



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:57 PM GMT

PDB ID : 4JTC
Title : Crystal structure of Kv1.2-2.1 paddle chimera channel in complex with Charyb-dotoxin in Cs+
Authors : Banerjee, A.; Lee, A.; Campbell, E.; MacKinnon, R.
Deposited on : 2013-03-23
Resolution : 2.56 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

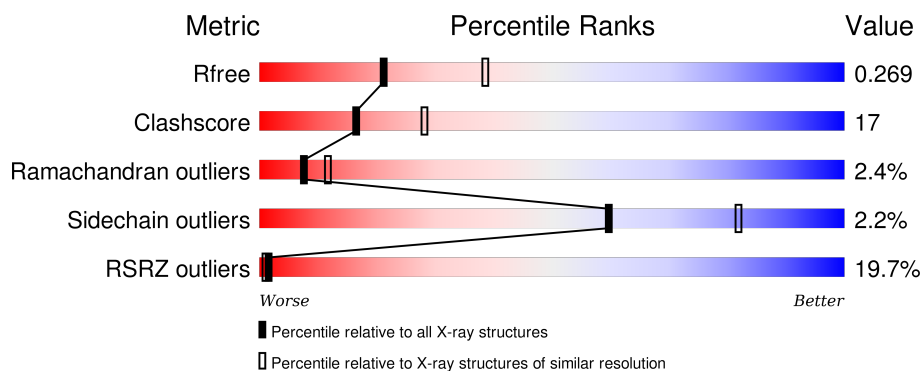
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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}	91344	3324 (2.60-2.52)
Clashscore	102246	3729 (2.60-2.52)
Ramachandran outliers	100387	3673 (2.60-2.52)
Sidechain outliers	100360	3673 (2.60-2.52)
RSRZ outliers	91569	3333 (2.60-2.52)

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	 2% 79% 17% ..
1	G	333	 2% 78% 19% ..
2	B	514	 13% 48% 25% • 25%
2	H	514	 32% 37% 31% • 29%
3	Y	37	 97% 59% 38% •

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	504	-	-	-	X
6	PGW	B	505	-	-	-	X
6	PGW	B	509	-	-	-	X
6	PGW	B	510	-	-	-	X
6	PGW	B	513	-	-	-	X
6	PGW	B	515	-	-	-	X
6	PGW	B	516	-	-	-	X
6	PGW	B	517	-	-	-	X
6	PGW	B	518	-	-	-	X
6	PGW	H	504	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11770 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

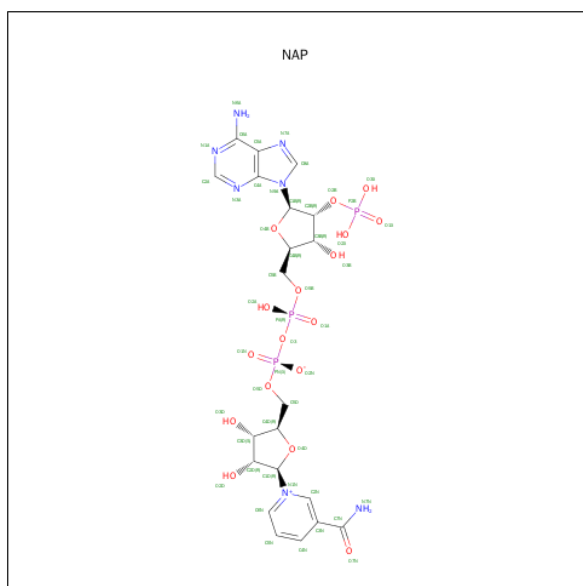
- Molecule 3 is a protein called Potassium channel toxin alpha-KTx 1.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Y	37	Total	C	N	O	S	0	0	0
			295	176	57	55	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	1	PCA	GLN	MODIFIED RESIDUE	UNP P13487

