



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2017 – 02:44 PM EST

PDB ID : 4JTD
Title : Crystal structure of Kv1.2-2.1 paddle chimera channel in complex with Lys27Met mutant of Charybdotoxin
Authors : Banerjee, A.; Lee, A.; Campbell, E.; MacKinnon, R.
Deposited on : unknown
Resolution : 2.54 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

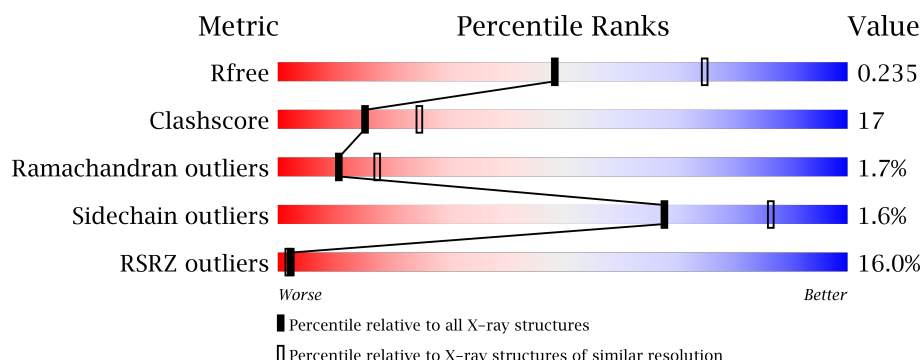
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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}	100719	4993 (2.58-2.50)
Clashscore	112137	5755 (2.58-2.50)
Ramachandran outliers	110173	5652 (2.58-2.50)
Sidechain outliers	110143	5654 (2.58-2.50)
RSRZ outliers	101464	5026 (2.58-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	333	
1	G	333	
2	B	514	
2	H	514	
3	Y	37	

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
4	NAP	G	1001	-	-	-	X
6	PGW	B	505	-	-	-	X
6	PGW	B	506	-	-	-	X
6	PGW	B	510	-	-	-	X
6	PGW	B	511	-	-	-	X
6	PGW	B	514	-	-	-	X
6	PGW	B	515	-	-	-	X
6	PGW	B	516	-	-	-	X
6	PGW	B	517	-	-	-	X
6	PGW	B	518	-	-	-	X
6	PGW	H	505	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12082 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 Voltage-gated potassium channel subunit beta-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2556	1627	443	470	16			
1	G	326	Total	C	N	O	S	0	0	0
			2556	1627	443	470	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	MET	-	EXPRESSION TAG	UNP P62483
G	35	MET	-	EXPRESSION TAG	UNP P62483

- Molecule 2 is a protein called Potassium voltage-gated channel subfamily A member 2, Potassium voltage-gated channel subfamily B member 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	386	Total	C	N	O	S	0	0	0
			3088	2022	504	548	14			
2	H	363	Total	C	N	O	S	0	0	0
			2959	1950	478	518	13			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	MET	-	EXPRESSION TAG	UNP P63142
B	-17	ALA	-	EXPRESSION TAG	UNP P63142
B	-16	HIS	-	EXPRESSION TAG	UNP P63142
B	-15	HIS	-	EXPRESSION TAG	UNP P63142
B	-14	HIS	-	EXPRESSION TAG	UNP P63142
B	-13	HIS	-	EXPRESSION TAG	UNP P63142
B	-12	HIS	-	EXPRESSION TAG	UNP P63142
B	-11	HIS	-	EXPRESSION TAG	UNP P63142
B	-10	HIS	-	EXPRESSION TAG	UNP P63142

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	HIS	-	EXPRESSION TAG	UNP P63142
B	-8	HIS	-	EXPRESSION TAG	UNP P63142
B	-7	HIS	-	EXPRESSION TAG	UNP P63142
B	-6	GLY	-	EXPRESSION TAG	UNP P63142
B	-5	LEU	-	EXPRESSION TAG	UNP P63142
B	-4	VAL	-	EXPRESSION TAG	UNP P63142
B	-3	PRO	-	EXPRESSION TAG	UNP P63142
B	-2	ARG	-	EXPRESSION TAG	UNP P63142
B	-1	GLY	-	EXPRESSION TAG	UNP P63142
B	0	SER	-	EXPRESSION TAG	UNP P63142
B	31	SER	CYS	ENGINEERED MUTATION	UNP P63142
B	32	SER	CYS	ENGINEERED MUTATION	UNP P63142
B	207	GLN	ASN	ENGINEERED MUTATION	UNP P63142
B	431	SER	CYS	ENGINEERED MUTATION	UNP P63142
B	478	SER	CYS	ENGINEERED MUTATION	UNP P63142
H	-18	MET	-	EXPRESSION TAG	UNP P63142
H	-17	ALA	-	EXPRESSION TAG	UNP P63142
H	-16	HIS	-	EXPRESSION TAG	UNP P63142
H	-15	HIS	-	EXPRESSION TAG	UNP P63142
H	-14	HIS	-	EXPRESSION TAG	UNP P63142
H	-13	HIS	-	EXPRESSION TAG	UNP P63142
H	-12	HIS	-	EXPRESSION TAG	UNP P63142
H	-11	HIS	-	EXPRESSION TAG	UNP P63142
H	-10	HIS	-	EXPRESSION TAG	UNP P63142
H	-9	HIS	-	EXPRESSION TAG	UNP P63142
H	-8	HIS	-	EXPRESSION TAG	UNP P63142
H	-7	HIS	-	EXPRESSION TAG	UNP P63142
H	-6	GLY	-	EXPRESSION TAG	UNP P63142
H	-5	LEU	-	EXPRESSION TAG	UNP P63142
H	-4	VAL	-	EXPRESSION TAG	UNP P63142
H	-3	PRO	-	EXPRESSION TAG	UNP P63142
H	-2	ARG	-	EXPRESSION TAG	UNP P63142
H	-1	GLY	-	EXPRESSION TAG	UNP P63142
H	0	SER	-	EXPRESSION TAG	UNP P63142
H	31	SER	CYS	ENGINEERED MUTATION	UNP P63142
H	32	SER	CYS	ENGINEERED MUTATION	UNP P63142
H	207	GLN	ASN	ENGINEERED MUTATION	UNP P63142
H	431	SER	CYS	ENGINEERED MUTATION	UNP P63142
H	478	SER	CYS	ENGINEERED MUTATION	UNP P63142

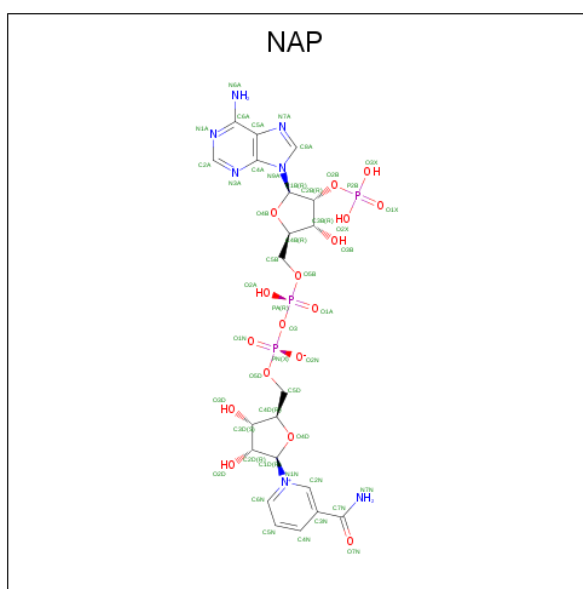
- Molecule 3 is a protein called Potassium channel toxin alpha-KTx 1.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Y	37	Total	C	N	O	S	0	0	0
			294	175	56	55	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	1	PCA	GLN	MODIFIED RESIDUE	UNP P13487
Y	27	MET	LYS	ENGINEERED MUTATION	UNP P13487

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



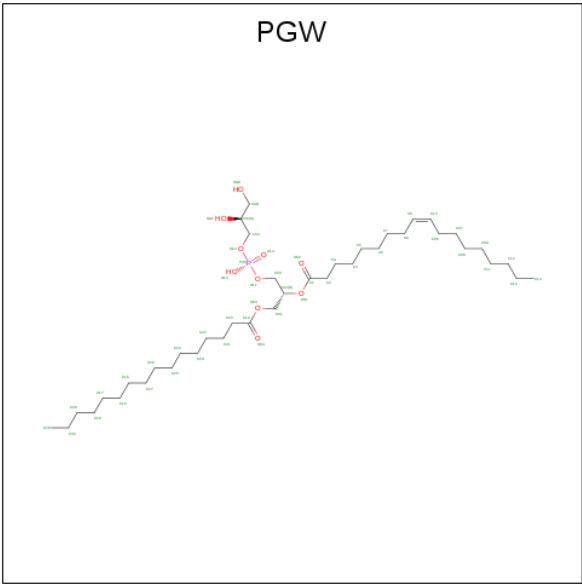
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
4	G	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	4	Total K 4 4	0	0
5	B	4	Total K 4 4	0	0

- Molecule 6 is (1R)-2-{[(S)-{(2S)-2,3-dihydroxypropyl}oxy}(hydroxy)phosphoryl]oxy}-1-[(

hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (three-letter code: PGW) (formula: C₄₀H₇₇O₁₀P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 22 17 5	0	0
6	B	1	Total C 9 9	0	0
6	B	1	Total C 9 9	0	0
6	B	1	Total C 9 9	0	0
6	B	1	Total C 9 9	0	0
6	B	1	Total C 9 9	0	0
6	B	1	Total C 9 9	0	0
6	B	1	Total C 7 7	0	0
6	B	1	Total C 9 9	0	0
6	B	1	Total C 8 8	0	0
6	B	1	Total C O P 23 14 8 1	0	0
6	B	1	Total C 8 8	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O P 36 25 10 1	0	0
6	B	1	Total C 7 7	0	0
6	B	1	Total C 8 8	0	0
6	B	1	Total C 8 8	0	0
6	H	1	Total C O 22 17 5	0	0

