	Atoms
2	A	395	GDD	O4'-C4'-C5'-O5'
2	A	395	GDD	C5'-O5'-PA-O2A
2	B	395	GDD	O51-C11-O1B-PB
2	A	395	GDD	C3'-C4'-C5'-O5'
2	A	395	GDD	O51-C51-C61-O6A
2	B	395	GDD	O51-C51-C61-O6A
2	B	395	GDD	PB-O3A-PA-O2A
2	A	395	GDD	O51-C11-O1B-PB
2	B	395	GDD	PB-O3A-PA-O1A

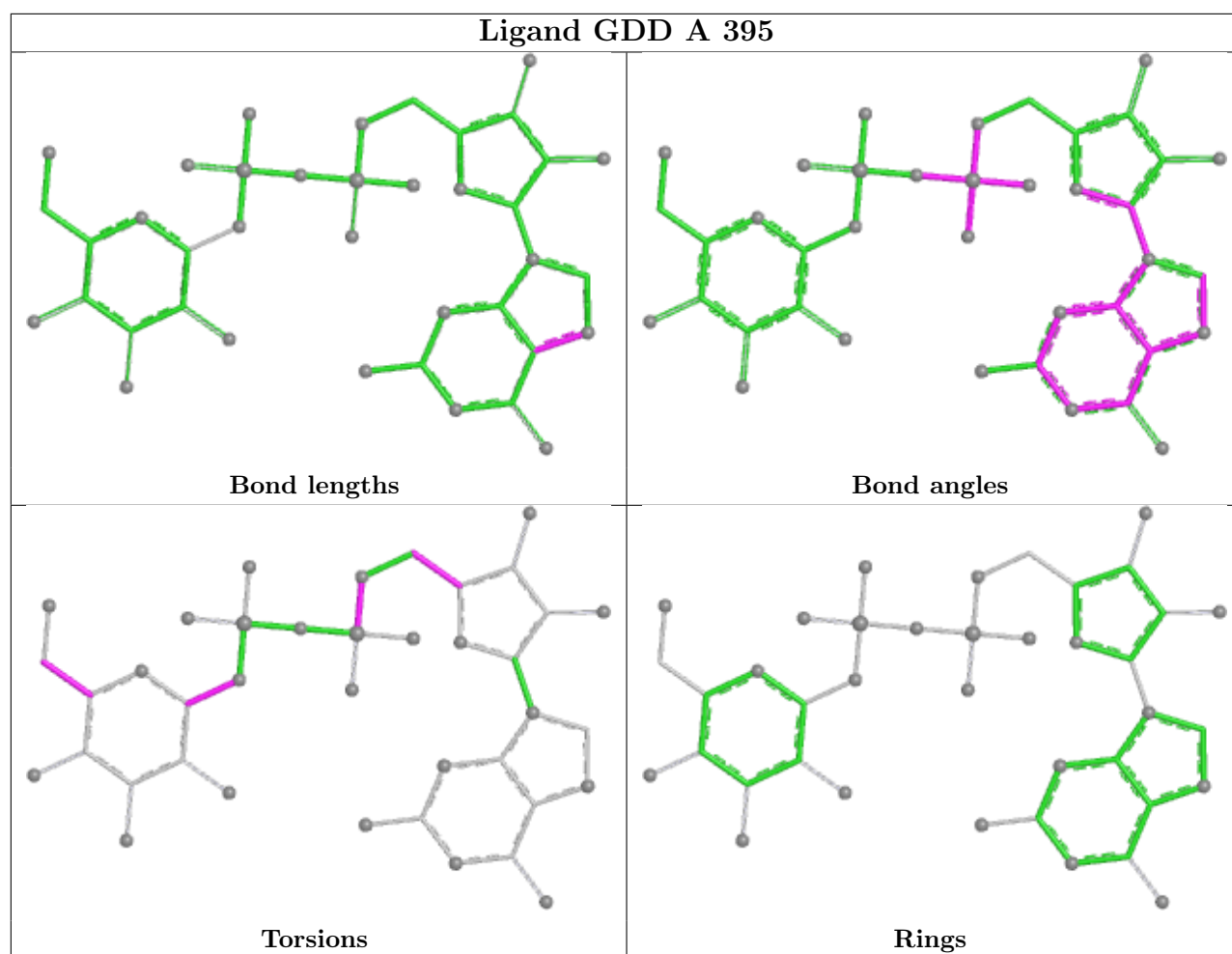
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	395	GDD	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	358/394 (90%)	0.23	11 (3%) 51 47	12, 27, 45, 67	0
1	B	354/394 (89%)	0.26	12 (3%) 48 44	15, 30, 49, 59	0
All	All	712/788 (90%)	0.24	23 (3%) 50 46	12, 29, 48, 67	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	44	GLU	4.0
1	A	348	ASP	3.7
1	B	10	GLU	3.3
1	B	351	ASP	3.2
1	A	351	ASP	3.1
1	B	37	THR	2.7
1	A	65	HIS	2.7
1	B	137	GLU	2.6
1	A	218	TRP	2.5
1	B	162	GLU	2.5
1	B	339	ASP	2.5
1	B	48	ASP	2.3
1	B	352	HIS	2.3
1	B	8	TYR	2.3
1	A	286	GLU	2.2
1	A	358	ASN	2.2
1	A	102	ARG	2.2
1	A	354	ILE	2.2
1	A	317	LYS	2.2
1	B	12	PHE	2.1
1	A	372	GLU	2.1
1	A	353	GLY	2.0
1	B	47	TYR	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](#)