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



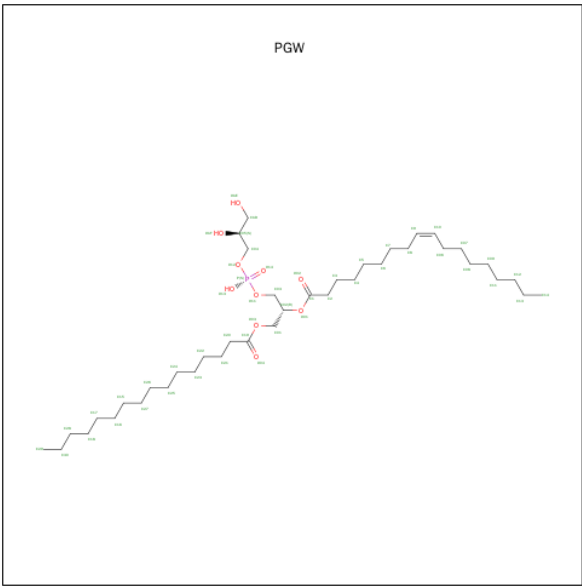
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 5 is CESIUM ION (three-letter code: CS) (formula: Cs).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	4	Total Cs 4 4	0	0
5	B	4	Total Cs 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-ENOIC ACID

TE (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
6	B	1	Total C O P 36 25 10 1	0	0

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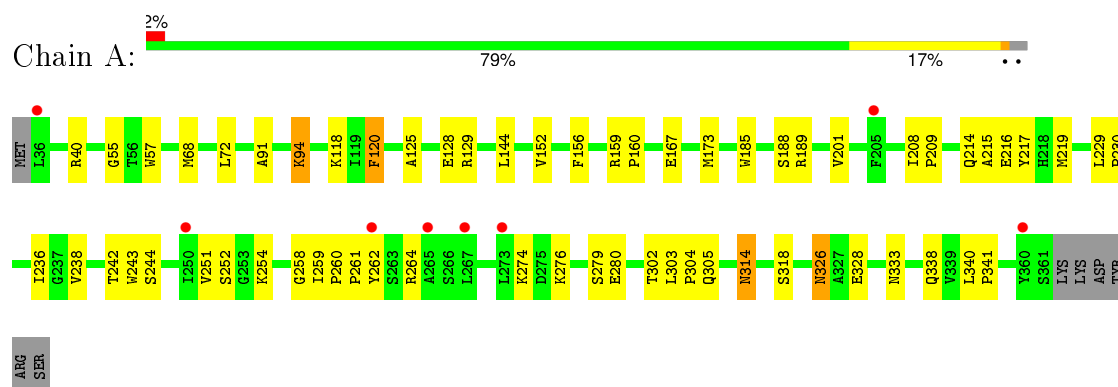
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C 7 7	0	0
6	B	1	Total C 8 8	0	0
6	B	1	Total C 8 8	0	0
6	H	1	Total C O 22 17 5	0	0

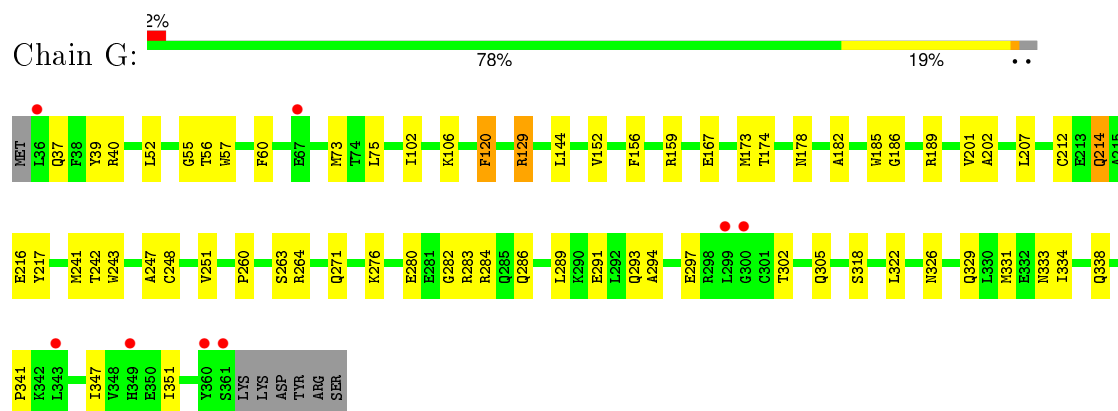
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