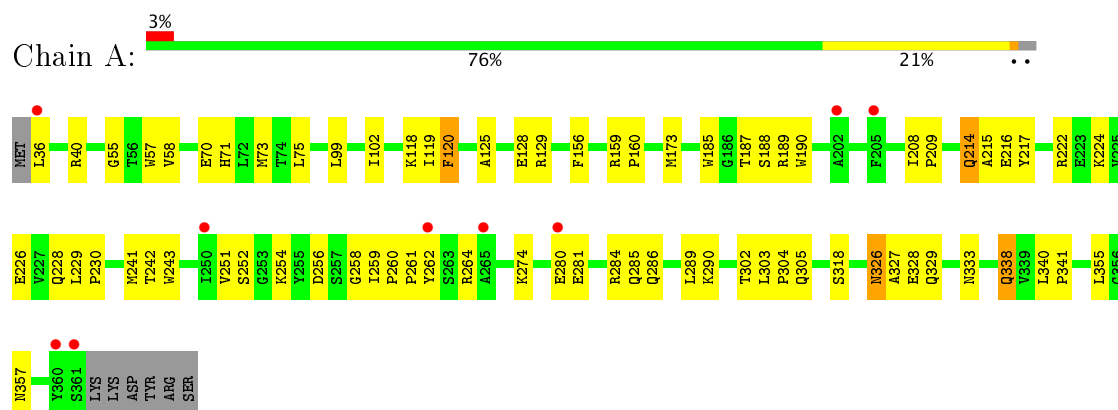
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	140	Total O 140 140	0	0
7	B	50	Total O 50 50	0	0
7	G	102	Total O 102 102	0	0
7	H	21	Total O 21 21	0	0

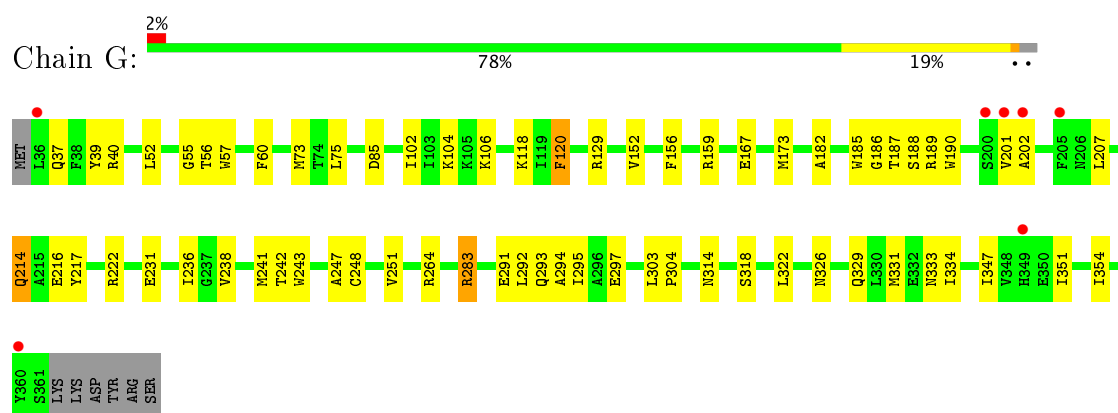
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

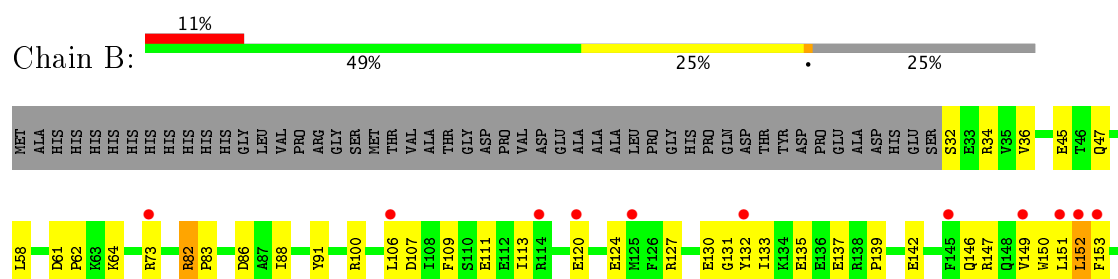
- Molecule 1: Voltage-gated potassium channel subunit beta-2

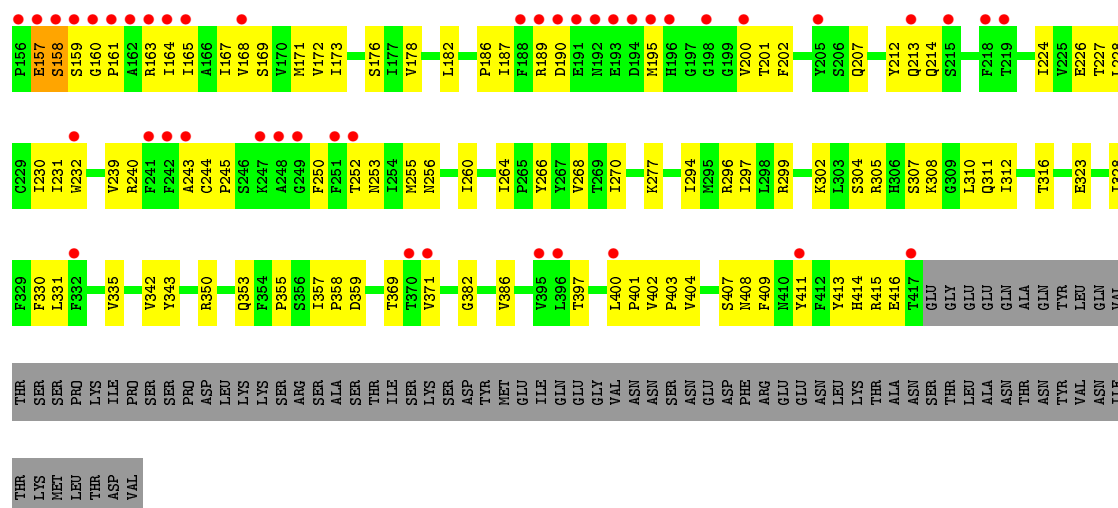


- Molecule 1: Voltage-gated potassium channel subunit beta-2

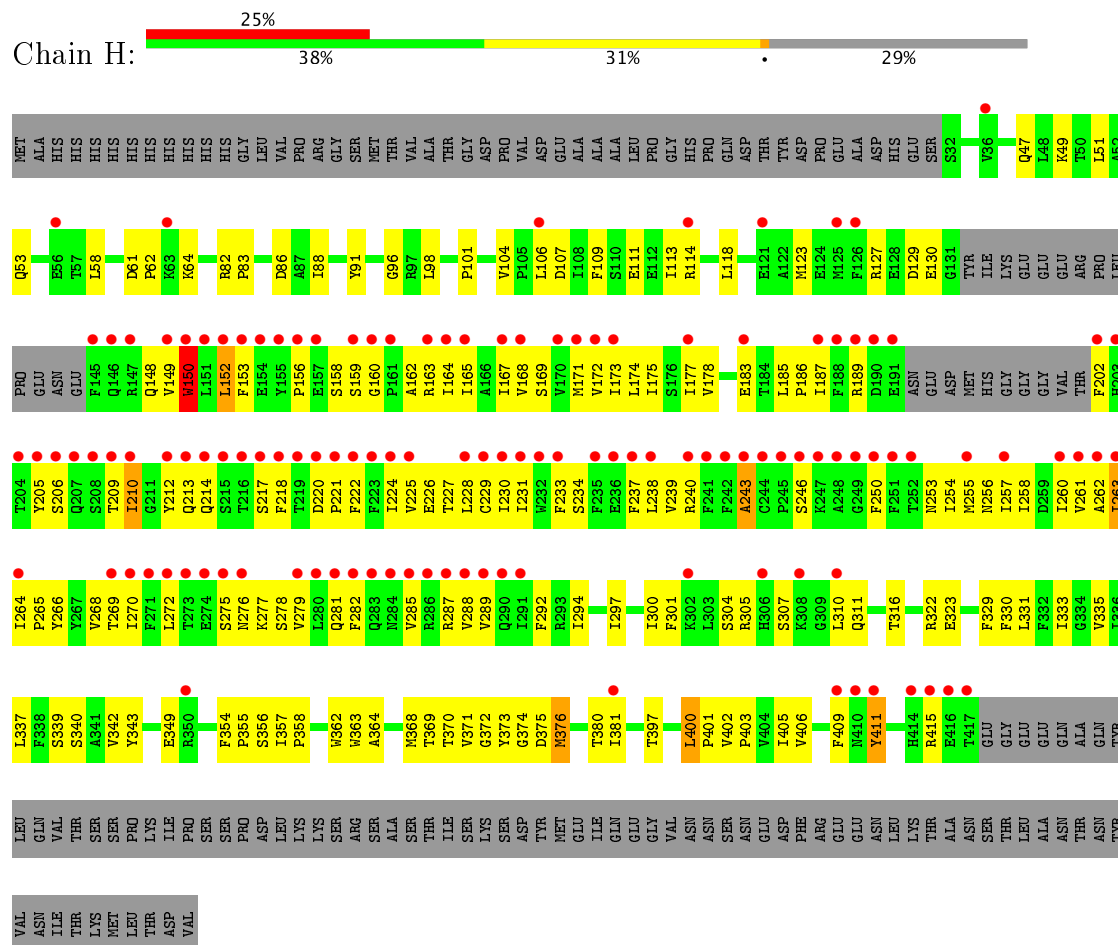


- Molecule 2: Potassium voltage-gated channel subfamily A member 2, Potassium voltage-gated channel subfamily B member 1