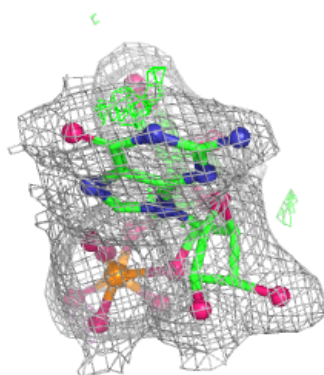
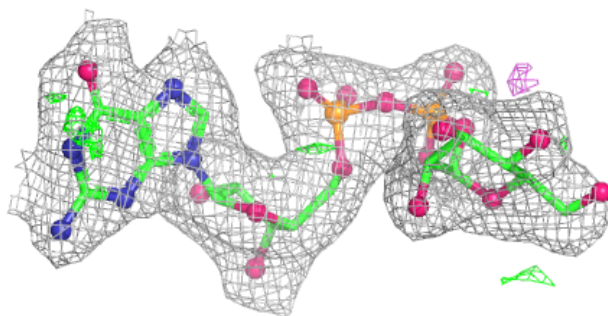
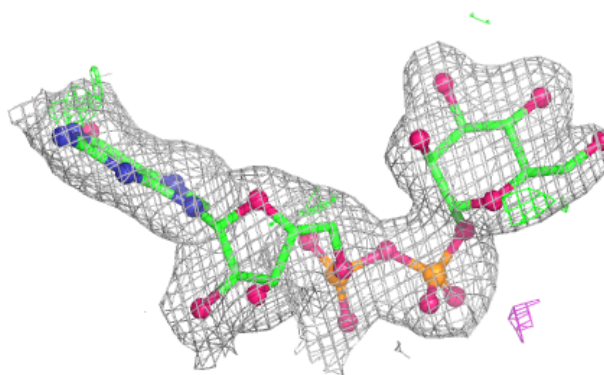
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GDD	A	395	39/39	0.93	0.08	19,25,29,31	0
2	GDD	B	395	39/39	0.94	0.08	19,25,31,33	0

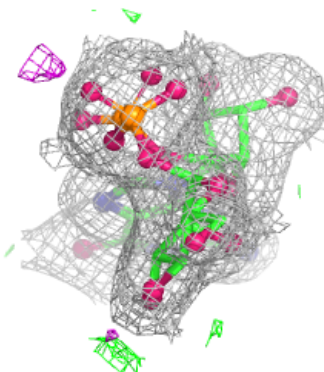
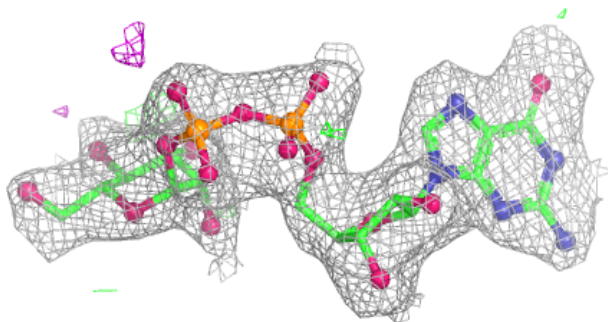
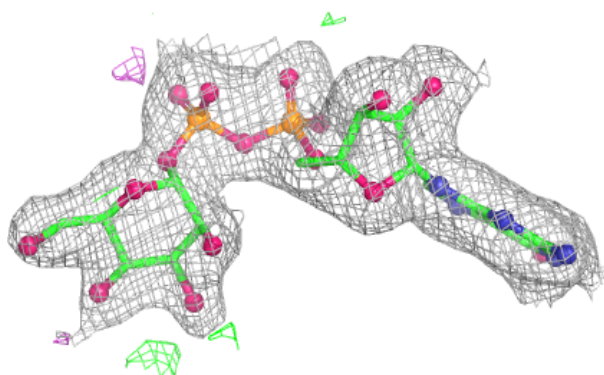
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GDD A 395:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around GDD B 395:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.