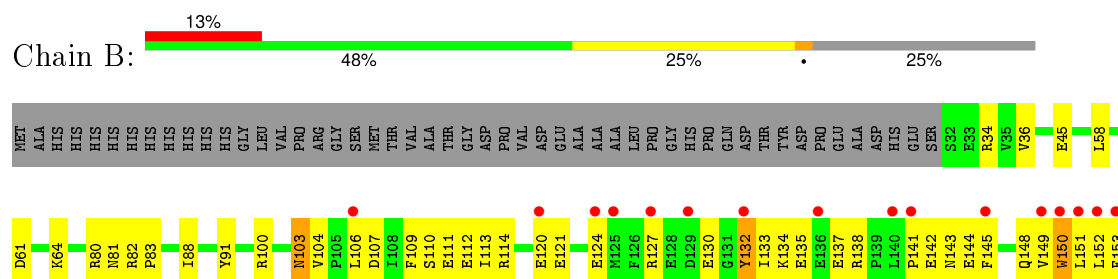
- Molecule 1: Voltage-gated potassium channel subunit beta-2

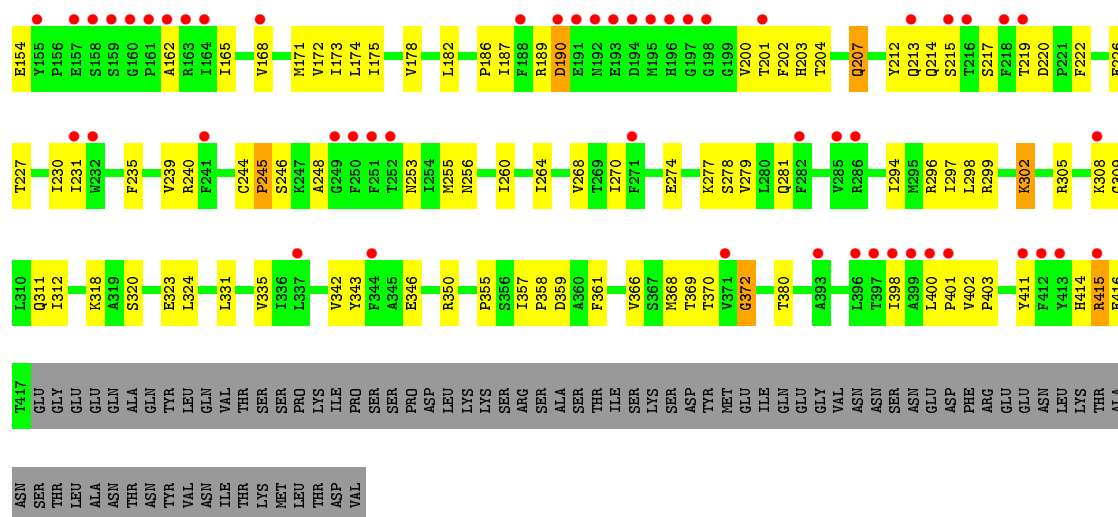


- Molecule 1: Voltage-gated potassium channel subunit beta-2

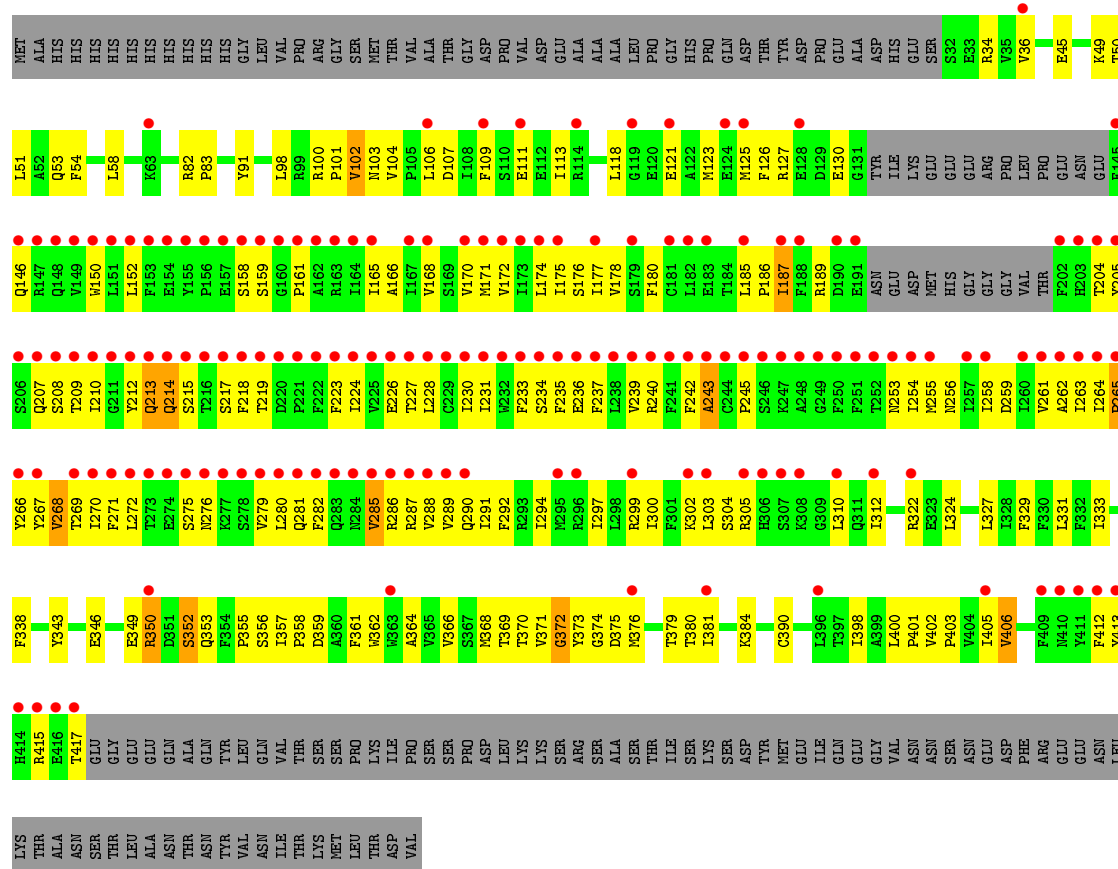


- Molecule 2: Potassium voltage-gated channel subfamily A member 2, Potassium voltage-gated channel subfamily B member 1



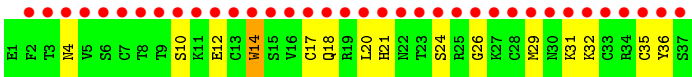


- Molecule 2: Potassium voltage-gated channel subfamily A member 2, Potassium voltage-gated channel subfamily B member 1



- 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	145.43 Å 145.43 Å 285.59 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.56 49.93 – 2.56	Depositor EDS
% Data completeness (in resolution range)	91.9 (50.00-2.56) 92.1 (49.93-2.56)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.54 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.237 , 0.262 0.243 , 0.269	Depositor DCC
R_{free} test set	4652 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 99051 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11770	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CS, PGW, NAP, PCA

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	0.42	0/2608	0.61	0/3524
1	G	0.39	0/2608	0.60	0/3524
2	B	0.37	0/3169	0.55	0/4292
2	H	0.33	0/3036	0.50	0/4114
3	Y	0.26	0/292	0.46	0/389
All	All	0.38	0/11713	0.56	0/15843