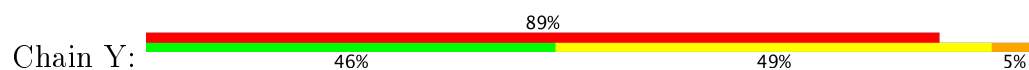




- Molecule 2: Potassium voltage-gated channel subfamily A member 2, Potassium voltage-gated channel subfamily B member 1



- Molecule 3: Potassium channel toxin alpha-KTx 1.1





4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	144.87Å 144.87Å 284.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.54 49.71 – 2.54	Depositor EDS
% Data completeness (in resolution range)	93.1 (50.00-2.54) 94.8 (49.71-2.54)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.54Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.210 , 0.235 0.211 , 0.235	Depositor DCC
R_{free} test set	4406 reflections (4.96%)	DCC
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 66.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12082	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PGW, K, PCA, NAP

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	0.38	0/2608	0.57	0/3524
1	G	0.36	0/2608	0.56	0/3524
2	B	0.35	0/3169	0.52	0/4292
2	H	0.32	0/3036	0.49	0/4114
3	Y	0.27	0/291	0.46	0/388
All	All	0.35	0/11712	0.53	0/15842

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2556	0	2582	54	0
1	G	2556	0	2582	48	0
2	B	3088	0	3034	95	0
2	H	2959	0	2956	166	0
3	Y	294	0	278	18	0
4	A	48	0	25	11	0
4	G	48	0	25	13	0
5	B	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	4	0	0	0	0
6	B	190	0	251	11	0
6	H	22	0	25	5	0
7	A	140	0	0	0	0
7	B	50	0	0	3	0
7	G	102	0	0	1	0
7	H	21	0	0	1	0
All	All	12082	0	11758	393	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 17.