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	44	0
1	G	2556	0	2582	46	0
2	B	3088	0	3034	118	0
2	H	2959	0	2956	161	0
3	Y	295	0	282	10	0
4	A	48	0	25	11	0
4	G	48	0	25	12	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	18	0
6	H	22	0	25	7	0
All	All	11770	0	11762	391	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 (391) 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)
2:B:400:LEU:HB2	2:B:401:PRO:HD3	1.43	1.00
1:G:55:GLY:HA3	4:G:1001:NAP:O3D	1.68	0.93
2:H:213:GLN:HE21	2:H:215:SER:HB3	1.31	0.91
2:H:146:GLN:HB3	2:H:243:ALA:HA	1.51	0.90
1:A:55:GLY:HA3	4:A:1001:NAP:O3D	1.73	0.89
1:A:314:ASN:H	1:A:314:ASN:ND2	1.69	0.88
2:H:350:ARG:HB3	2:H:350:ARG:HH11	1.40	0.87
1:G:333:ASN:HD21	4:G:1001:NAP:H61A	1.22	0.87
2:H:358:PRO:HB3	6:H:504:PGW:H20A	1.61	0.83
1:G:40:ARG:HD2	1:G:318:SER:O	1.77	0.82
1:A:314:ASN:H	1:A:314:ASN:HD22	1.26	0.81
3:Y:4:ASN:HA	3:Y:32:LYS:HD3	1.62	0.81
2:H:185:LEU:HD12	2:H:186:PRO:HD2	1.63	0.80
1:A:333:ASN:HD21	4:A:1001:NAP:H61A	1.31	0.78
1:G:189:ARG:HH21	4:G:1001:NAP:H71N	1.32	0.78
2:H:358:PRO:HB3	6:H:504:PGW:C20	2.14	0.78
2:H:349:GLU:HB2	2:H:352:SER:HB2	1.66	0.76
2:B:311:GLN:HG2	6:B:516:PGW:H3	1.67	0.75
3:Y:26:GLY:HA3	3:Y:35:CYS:HA	1.69	0.74
2:H:213:GLN:HE21	2:H:215:SER:CB	2.01	0.73
1:G:293:GLN:O	1:G:297:GLU:HG3	1.89	0.72
2:H:412:PHE:HD1	2:H:415:ARG:HH21	1.34	0.72
2:B:400:LEU:O	2:B:403:PRO:HD2	1.88	0.72
2:B:227:THR:O	2:B:231:ILE:HG12	1.88	0.72
1:G:129:ARG:HB3	1:G:129:ARG:HH11	1.53	0.72
2:H:113:ILE:HG23	2:H:118:LEU:HD12	1.72	0.71
2:B:253:ASN:ND2	2:B:255:MET:HB2	2.04	0.71
2:H:177:ILE:HD11	2:H:300:ILE:HA	1.71	0.71
2:H:270:ILE:H	2:H:270:ILE:HD12	1.55	0.71
2:H:366:VAL:HG12	2:H:372:GLY:HA2	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:ASN:H	2:B:103:ASN:HD22	1.39	0.70
2:H:400:LEU:HB2	2:H:401:PRO:HD3	1.72	0.70
2:H:375:ASP:O	2:H:376:MET:HG3	1.92	0.70
2:B:120:GLU:O	2:B:124:GLU:HG3	1.92	0.69
1:A:258:GLY:O	1:A:260:PRO:HD3	1.92	0.69
1:A:118:LYS:HG3	1:A:156:PHE:HB2	1.72	0.69
2:H:364:ALA:O	2:H:368:MET:HG3	1.93	0.67
2:B:100:ARG:NH1	2:B:106:LEU:HB2	2.10	0.67
2:B:226:GLU:O	2:B:230:ILE:HD13	1.94	0.67
2:H:109:PHE:CE2	2:H:113:ILE:HD11	2.28	0.66
2:B:350:ARG:HB3	2:B:350:ARG:NH1	2.11	0.66