All (393) 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)
3:Y:4:ASN:HA	3:Y:32:LYS:HD3	1.44	0.96
1:G:333:ASN:HD21	4:G:1001:NAP:H61A	1.15	0.91
2:H:400:LEU:HB2	2:H:401:PRO:HD3	1.56	0.87
1:G:55:GLY:HA3	4:G:1001:NAP:O3D	1.74	0.86
2:B:400:LEU:HB2	2:B:401:PRO:HD3	1.57	0.86
2:H:148:GLN:HE21	2:H:152:LEU:HD23	1.38	0.85
2:B:311:GLN:HG2	6:B:517:PGW:H3	1.59	0.85
2:H:210:ILE:HD13	2:H:214:GLN:HB3	1.57	0.85
1:A:55:GLY:HA3	4:A:1001:NAP:O3D	1.78	0.84
2:B:58:LEU:HD12	2:B:64:LYS:HB3	1.57	0.83
2:H:185:LEU:HD12	2:H:186:PRO:HD2	1.61	0.83
2:H:287:ARG:HB2	2:H:287:ARG:NH1	1.95	0.81
1:A:118:LYS:HG3	1:A:156:PHE:HB2	1.66	0.77
2:H:285:VAL:HG23	2:H:288:VAL:HB	1.65	0.77
2:H:213:GLN:HG2	2:H:220:ASP:HB2	1.65	0.77
1:A:333:ASN:HD21	4:A:1001:NAP:H61A	1.34	0.75
2:H:358:PRO:HB3	6:H:505:PGW:H20A	1.69	0.75
1:G:40:ARG:HD2	1:G:318:SER:O	1.86	0.74
1:G:189:ARG:HH21	4:G:1001:NAP:H71N	1.35	0.72
2:H:163:ARG:NH1	2:H:163:ARG:HB2	2.04	0.72
2:H:210:ILE:HG21	2:H:214:GLN:HB2	1.73	0.69
1:A:36:LEU:HG	1:A:341:PRO:HG3	1.75	0.68
2:B:227:THR:O	2:B:231:ILE:HG12	1.93	0.68
2:H:227:THR:O	2:H:231:ILE:HG12	1.94	0.68
2:H:287:ARG:HB2	2:H:287:ARG:HH11	1.60	0.67
2:B:253:ASN:ND2	2:B:255:MET:HB2	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:1001:NAP:H52A	4:G:1001:NAP:H8A	1.76	0.67
2:H:107:ASP:O	2:H:111:GLU:HG3	1.94	0.67
2:B:176:SER:OG	2:B:299:ARG:HD3	1.94	0.66
4:A:1001:NAP:H52A	4:A:1001:NAP:H8A	1.77	0.66
2:H:148:GLN:NE2	2:H:152:LEU:HD23	2.08	0.66
3:Y:17:CYS:O	3:Y:21:HIS:HB2	1.97	0.65
1:A:159:ARG:HA	1:A:188:SER:O	1.97	0.65
2:B:226:GLU:O	2:B:230:ILE:HD13	1.97	0.65
2:H:264:ILE:HB	2:H:265:PRO:HD3	1.79	0.64
2:B:253:ASN:HD21	2:B:255:MET:HB2	1.63	0.64
2:H:152:LEU:HD12	2:H:153:PHE:N	2.12	0.63
1:A:259:ILE:HG13	1:A:274:LYS:HE3	1.80	0.63
2:H:240:ARG:HH22	2:H:305:ARG:HD3	1.63	0.63
2:H:363:TRP:HB2	2:H:376:MET:HE2	1.79	0.62
2:B:304:SER:HA	2:B:310:LEU:HD23	1.82	0.62
2:H:263:ILE:H	2:H:263:ILE:HD13	1.65	0.62
3:Y:13:CYS:SG	3:Y:28:CYS:HB2	2.39	0.62
1:A:189:ARG:HH21	4:A:1001:NAP:H71N	1.46	0.61
2:B:214:GLN:NE2	2:B:270:ILE:HG12	2.16	0.61
2:H:357:ILE:HB	2:H:358:PRO:HD3	1.81	0.60
3:Y:14:TRP:HA	3:Y:14:TRP:HE3	1.66	0.60
2:B:146:GLN:HG3	2:B:243:ALA:HA	1.82	0.60
2:H:205:TYR:HE2	2:H:282:PHE:HB3	1.66	0.60
3:Y:14:TRP:HA	3:Y:14:TRP:CE3	2.35	0.60
2:H:174:LEU:O	2:H:178:VAL:HG23	2.02	0.60
2:H:381:ILE:HD12	2:H:381:ILE:N	2.16	0.60
2:H:272:LEU:HD13	2:H:289:VAL:HG22	1.84	0.60
2:H:400:LEU:O	2:H:403:PRO:HD2	2.02	0.59
1:A:258:GLY:O	1:A:260:PRO:HD3	2.03	0.59
2:H:253:ASN:HB3	2:H:256:ASN:HD22	1.68	0.59
2:B:255:MET:CE	2:B:305:ARG:HA	2.33	0.59
2:H:265:PRO:O	2:H:269:THR:HG23	2.03	0.58
2:B:330:PHE:HB3	2:B:397:THR:HG23	1.85	0.58
2:H:169:SER:O	2:H:173:ILE:HG13	2.03	0.58
2:B:328:ILE:HG23	6:B:505:PGW:C9	2.33	0.58
2:B:61:ASP:OD2	2:B:64:LYS:HG3	2.04	0.58
2:B:186:PRO:O	2:B:190:ASP:HB2	2.03	0.58
2:B:253:ASN:HB3	2:B:256:ASN:ND2	2.18	0.58
1:A:159:ARG:HB2	1:A:160:PRO:HD2	1.86	0.58
2:H:362:TRP:HB2	6:H:505:PGW:H2A	1.86	0.58
2:B:294:ILE:O	2:B:297:ILE:HG22	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:305:ARG:HG3	2:B:305:ARG:HH11	1.68	0.57
2:H:101:PRO:HB2	2:H:104:VAL:HG23	1.86	0.57
2:H:369:THR:OG1	2:H:371:VAL:HG23	2.04	0.57
2:H:98:LEU:HD21	2:H:113:ILE:HD13	1.86	0.57
2:H:149:VAL:O	2:H:243:ALA:HB1	2.03	0.57
2:H:189:ARG:HH11	2:H:189:ARG:HG3	1.70	0.57
2:H:331:LEU:O	2:H:335:VAL:HG23	2.05	0.57
1:G:251:VAL:O	1:G:251:VAL:HG12	2.04	0.57
2:H:304:SER:HA	2:H:310:LEU:HD23	1.85	0.57
1:G:293:GLN:HE21	1:G:297:GLU:HG3	1.69	0.56
2:B:100:ARG:HG3	2:B:109:PHE:CG	2.41	0.56
2:H:276:ASN:HA	2:H:281:GLN:NE2	2.19	0.56
2:H:168:VAL:HA	2:H:171:MET:HG2	1.88	0.56
2:H:330:PHE:HB3	2:H:397:THR:HG23	1.87	0.56
2:B:323:GLU:CD	2:B:323:GLU:H	2.09	0.56
2:H:212:TYR:HB3	2:H:222:PHE:HB2	1.88	0.55
2:H:402:VAL:O	2:H:406:VAL:HG23	2.06	0.55
6:H:505:PGW:O02	6:H:505:PGW:H03A	2.07	0.55
2:H:158:SER:HB3	2:H:162:ALA:HB1	1.87	0.55
2:H:88:ILE:O	2:H:91:TYR:HB3	2.07	0.55
1:A:55:GLY:CA	4:A:1001:NAP:O3D	2.54	0.55
2:B:164:ILE:O	2:B:168:VAL:HG23	2.07	0.55
2:B:169:SER:HA	2:B:232:TRP:HE1	1.71	0.55
2:B:260:ILE:O	2:B:264:ILE:HG13	2.05	0.55
1:G:333:ASN:ND2	4:G:1001:NAP:H61A	1.94	0.55
2:B:120:GLU:O	2:B:124:GLU:HG3	2.07	0.54
2:B:142:GLU:H	2:B:147:ARG:CB	2.21	0.54
2:H:258:ILE:HG21	2:H:301:PHE:O	2.07	0.54
6:B:515:PGW:O02	6:B:515:PGW:O11	2.25	0.54
1:G:55:GLY:CA	4:G:1001:NAP:O3D	2.51	0.54
2:H:123:MET:O	2:H:127:ARG:HG3	2.07	0.54
2:H:253:ASN:O	2:H:257:ILE:HG12	2.08	0.54
2:H:187:ILE:O	2:H:187:ILE:HG22	2.06	0.54
1:A:251:VAL:HG12	1:A:251:VAL:O	2.07	0.54
2:B:107:ASP:O	2:B:111:GLU:HG3	2.08	0.54
6:B:517:PGW:O02	6:B:517:PGW:H03A	2.07	0.54
2:H:58:LEU:HD23	2:H:58:LEU:C	2.28	0.54
2:B:308:LYS:NZ	6:B:517:PGW:HAD	2.23	0.54
1:G:189:ARG:HE	4:G:1001:NAP:H72N	1.56	0.54
2:H:230:ILE:H	2:H:230:ILE:HD12	1.72	0.54
2:B:304:SER:CA	2:B:310:LEU:HD23	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:173:ILE:O	2:B:176:SER:HB3	2.08	0.53
2:H:202:PHE:HB3	2:H:279:VAL:HG22	1.91	0.53
2:H:307:SER:O	2:H:311:GLN:HG3	2.09	0.53
2:B:73:ARG:HD3	7:B:642:HOH:O	2.09	0.53
1:G:57:TRP:HB3	4:G:1001:NAP:H3D	1.91	0.53
2:H:213:GLN:CG	2:H:220:ASP:HB2	2.36	0.53
6:H:505:PGW:O02	6:H:505:PGW:H01	2.08	0.53
3:Y:29:MET:C	3:Y:31:LYS:H	2.12	0.53
2:B:159:SER:HB2	2:B:161:PRO:HD2	1.90	0.53
3:Y:28:CYS:HB2	3:Y:33:CYS:HA	1.91	0.53
2:B:157:GLU:O	2:B:158:SER:O	2.27	0.52
6:B:505:PGW:H01	6:B:505:PGW:O02	2.09	0.52
2:H:285:VAL:CG2	2:H:288:VAL:HB	2.36	0.52
2:H:106:LEU:CD1	2:H:130:GLU:HG2	2.39	0.52
2:H:285:VAL:HG22	2:H:289:VAL:HG23	1.90	0.52
2:H:230:ILE:HD12	2:H:230:ILE:N	2.24	0.52
2:H:246:SER:O	2:H:250:PHE:HB2	2.09	0.52
1:G:120:PHE:CD1	1:G:159:ARG:HG3	2.44	0.52
1:G:37:GLN:HG3	1:G:39:TYR:O	2.10	0.52
2:H:172:VAL:HG12	2:H:233:PHE:CZ	2.44	0.52
2:H:263:ILE:HD13	2:H:263:ILE:N	2.24	0.52
2:H:268:VAL:HB	2:H:292:PHE:CE2	2.45	0.52
2:H:329:PHE:O	2:H:333:ILE:HG12	2.09	0.52
3:Y:18:GLN:HG3	3:Y:23:THR:O	2.09	0.52
2:H:287:ARG:HH11	2:H:287:ARG:CB	2.21	0.52
2:B:149:VAL:O	2:B:152:LEU:HD12	2.10	0.52
1:A:125:ALA:HB3	1:A:128:GLU:HG3	1.91	0.52
2:B:250:PHE:C	2:B:252:THR:H	2.14	0.52
2:H:411:TYR:CZ	2:H:415:ARG:HD3	2.45	0.52
2:B:316:THR:HG21	2:B:409:PHE:HB2	1.92	0.51
1:G:295:ILE:HD12	1:G:295:ILE:H	1.74	0.51
1:A:261:PRO:O	1:A:262:TYR:HB2	2.10	0.51
2:B:256:ASN:O	2:B:260:ILE:HG13	2.10	0.51
1:G:85:ASP:OD1	1:G:118:LYS:NZ	2.43	0.51
1:A:329:GLN:OE1	4:A:1001:NAP:H2B	2.10	0.51
1:A:120:PHE:CD1	1:A:159:ARG:HG3	2.46	0.51
2:B:240:ARG:NH2	2:B:305:ARG:HD3	2.26	0.51
2:H:237:PHE:CE1	2:H:260:ILE:HG12	2.46	0.51
1:G:331:MET:HE2	1:G:334:ILE:HD12	1.91	0.51
2:H:163:ARG:HH11	2:H:163:ARG:HB2	1.73	0.51
2:B:404:VAL:O	2:B:407:SER:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:511:PGW:H2A	6:B:516:PGW:H16	1.91	0.51
1:G:295:ILE:HD12	1:G:295:ILE:N	2.26	0.51
2:H:368:MET:C	2:H:370:THR:H	2.12	0.51
2:H:109:PHE:CE2	2:H:113:ILE:HD11	2.46	0.51
2:H:159:SER:O	2:H:163:ARG:HG3	2.11	0.51
1:A:36:LEU:HD12	1:A:36:LEU:N	2.26	0.51
2:H:217:SER:O	2:H:218:PHE:HB2	2.12	0.50
2:H:86:ASP:HB2	7:H:616:HOH:O	2.11	0.50
2:B:240:ARG:O	2:B:244:CYS:HB2	2.10	0.50
1:G:118:LYS:HG2	1:G:156:PHE:HB2	1.92	0.50
1:G:291:GLU:O	1:G:294:ALA:HB3	2.11	0.50
2:H:230:ILE:HG12	2:H:266:TYR:CG	2.46	0.50
2:B:127:ARG:HG2	2:B:127:ARG:HH11	1.77	0.50
1:G:236:ILE:HG13	1:G:238:VAL:HG23	1.92	0.50
2:H:224:ILE:O	2:H:228:LEU:HG	2.11	0.50
1:A:340:LEU:HB3	1:A:341:PRO:HD3	1.93	0.50
2:H:258:ILE:O	2:H:262:ALA:HB2	2.11	0.50
1:G:214:GLN:HA	1:G:241:MET:O	2.10	0.50
1:G:326:ASN:OD1	1:G:329:GLN:HG3	2.12	0.50
2:H:415:ARG:HG2	2:H:415:ARG:HH11	1.76	0.50
3:Y:25:ARG:NH1	3:Y:25:ARG:HB2	2.27	0.50
1:A:57:TRP:HB3	4:A:1001:NAP:H3D	1.93	0.49
2:B:350:ARG:HB3	2:B:350:ARG:NH1	2.27	0.49
2:B:355:PRO:HB2	2:B:359:ASP:OD2	2.12	0.49
1:G:189:ARG:NH2	4:G:1001:NAP:H71N	2.08	0.49
3:Y:20:LEU:HD12	3:Y:20:LEU:N	2.27	0.49
2:B:109:PHE:CE2	2:B:113:ILE:HD11	2.47	0.49
1:G:173:MET:HG3	1:G:185:TRP:CE3	2.48	0.49
2:H:374:GLY:C	2:H:376:MET:H	2.15	0.49
2:B:167:ILE:O	2:B:171:MET:HG2	2.13	0.49
2:B:331:LEU:O	2:B:335:VAL:HG23	2.12	0.49
2:H:264:ILE:O	2:H:268:VAL:HG23	2.12	0.49
1:G:329:GLN:OE1	4:G:1001:NAP:H2B	2.13	0.49
2:H:294:ILE:O	2:H:297:ILE:HG22	2.13	0.49
2:H:148:GLN:HE21	2:H:152:LEU:CD2	2.18	0.49
2:H:163:ARG:HH11	2:H:163:ARG:CB	2.26	0.49
2:H:322:ARG:HG3	2:H:322:ARG:HH11	1.78	0.49
2:B:168:VAL:O	2:B:172:VAL:HG23	2.12	0.49
1:G:292:LEU:HA	1:G:295:ILE:HD13	1.95	0.48
2:H:47:GLN:NE2	2:H:49:LYS:HE2	2.28	0.48
2:B:153:PHE:CD2	2:B:239:VAL:HG11	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:212:TYR:OH	2:H:226:GLU:HG2	2.13	0.48
2:H:260:ILE:O	2:H:264:ILE:HG13	2.13	0.48
2:H:159:SER:H	2:H:162:ALA:HB3	1.78	0.48
2:H:171:MET:O	2:H:175:ILE:HG13	2.13	0.48
2:H:230:ILE:HG12	2:H:266:TYR:CB	2.43	0.48
1:A:224:LYS:HA	1:A:228:GLN:HG3	1.96	0.48
1:A:73:MET:SD	1:A:99:LEU:HD12	2.53	0.48
2:B:201:THR:HG22	2:B:202:PHE:N	2.28	0.48
2:H:202:PHE:N	2:H:206:SER:HB3	2.28	0.48
2:H:281:GLN:O	2:H:285:VAL:HG12	2.13	0.48
2:H:255:MET:CE	2:H:305:ARG:HA	2.44	0.48
1:A:355:LEU:HB3	1:A:357:ASN:OD1	2.14	0.48
2:H:268:VAL:HB	2:H:292:PHE:HE2	1.79	0.48
2:H:240:ARG:HH12	2:H:305:ARG:CZ	2.27	0.48
2:B:149:VAL:C	2:B:151:LEU:H	2.18	0.47
2:B:36:VAL:HG22	2:B:45:GLU:HG2	1.96	0.47
2:H:316:THR:HG21	2:H:409:PHE:HB2	1.95	0.47
2:H:400:LEU:C	2:H:403:PRO:HD2	2.34	0.47
2:B:150:TRP:HB2	2:B:243:ALA:O	2.14	0.47
2:B:230:ILE:HG21	2:B:266:TYR:CD2	2.49	0.47
2:B:299:ARG:O	2:B:302:LYS:HB2	2.15	0.47
2:H:106:LEU:HD13	2:H:130:GLU:HG2	1.96	0.47
2:H:221:PRO:O	2:H:225:VAL:HG23	2.15	0.47
2:H:381:ILE:H	2:H:381:ILE:HD12	1.77	0.47
2:H:277:LYS:O	2:H:277:LYS:HG3	2.15	0.47
1:G:247:ALA:O	1:G:248:CYS:HB2	2.15	0.47
1:A:338:GLN:HE21	1:A:338:GLN:HA	1.80	0.47
2:H:270:ILE:HD12	2:H:270:ILE:N	2.29	0.47
2:H:339:SER:O	2:H:342:VAL:HG12	2.14	0.47
2:H:354:PHE:HE1	2:H:376:MET:HE2	1.80	0.47
2:H:212:TYR:HB3	2:H:222:PHE:CB	2.45	0.47
3:Y:17:CYS:HB2	3:Y:23:THR:O	2.15	0.47
1:A:286:GLN:NE2	1:A:289:LEU:HD12	2.30	0.47
2:B:264:ILE:O	2:B:268:VAL:HG23	2.15	0.47
2:H:285:VAL:O	2:H:285:VAL:HG22	2.14	0.47
2:B:415:ARG:HH11	2:B:415:ARG:HG2	1.80	0.47
2:B:357:ILE:HB	2:B:358:PRO:HD3	1.97	0.46
2:H:337:LEU:HD23	2:H:337:LEU:C	2.36	0.46
1:A:216:GLU:HB2	1:A:243:TRP:CH2	2.50	0.46
1:A:326:ASN:HD22	1:A:328:GLU:H	1.62	0.46
2:B:212:TYR:CE2	2:B:226:GLU:HG2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:158:SER:HB3	2:H:162:ALA:CB	2.45	0.46
2:B:160:GLY:N	2:B:161:PRO:CD	2.78	0.46
2:H:212:TYR:HA	2:H:220:ASP:OD1	2.16	0.46
2:H:239:VAL:O	2:H:243:ALA:HB3	2.15	0.46
2:H:372:GLY:O	2:H:374:GLY:N	2.49	0.46
1:A:256:ASP:HB2	1:A:290:LYS:NZ	2.30	0.46
1:G:216:GLU:HB2	1:G:243:TRP:CH2	2.51	0.46
2:H:111:GLU:O	2:H:114:ARG:HB3	2.15	0.46
4:G:1001:NAP:H6N	4:G:1001:NAP:H52N	1.98	0.46
1:G:217:TYR:HB3	1:G:242:THR:HB	1.97	0.46
2:H:255:MET:HB3	2:H:305:ARG:NH2	2.30	0.46
2:H:268:VAL:HG12	2:H:268:VAL:O	2.15	0.46
2:H:305:ARG:HH11	2:H:305:ARG:HG3	1.81	0.46
2:B:305:ARG:HG3	2:B:305:ARG:NH1	2.30	0.46
1:G:167:GLU:HA	1:G:201:VAL:HG11	1.96	0.46
6:B:511:PGW:C1	6:B:516:PGW:H16	2.46	0.46
2:B:163:ARG:O	2:B:167:ILE:HG12	2.16	0.46
1:A:303:LEU:HB3	1:A:304:PRO:HD3	1.98	0.46
2:B:127:ARG:HG2	2:B:127:ARG:NH1	2.30	0.46
2:B:353:GLN:O	2:B:355:PRO:HD3	2.16	0.46
2:H:343:TYR:CE1	2:H:356:SER:HA	2.51	0.46
2:H:364:ALA:O	2:H:368:MET:HG3	2.16	0.46
2:H:254:ILE:O	2:H:258:ILE:HG13	2.16	0.46
3:Y:10:SER:C	3:Y:12:GLU:H	2.19	0.46
1:A:264:ARG:NH2	4:A:1001:NAP:H4B	2.31	0.45
2:H:276:ASN:ND2	2:H:285:VAL:HG21	2.31	0.45
1:A:326:ASN:ND2	1:A:328:GLU:HB2	2.31	0.45
2:B:106:LEU:HD13	2:B:130:GLU:HG2	1.99	0.45
2:H:82:ARG:HB2	2:H:83:PRO:HD3	1.97	0.45
2:B:189:ARG:HG3	2:B:189:ARG:HH11	1.81	0.45
2:H:229:CYS:HB3	2:H:233:PHE:HE2	1.82	0.45
2:H:189:ARG:NH1	2:H:189:ARG:HG3	2.32	0.45
1:A:217:TYR:HB3	1:A:242:THR:HB	1.99	0.45
1:A:252:SER:OG	1:A:254:LYS:HG2	2.16	0.45
2:B:253:ASN:HB3	2:B:256:ASN:HD22	1.80	0.45
2:B:307:SER:OG	2:B:310:LEU:HB2	2.16	0.45
1:A:216:GLU:HB2	1:A:243:TRP:CZ2	2.51	0.45
1:A:71:HIS:CD2	1:A:327:ALA:HB2	2.52	0.45
1:G:52:LEU:HD13	1:G:322:LEU:HD11	1.98	0.45
2:H:272:LEU:CD1	2:H:289:VAL:HG22	2.45	0.45
2:H:113:ILE:HG23	2:H:118:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:16:VAL:C	3:Y:18:GLN:H	2.19	0.45
1:A:254:LYS:HE3	4:A:1001:NAP:N3A	2.31	0.44
1:A:214:GLN:HA	1:A:241:MET:O	2.16	0.44
2:H:230:ILE:H	2:H:230:ILE:CD1	2.30	0.44
2:B:328:ILE:HG13	6:B:511:PGW:C9	2.48	0.44
1:G:303:LEU:HB3	1:G:304:PRO:HD3	1.99	0.44
2:B:382:GLY:O	2:B:386:VAL:HG23	2.18	0.44
2:H:213:GLN:HA	2:H:213:GLN:NE2	2.31	0.44
2:H:234:SER:O	2:H:238:LEU:HG	2.17	0.44
2:B:32:SER:HB3	2:B:47:GLN:HE21	1.83	0.44
1:G:120:PHE:O	1:G:129:ARG:HA	2.17	0.44
2:H:213:GLN:HA	2:H:213:GLN:HE21	1.83	0.44
2:H:177:ILE:HD13	2:H:300:ILE:CD1	2.47	0.44
2:H:400:LEU:HB2	2:H:401:PRO:CD	2.39	0.44
6:B:505:PGW:H03A	6:B:505:PGW:O02	2.18	0.44
1:G:37:GLN:HA	1:G:37:GLN:NE2	2.33	0.44
2:H:343:TYR:HE1	2:H:355:PRO:O	2.01	0.44
2:B:224:ILE:O	2:B:228:LEU:HG	2.17	0.44
2:H:150:TRP:HA	2:H:150:TRP:CE3	2.53	0.44
2:H:210:ILE:HG21	2:H:214:GLN:CB	2.43	0.44
2:H:229:CYS:HB3	2:H:233:PHE:CE2	2.52	0.44
2:B:82:ARG:HB2	2:B:83:PRO:HD3	1.98	0.44
1:G:104:LYS:HG3	7:G:1163:HOH:O	2.18	0.44
1:G:56:THR:HB	1:G:60:PHE:HB2	1.99	0.44
2:H:150:TRP:HE3	2:H:150:TRP:HA	1.82	0.44
2:H:173:ILE:HG12	2:H:233:PHE:HE1	1.83	0.44
2:H:270:ILE:O	2:H:270:ILE:HG22	2.16	0.44
1:G:102:ILE:O	1:G:106:LYS:HG2	2.17	0.43
1:G:37:GLN:HA	1:G:37:GLN:HE21	1.83	0.43
2:H:91:TYR:CE2	2:H:118:LEU:HD22	2.53	0.43
2:H:162:ALA:HA	2:H:165:ILE:CD1	2.48	0.43
2:H:261:VAL:HA	2:H:264:ILE:HG13	2.00	0.43
2:H:368:MET:C	2:H:370:THR:N	2.72	0.43
1:A:188:SER:O	1:A:189:ARG:HB2	2.18	0.43
1:G:264:ARG:NH2	4:G:1001:NAP:H4B	2.33	0.43
2:H:261:VAL:O	2:H:261:VAL:HG12	2.18	0.43
1:A:229:LEU:N	1:A:230:PRO:CD	2.82	0.43
1:A:302:THR:OG1	1:A:305:GLN:HG3	2.17	0.43
2:B:414:HIS:C	2:B:416:GLU:N	2.70	0.43
3:Y:29:MET:HG3	3:Y:31:LYS:HB3	2.00	0.43
2:H:256:ASN:O	2:H:260:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:GLU:HA	1:A:102:ILE:HD13	2.01	0.43
2:B:414:HIS:C	2:B:416:GLU:H	2.21	0.43
1:G:283:ARG:HG3	1:G:283:ARG:HH11	1.83	0.43
1:A:281:GLU:O	1:A:285:GLN:HG3	2.17	0.43
2:B:277:LYS:O	2:B:277:LYS:HG3	2.18	0.43
2:H:337:LEU:HD23	2:H:337:LEU:O	2.19	0.43
2:B:178:VAL:O	2:B:182:LEU:HG	2.19	0.43
2:B:255:MET:HE3	2:B:305:ARG:HA	2.00	0.43
1:G:156:PHE:HA	1:G:186:GLY:O	2.18	0.43
2:H:276:ASN:HD21	2:H:285:VAL:HG21	1.83	0.43
2:B:350:ARG:CB	2:B:350:ARG:NH1	2.81	0.43
2:H:152:LEU:HA	2:H:158:SER:OG	2.18	0.43
2:H:209:THR:HG22	2:H:209:THR:O	2.18	0.43
2:H:230:ILE:HG21	2:H:266:TYR:CD2	2.54	0.43
1:A:222:ARG:HB3	1:A:226:GLU:OE2	2.18	0.43
2:H:156:PRO:O	2:H:163:ARG:HA	2.19	0.43
2:H:278:SER:OG	2:H:281:GLN:HG3	2.19	0.43
2:H:358:PRO:HB3	6:H:505:PGW:C20	2.42	0.43
2:H:402:VAL:HB	2:H:403:PRO:HD3	2.01	0.43
2:B:195:MET:HE3	7:B:626:HOH:O	2.18	0.42
1:G:55:GLY:HA3	4:G:1001:NAP:HO3N	1.76	0.42
2:H:287:ARG:HB2	2:H:287:ARG:CZ	2.50	0.42
2:H:349:GLU:HG3	2:H:380:THR:CG2	2.49	0.42
1:A:119:ILE:O	1:A:120:PHE:HB2	2.19	0.42
1:G:152:VAL:O	1:G:182:ALA:HA	2.18	0.42
1:G:347:ILE:O	1:G:351:ILE:HG13	2.19	0.42
2:B:408:ASN:O	2:B:411:TYR:HB3	2.20	0.42
1:A:208:ILE:HA	1:A:209:PRO:HD3	1.84	0.42
1:A:215:ALA:O	1:A:242:THR:HA	2.20	0.42
1:A:280:GLU:HG3	1:A:284:ARG:HH12	1.84	0.42
2:B:207:GLN:HG3	2:B:213:GLN:HB2	2.01	0.42
1:G:251:VAL:CG1	1:G:251:VAL:O	2.68	0.42
2:B:342:VAL:HG13	2:B:343:TYR:N	2.34	0.42
1:G:202:ALA:HA	1:G:207:LEU:HB2	2.02	0.42
2:H:177:ILE:HD13	2:H:300:ILE:HD12	2.02	0.42
1:A:173:MET:HG3	1:A:185:TRP:CE3	2.55	0.42
2:H:163:ARG:O	2:H:167:ILE:HG12	2.19	0.42
2:H:51:LEU:C	2:H:53:GLN:H	2.23	0.42
1:A:187:THR:HB	1:A:190:TRP:CG	2.55	0.42
2:B:187:ILE:HG22	2:B:187:ILE:O	2.20	0.42
2:B:308:LYS:HZ1	6:B:517:PGW:HAD	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:164:ILE:HA	2:H:167:ILE:HB	2.02	0.42
2:B:312:ILE:HD13	2:B:413:TYR:HA	2.01	0.42
3:Y:10:SER:C	3:Y:12:GLU:N	2.74	0.42
1:A:120:PHE:O	1:A:129:ARG:HA	2.19	0.41
2:B:214:GLN:HE22	2:B:270:ILE:HG12	1.83	0.41
2:H:185:LEU:CD1	2:H:186:PRO:HD2	2.42	0.41
3:Y:9:THR:O	3:Y:12:GLU:N	2.43	0.41
1:A:40:ARG:HD2	1:A:318:SER:O	2.20	0.41
2:H:354:PHE:CE1	2:H:376:MET:HE2	2.55	0.41
2:H:375:ASP:O	2:H:376:MET:HB2	2.20	0.41
2:B:152:LEU:HB2	2:B:165:ILE:HD12	2.03	0.41
2:B:200:VAL:O	2:B:200:VAL:HG23	2.21	0.41
2:B:350:ARG:HH11	2:B:350:ARG:CB	2.33	0.41
2:B:61:ASP:HA	2:B:62:PRO:HD3	1.91	0.41
1:G:159:ARG:HA	1:G:188:SER:O	2.21	0.41
4:A:1001:NAP:H52N	4:A:1001:NAP:H6N	2.03	0.41
1:A:264:ARG:HB2	4:A:1001:NAP:O3X	2.21	0.41
1:A:326:ASN:HD22	1:A:328:GLU:N	2.18	0.41
2:B:369:THR:OG1	2:B:371:VAL:HG23	2.20	0.41
2:H:340:SER:HB3	2:H:357:ILE:HD13	2.02	0.41
1:A:286:GLN:HA	1:A:286:GLN:NE2	2.35	0.41
2:B:402:VAL:HB	2:B:403:PRO:HD3	2.03	0.41
1:G:295:ILE:HD11	1:G:354:ILE:HD11	2.03	0.41
2:H:304:SER:CA	2:H:310:LEU:HD23	2.48	0.41
3:Y:28:CYS:SG	3:Y:33:CYS:HA	2.61	0.41
1:A:286:GLN:O	1:A:290:LYS:HG3	2.21	0.41
2:B:296:ARG:HE	2:B:299:ARG:NH2	2.19	0.41
1:G:187:THR:HB	1:G:190:TRP:CG	2.55	0.41
2:H:261:VAL:HA	2:H:264:ILE:CD1	2.51	0.41
2:H:261:VAL:HA	2:H:264:ILE:HD12	2.02	0.41
2:H:323:GLU:HB2	2:H:405:ILE:CG1	2.51	0.41
2:H:61:ASP:HA	2:H:62:PRO:HD3	1.95	0.41
2:B:214:GLN:NE2	7:B:634:HOH:O	2.54	0.40
2:B:88:ILE:O	2:B:91:TYR:HB3	2.21	0.40
1:A:57:TRP:CD2	1:A:58:VAL:HG23	2.55	0.40
2:H:240:ARG:HH11	2:H:240:ARG:HG3	1.86	0.40
2:H:183:GLU:C	2:H:185:LEU:H	2.25	0.40
3:Y:9:THR:O	3:Y:10:SER:C	2.60	0.40
2:H:61:ASP:OD2	2:H:64:LYS:HG3	2.22	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	324/333 (97%)	310 (96%)	13 (4%)	1 (0%)	44	64
1	G	324/333 (97%)	315 (97%)	8 (2%)	1 (0%)	44	64
2	B	384/514 (75%)	348 (91%)	27 (7%)	9 (2%)	7	11
2	H	357/514 (70%)	291 (82%)	55 (15%)	11 (3%)	5	6
3	Y	35/37 (95%)	17 (49%)	16 (46%)	2 (6%)	2	1
All	All	1424/1731 (82%)	1281 (90%)	119 (8%)	24 (2%)	11	17