1:A:314:ASN:N	1:A:314:ASN:HD22	1.92	0.65
2:H:230:ILE:HG12	2:H:266:TYR:HB2	1.78	0.65
4:G:1001:NAP:H52A	4:G:1001:NAP:H8A	1.77	0.65
1:G:338:GLN:O	1:G:341:PRO:HD2	1.96	0.65
2:H:350:ARG:HH11	2:H:350:ARG:CB	2.09	0.65
4:A:1001:NAP:H52A	4:A:1001:NAP:H8A	1.79	0.65
2:B:61:ASP:HB3	2:B:64:LYS:HB2	1.79	0.65
2:B:366:VAL:HG12	2:B:372:GLY:HA2	1.80	0.64
2:B:416:GLU:HA	6:B:516:PGW:HADA	1.78	0.64
2:H:276:ASN:HB3	2:H:282:PHE:HB2	1.80	0.63
2:H:276:ASN:OD1	2:H:281:GLN:HG2	1.99	0.63
2:B:253:ASN:HD21	2:B:255:MET:HB2	1.63	0.62
2:H:213:GLN:NE2	2:H:215:SER:HB3	2.09	0.62
2:H:402:VAL:O	2:H:406:VAL:HG23	1.99	0.62
2:H:207:GLN:HE21	2:H:213:GLN:HA	1.64	0.62
2:H:270:ILE:HD12	2:H:270:ILE:N	2.15	0.62
2:B:58:LEU:HD12	2:B:64:LYS:HB3	1.80	0.62
2:H:305:ARG:HH11	2:H:305:ARG:HG2	1.65	0.62
2:H:210:ILE:HD11	2:H:214:GLN:N	2.15	0.62
2:B:400:LEU:CB	2:B:401:PRO:HD3	2.25	0.61
2:H:331:LEU:HD11	2:H:398:ILE:HG12	1.82	0.61
2:H:212:TYR:O	2:H:213:GLN:HB2	2.01	0.61
2:B:253:ASN:HB3	2:B:256:ASN:ND2	2.15	0.61
2:H:362:TRP:HB2	6:H:504:PGW:H2A	1.82	0.61
2:H:302:LYS:HA	2:H:302:LYS:HE2	1.82	0.61
2:H:230:ILE:HD12	2:H:230:ILE:N	2.16	0.61
2:H:294:ILE:O	2:H:297:ILE:HG22	2.01	0.61
2:B:187:ILE:HG21	6:B:512:PGW:H2A	1.82	0.61
2:B:100:ARG:HH11	2:B:106:LEU:HB2	1.65	0.60
2:H:381:ILE:H	2:H:381:ILE:HD12	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:331:LEU:O	2:B:335:VAL:HG23	2.01	0.60
1:A:91:ALA:O	1:A:94:LYS:HB2	2.01	0.60
2:B:255:MET:CE	2:B:305:ARG:HA	2.32	0.59
1:G:302:THR:OG1	1:G:305:GLN:HG3	2.02	0.59
2:H:36:VAL:HG22	2:H:45:GLU:HG3	1.83	0.59
2:B:186:PRO:O	2:B:190:ASP:HB2	2.02	0.59
2:B:323:GLU:CD	2:B:323:GLU:H	2.06	0.59
2:H:357:ILE:HB	2:H:358:PRO:HD3	1.83	0.59
2:B:414:HIS:C	2:B:416:GLU:H	2.04	0.58
2:H:398:ILE:HG22	2:H:398:ILE:O	2.03	0.58
3:Y:14:TRP:HA	3:Y:14:TRP:HE3	1.68	0.58
1:G:55:GLY:HA3	4:G:1001:NAP:HO3N	1.69	0.58
2:H:381:ILE:HD12	2:H:381:ILE:N	2.18	0.58
2:H:264:ILE:HB	2:H:265:PRO:HD3	1.86	0.58
6:B:516:PGW:O02	6:B:516:PGW:H03A	2.04	0.58
3:Y:14:TRP:HA	3:Y:14:TRP:CE3	2.38	0.58
2:H:161:PRO:O	2:H:165:ILE:HG13	2.04	0.58
2:B:171:MET:O	2:B:175:ILE:HG13	2.03	0.58
1:G:120:PHE:CD1	1:G:159:ARG:HG3	2.39	0.57
2:H:402:VAL:HB	2:H:403:PRO:HD3	1.86	0.57
2:H:207:GLN:NE2	2:H:213:GLN:HG3	2.18	0.57
2:H:231:ILE:O	2:H:235:PHE:HB2	2.04	0.57