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	133	ILE
2	B	137	GLU
2	B	158	SER
2	H	373	TYR
3	Y	22	ASN
1	A	120	PHE
2	B	135	GLU
1	G	120	PHE
2	H	243	ALA
2	B	132	TYR
2	B	245	PRO
2	H	150	TRP
2	B	157	GLU
2	H	129	ASP
2	H	275	SER
3	Y	10	SER
2	B	139	PRO
2	H	160	GLY
2	H	376	MET
2	H	411	TYR
2	H	210	ILE

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Mol	Chain	Res	Type
2	B	131	GLY
2	H	96	GLY
2	H	400	LEU

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	273/280 (98%)	269 (98%)	4 (2%)	70	87
1	G	273/280 (98%)	266 (97%)	7 (3%)	51	76
2	B	332/459 (72%)	328 (99%)	4 (1%)	75	90
2	H	324/459 (71%)	321 (99%)	3 (1%)	82	93
3	Y	35/35 (100%)	33 (94%)	2 (6%)	24	41
All	All	1237/1513 (82%)	1217 (98%)	20 (2%)	68	86

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	LEU
1	A	214	GLN
1	A	326	ASN
1	A	338	GLN
2	B	34	ARG
2	B	82	ARG
2	B	86	ASP
2	B	152	LEU
1	G	73	MET
1	G	75	LEU
1	G	214	GLN
1	G	222	ARG
1	G	231	GLU
1	G	283	ARG
1	G	314	ASN
2	H	150	TRP

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Mol	Chain	Res	Type
2	H	152	LEU
2	H	263	ILE
3	Y	14	TRP
3	Y	27	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	HIS
1	A	286	GLN
1	A	326	ASN
1	A	333	ASN
1	A	338	GLN
2	B	47	GLN
2	B	53	GLN
2	B	103	ASN
2	B	146	GLN
2	B	214	GLN
2	B	253	ASN
2	B	256	ASN
2	B	414	HIS
1	G	37	GLN
1	G	71	HIS
1	G	148	GLN
1	G	204	GLN
1	G	286	GLN
1	G	293	GLN
1	G	333	ASN
2	H	53	GLN
2	H	148	GLN
2	H	213	GLN
2	H	256	ASN
2	H	281	GLN
2	H	311	GLN
2	H	414	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PCA	Y	1	3	8,8,9	0.74	0	9,10,12	0.91	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCA	Y	1	3	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 27 ligands modelled in this entry, 8 are monoatomic - leaving 19 for Mogul analysis.

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
4	NAP	A	1001	-	44,52,52	1.55	4 (9%)	51,80,80	1.78	11 (21%)
6	PGW	B	505	-	21,21,50	0.60	0	23,23,56	1.29	4 (17%)
6	PGW	B	506	-	8,8,50	0.34	0	7,7,56	0.51	0
6	PGW	B	507	-	8,8,50	0.34	0	7,7,56	0.50	0
6	PGW	B	508	-	8,8,50	0.34	0	7,7,56	0.52	0
6	PGW	B	509	-	8,8,50	0.34	0	7,7,56	0.52	0
6	PGW	B	510	-	8,8,50	0.34	0	7,7,56	0.52	0
6	PGW	B	511	-	8,8,50	0.34	0	7,7,56	0.53	0
6	PGW	B	512	-	6,6,50	0.35	0	5,5,56	0.44	0
6	PGW	B	513	-	8,8,50	0.34	0	7,7,56	0.51	0
6	PGW	B	514	-	7,7,50	0.34	0	6,6,56	0.50	0
6	PGW	B	515	-	22,22,50	0.77	0	26,27,56	1.30	5 (19%)
6	PGW	B	516	-	7,7,50	0.34	0	6,6,56	0.50	0
6	PGW	B	517	-	35,35,50	0.65	0	36,41,56	0.97	2 (5%)
6	PGW	B	518	-	6,6,50	0.35	0	5,5,56	0.43	0
6	PGW	B	519	-	7,7,50	0.34	0	6,6,56	0.49	0
6	PGW	B	520	-	7,7,50	0.34	0	6,6,56	0.49	0
4	NAP	G	1001	-	44,52,52	1.60	6 (13%)	51,80,80	1.75	10 (19%)
6	PGW	H	505	-	21,21,50	0.60	0	23,23,56	1.36	4 (17%)

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
4	NAP	A	1001	-	-	0/27/67/67	0/5/5/5
6	PGW	B	505	-	-	0/23/23/55	0/0/0/0
6	PGW	B	506	-	-	0/6/6/55	0/0/0/0
6	PGW	B	507	-	-	0/6/6/55	0/0/0/0
6	PGW	B	508	-	-	0/6/6/55	0/0/0/0
6	PGW	B	509	-	-	0/6/6/55	0/0/0/0
6	PGW	B	510	-	-	0/6/6/55	0/0/0/0
6	PGW	B	511	-	-	0/6/6/55	0/0/0/0
6	PGW	B	512	-	-	0/4/4/55	0/0/0/0
6	PGW	B	513	-	-	0/6/6/55	0/0/0/0
6	PGW	B	514	-	-	0/5/5/55	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PGW	B	515	-	-	0/24/24/55	0/0/0/0
6	PGW	B	516	-	-	0/5/5/55	0/0/0/0
6	PGW	B	517	-	-	0/40/40/55	0/0/0/0
6	PGW	B	518	-	-	0/4/4/55	0/0/0/0
6	PGW	B	519	-	-	0/5/5/55	0/0/0/0
6	PGW	B	520	-	-	0/5/5/55	0/0/0/0
4	NAP	G	1001	-	-	0/27/67/67	0/5/5/5
6	PGW	H	505	-	-	0/23/23/55	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1001	NAP	C8A-N7A	-2.59	1.29	1.34
4	G	1001	NAP	O3D-C3D	-2.12	1.38	1.43
4	A	1001	NAP	C4N-C3N	2.44	1.43	1.39
4	G	1001	NAP	C4N-C3N	2.74	1.43	1.39
4	G	1001	NAP	C2N-C3N	3.29	1.44	1.39
4	A	1001	NAP	C2N-C3N	3.43	1.44	1.39
4	A	1001	NAP	O4D-C1D	4.03	1.46	1.41
4	G	1001	NAP	O4D-C1D	4.28	1.47	1.41
4	G	1001	NAP	O4B-C1B	5.37	1.48	1.41
4	A	1001	NAP	O4B-C1B	5.50	1.48	1.41

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1001	NAP	N3A-C2A-N1A	-8.04	121.86	128.86
4	A	1001	NAP	N3A-C2A-N1A	-7.90	121.97	128.86
6	B	515	PGW	C03-C02-C01	-3.02	105.05	111.86
4	A	1001	NAP	O4B-C4B-C5B	-2.48	101.04	109.40
6	B	515	PGW	C01-O03-C19	-2.39	109.95	117.13
6	H	505	PGW	C02-O01-C1	-2.32	112.39	117.88
4	A	1001	NAP	O7N-C7N-N7N	-2.28	119.34	122.58
4	G	1001	NAP	C5D-C4D-C3D	-2.25	106.70	115.29
6	H	505	PGW	C01-O03-C19	-2.24	110.39	117.13
4	A	1001	NAP	C4A-C5A-N7A	-2.24	107.25	109.41
6	B	505	PGW	C02-O01-C1	-2.20	112.68	117.88
4	G	1001	NAP	O7N-C7N-N7N	-2.17	119.50	122.58
6	B	517	PGW	O01-C02-C01	-2.17	100.56	108.44
6	B	505	PGW	C01-O03-C19	-2.17	110.61	117.13
4	A	1001	NAP	C5D-C4D-C3D	-2.13	107.16	115.29
4	G	1001	NAP	C4A-C5A-N7A	-2.04	107.44	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1001	NAP	O4B-C4B-C5B	-2.01	102.61	109.40
4	A	1001	NAP	C3N-C7N-N7N	2.01	120.07	117.77
4	A	1001	NAP	O5B-PA-O1A	2.03	117.45	109.25
6	B	515	PGW	O11-P-O14	2.17	112.55	106.47
4	G	1001	NAP	O2B-C2B-C1B	2.23	118.36	110.06
4	G	1001	NAP	O5B-PA-O1A	2.32	118.61	109.25
4	G	1001	NAP	O4D-C4D-C3D	2.34	109.83	105.17
4	A	1001	NAP	O4D-C4D-C3D	2.38	109.90	105.17
6	B	517	PGW	O01-C1-C2	2.43	116.60	111.55
6	B	515	PGW	O03-C19-C20	2.48	119.13	111.90
6	H	505	PGW	O03-C19-C20	2.58	119.40	111.90
6	B	505	PGW	O03-C19-C20	2.58	119.42	111.90
4	G	1001	NAP	C4B-O4B-C1B	2.59	112.53	109.77
4	A	1001	NAP	C4B-O4B-C1B	2.74	112.69	109.77
4	A	1001	NAP	O2B-C2B-C3B	2.89	122.34	111.63
6	B	515	PGW	O01-C1-C2	2.97	117.71	111.55
6	B	505	PGW	O01-C1-C2	3.43	118.68	111.55
4	G	1001	NAP	C2B-C3B-C4B	3.74	110.45	101.95
4	A	1001	NAP	C2B-C3B-C4B	3.80	110.60	101.95
6	H	505	PGW	O01-C1-C2	3.89	119.63	111.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1001	NAP	11	0
6	B	505	PGW	3	0
6	B	511	PGW	3	0
6	B	515	PGW	1	0
6	B	516	PGW	2	0
6	B	517	PGW	4	0
4	G	1001	NAP	13	0
6	H	505	PGW	5	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	326/333 (97%)	0.21	9 (2%) 53 57	24, 41, 66, 89	0
1	G	326/333 (97%)	0.08	7 (2%) 64 67	27, 45, 77, 100	0
2	B	386/514 (75%)	0.79	55 (14%) 3 3	34, 70, 120, 128	0
2	H	363/514 (70%)	2.36	126 (34%) 0 0	44, 115, 191, 202	0
3	Y	36/37 (97%)	4.15	33 (91%) 0 0	80, 83, 88, 90	36 (100%)
All	All	1437/1731 (83%)	0.98	230 (16%) 2 2	24, 61, 175, 202	36 (2%)

All (230) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	272	LEU	15.6
2	H	244	CYS	14.5
2	H	280	LEU	14.1
2	H	214	GLN	13.7
2	H	215	SER	13.2
2	H	149	VAL	13.1
2	H	218	PHE	12.7
2	H	153	PHE	11.9
2	H	242	PHE	11.8
2	H	247	LYS	11.8
2	H	248	ALA	11.0
2	H	216	THR	10.6
2	H	161	PRO	10.3
2	H	282	PHE	10.2
2	H	190	ASP	10.2
2	H	241	PHE	10.1
2	H	251	PHE	9.5
2	H	245	PRO	9.3
2	H	233	PHE	8.8
2	H	150	TRP	8.8

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Mol	Chain	Res	Type	RSRZ
3	Y	17	CYS	8.8
2	H	208	SER	8.6
2	H	146	GLN	8.5
2	H	286	ARG	8.4
2	H	145	PHE	8.4
3	Y	8	THR	8.3
2	H	151	LEU	8.2
2	H	246	SER	8.2
2	H	283	GLN	8.1
2	H	250	PHE	8.1
2	H	224	ILE	7.9
2	H	285	VAL	7.9
2	H	222	PHE	7.8
2	H	217	SER	7.7
3	Y	3	THR	7.5
2	B	193	GLU	7.5
2	H	188	PHE	7.3
2	H	187	ILE	7.2
3	Y	23	THR	7.2
3	Y	5	VAL	7.2
2	H	288	VAL	7.1
2	H	203	HIS	7.1
2	H	219	THR	6.8
2	H	279	VAL	6.8
2	H	225	VAL	6.7
2	H	205	TYR	6.6
2	H	229	CYS	6.5
2	H	235	PHE	6.1
2	H	273	THR	6.1
3	Y	36	TYR	5.9
2	H	213	GLN	5.8
3	Y	4	ASN	5.8
2	H	212	TYR	5.8
2	H	249	GLY	5.7
2	H	209	THR	5.6
2	H	240	ARG	5.6
2	H	207	GLN	5.6
2	H	263	ILE	5.6
2	H	204	THR	5.6
2	H	284	ASN	5.5
2	H	164	ILE	5.5
2	H	270	ILE	5.4

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Mol	Chain	Res	Type	RSRZ
2	H	252	THR	5.3
2	H	167	ILE	5.3
2	H	238	LEU	5.2
2	H	271	PHE	5.2
2	H	232	TRP	5.1
3	Y	21	HIS	5.1
2	H	160	GLY	5.1
2	H	415	ARG	5.0
2	H	221	PRO	4.9
3	Y	16	VAL	4.9
3	Y	24	SER	4.8
2	H	262	ALA	4.8
2	H	157	GLU	4.7
3	Y	30	ASN	4.7
2	B	152	LEU	4.7
3	Y	25	ARG	4.6
2	H	276	ASN	4.6
2	B	149	VAL	4.6
3	Y	7	CYS	4.6
3	Y	9	THR	4.6
1	A	360	TYR	4.6
2	H	202	PHE	4.6
2	H	289	VAL	4.5
2	H	156	PRO	4.5
2	H	172	VAL	4.5
3	Y	28	CYS	4.4
2	H	236	GLU	4.4
1	G	36	LEU	4.4
2	H	231	ILE	4.4
2	B	192	ASN	4.3
2	B	156	PRO	4.3
2	B	157	GLU	4.3
3	Y	6	SER	4.3
2	H	154	GLU	4.3
1	G	360	TYR	4.3
2	H	287	ARG	4.3
2	B	191	GLU	4.3
2	H	147	ARG	4.2
2	B	153	PHE	4.2
2	H	189	ARG	4.1
2	B	196	HIS	4.1
2	H	417	THR	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	161	PRO	4.0
2	H	168	VAL	4.0
2	H	220	ASP	4.0
3	Y	12	GLU	4.0
2	H	106	LEU	4.0
2	H	152	LEU	4.0
2	B	162	ALA	3.9
3	Y	15	SER	3.9
3	Y	37	SER	3.9
3	Y	14	TRP	3.9
2	H	281	GLN	3.9
2	B	190	ASP	3.8
2	H	243	ALA	3.7
2	B	219	THR	3.6
2	H	165	ILE	3.6
2	H	416	GLU	3.5
2	H	228	LEU	3.5
3	Y	27	MET	3.5
2	H	414	HIS	3.5
2	B	165	ILE	3.5
2	H	155	TYR	3.4
2	H	290	GLN	3.4
2	B	158	SER	3.4
2	H	381	ILE	3.4
2	H	260	ILE	3.4
2	H	410	ASN	3.3
2	H	163	ARG	3.3
3	Y	2	PHE	3.3
2	H	237	PHE	3.3
3	Y	11	LYS	3.3
3	Y	26	GLY	3.3
2	H	63	LYS	3.3
2	B	163	ARG	3.3
2	H	223	PHE	3.2
2	H	302	LYS	3.2
1	A	36	LEU	3.2
3	Y	29	MET	3.2
2	H	173	ILE	3.1
2	H	210	ILE	3.1
2	H	411	TYR	3.1
2	H	125	MET	3.1
3	Y	18	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
2	H	206	SER	3.1
2	H	261	VAL	3.1
2	H	121	GLU	3.0
2	B	188	PHE	3.0
3	Y	20	LEU	3.0
2	H	409	PHE	3.0
1	G	349	HIS	3.0
2	B	198	GLY	2.9
2	H	306	HIS	2.9
2	B	195	MET	2.9
2	B	200	VAL	2.9
2	B	151	LEU	2.9
2	B	241	PHE	2.9
2	H	308	LYS	2.9
2	B	132	TYR	2.9
1	G	202	ALA	2.8
2	H	183	GLU	2.8
3	Y	33	CYS	2.8
2	B	125	MET	2.8
2	H	177	ILE	2.7
2	B	215	SER	2.7
3	Y	22	ASN	2.6
2	B	159	SER	2.6
2	B	160	GLY	2.6
2	H	264	ILE	2.6
2	B	247	LYS	2.6
2	H	114	ARG	2.6
2	H	171	MET	2.6
2	H	159	SER	2.6
2	B	411	TYR	2.6
2	B	168	VAL	2.5
2	B	164	ILE	2.5
2	H	291	ILE	2.5
2	H	170	VAL	2.5
2	B	242	PHE	2.5
2	H	230	ILE	2.5
2	B	218	PHE	2.5
2	B	205	TYR	2.5
2	H	255	MET	2.5
2	B	194	ASP	2.5
2	B	370	THR	2.5
2	B	114	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	262	TYR	2.4
2	H	36	VAL	2.4
2	B	120	GLU	2.4
2	B	371	VAL	2.4
2	B	251	PHE	2.3
2	B	252	THR	2.3
2	B	396	LEU	2.3
2	B	395	VAL	2.3
2	H	126	PHE	2.3
1	A	205	PHE	2.3
1	G	200	SER	2.3
2	H	274	GLU	2.3
1	A	280	GLU	2.2
2	H	257	ILE	2.2
2	H	350	ARG	2.2
2	B	232	TRP	2.2
2	B	145	PHE	2.2
2	B	106	LEU	2.2
2	B	332	PHE	2.1
3	Y	32	LYS	2.1
2	B	73	ARG	2.1
2	B	213	GLN	2.1
2	B	417	THR	2.1
2	B	189	ARG	2.1
2	H	310	LEU	2.1
2	B	243	ALA	2.1
1	G	205	PHE	2.1
3	Y	35	CYS	2.1
2	B	249	GLY	2.1
1	A	202	ALA	2.1
1	A	250	ILE	2.1
2	B	400	LEU	2.1
2	H	275	SER	2.1
2	H	191	GLU	2.1
2	H	269	THR	2.0
3	Y	10	SER	2.0
3	Y	31	LYS	2.0
1	A	265	ALA	2.0
1	G	201	VAL	2.0
2	B	248	ALA	2.0
1	A	361	SER	2.0
2	H	56	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	PCA	Y	1	8/9	0.81	0.25	-	90,90,90,91	8

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
6	PGW	B	505	22/51	0.36	0.82	19.35	92,107,120,121	0
6	PGW	B	510	9/51	0.72	0.98	14.29	104,106,107,107	0
6	PGW	H	505	22/51	0.33	0.73	8.54	139,145,148,148	0
6	PGW	B	516	8/51	0.63	0.55	8.30	90,94,99,99	0
6	PGW	B	514	8/51	0.72	0.53	4.51	80,82,84,85	0
6	PGW	B	511	9/51	0.74	0.41	3.61	122,123,124,124	0
6	PGW	B	506	9/51	0.61	0.31	3.15	81,84,88,88	0
6	PGW	B	515	23/51	0.73	0.36	2.92	128,136,138,138	0
6	PGW	B	518	7/51	0.57	0.40	2.56	72,74,75,75	0
4	NAP	G	1001	48/48	0.95	0.19	2.32	26,45,58,63	0
6	PGW	B	517	36/51	0.56	0.33	2.30	117,135,152,152	0
4	NAP	A	1001	48/48	0.96	0.19	1.07	32,42,52,55	0
5	K	B	503	1/1	0.97	0.19	-	34,34,34,34	1
6	PGW	B	512	7/51	0.82	0.19	-	76,78,79,79	0
5	K	B	504	1/1	0.99	0.16	-	39,39,39,39	1
6	PGW	B	509	9/51	0.32	0.89	-	115,115,116,116	0
6	PGW	B	507	9/51	0.54	0.35	-	94,97,98,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	K	H	501	1/1	0.99	0.41	-	53,53,53,53	1
5	K	H	502	1/1	0.95	0.30	-	55,55,55,55	1
6	PGW	B	519	8/51	0.59	0.73	-	111,114,115,115	0
5	K	B	502	1/1	0.96	0.16	-	39,39,39,39	1
6	PGW	B	520	8/51	0.38	0.41	-	96,100,103,104	0
6	PGW	B	513	9/51	0.25	0.53	-	127,129,129,129	0
5	K	H	503	1/1	0.92	0.18	-	56,56,56,56	1
5	K	B	501	1/1	1.00	0.29	-	42,42,42,42	1
5	K	H	504	1/1	0.76	0.42	-	55,55,55,55	1
6	PGW	B	508	9/51	0.79	0.40	-	96,97,98,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.