2:B:142:GLU:O	2:B:144:GLU:N	2.34	0.57
2:H:415:ARG:HG2	2:H:415:ARG:HH11	1.69	0.57
1:A:259:ILE:HG13	1:A:274:LYS:HE3	1.86	0.57
2:B:149:VAL:C	2:B:151:LEU:H	2.07	0.57
2:B:201:THR:HB	2:B:204:THR:OG1	2.05	0.57
2:B:222:PHE:CE1	6:B:513:PGW:H15A	2.39	0.57
2:B:153:PHE:CD2	2:B:239:VAL:HG11	2.40	0.56
1:G:280:GLU:HG2	1:G:284:ARG:NH1	2.19	0.56
2:B:213:GLN:HE22	2:B:219:THR:HB	1.70	0.56
2:B:152:LEU:N	2:B:152:LEU:HD12	2.21	0.56
1:A:251:VAL:HG12	1:A:251:VAL:O	2.05	0.56
1:A:125:ALA:HB3	1:A:128:GLU:HG3	1.85	0.56
2:H:152:LEU:HD22	2:H:161:PRO:HG2	1.87	0.56
2:H:400:LEU:O	2:H:403:PRO:HD2	2.06	0.56
2:B:152:LEU:HA	2:B:162:ALA:HB1	1.87	0.56
2:H:346:GLU:HG2	2:H:380:THR:CG2	2.35	0.56
1:A:216:GLU:HB2	1:A:243:TRP:CZ2	2.40	0.56
2:H:58:LEU:HD23	2:H:58:LEU:C	2.25	0.55
2:B:278:SER:OG	2:B:281:GLN:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:400:LEU:HB2	2:B:401:PRO:CD	2.27	0.55
2:H:91:TYR:CE2	2:H:118:LEU:HD22	2.42	0.55
2:H:101:PRO:HB2	2:H:104:VAL:HG23	1.89	0.55
1:G:214:GLN:HA	1:G:241:MET:O	2.06	0.55
2:H:82:ARG:HB2	2:H:83:PRO:HD3	1.87	0.55
1:A:159:ARG:HA	1:A:188:SER:O	2.06	0.55
2:H:180:PHE:CE2	2:H:297:ILE:HD13	2.42	0.55
2:H:355:PRO:HB2	2:H:359:ASP:OD2	2.07	0.55
2:B:277:LYS:O	2:B:277:LYS:HG3	2.07	0.55
2:B:103:ASN:HD22	2:B:103:ASN:N	2.05	0.54
1:G:286:GLN:HA	1:G:289:LEU:HD12	1.88	0.54
2:H:327:LEU:O	2:H:331:LEU:HD13	2.08	0.54
6:B:514:PGW:O02	6:B:514:PGW:O11	2.26	0.54
2:H:121:GLU:O	2:H:125:MET:HB2	2.08	0.54
1:G:144:LEU:HD21	1:G:152:VAL:HG13	1.89	0.54
2:H:230:ILE:HG12	2:H:266:TYR:CB	2.38	0.54
1:A:159:ARG:HB2	1:A:160:PRO:HD2	1.89	0.54
2:H:285:VAL:O	2:H:285:VAL:HG22	2.08	0.54
2:H:152:LEU:O	2:H:165:ILE:HD12	2.08	0.54
2:H:107:ASP:O	2:H:111:GLU:HG3	2.07	0.54
1:G:264:ARG:NH2	4:G:1001:NAP:H4B	2.22	0.54
1:G:216:GLU:HB2	1:G:243:TRP:CH2	2.43	0.54
1:A:276:LYS:O	1:A:279:SER:HB3	2.08	0.54
2:H:253:ASN:HB3	2:H:256:ASN:OD1	2.08	0.54
2:B:255:MET:HE1	2:B:305:ARG:HA	1.88	0.53
2:B:355:PRO:HB2	2:B:359:ASP:OD2	2.08	0.53
1:G:251:VAL:O	1:G:251:VAL:HG12	2.08	0.53
2:H:324:LEU:HD13	2:H:405:ILE:HD13	1.91	0.53
2:H:236:GLU:HA	2:H:239:VAL:CG2	2.38	0.53
2:B:201:THR:HG22	2:B:202:PHE:N	2.23	0.53
1:G:280:GLU:HG2	1:G:284:ARG:HH12	1.73	0.53
2:B:127:ARG:HG2	2:B:132:TYR:HB2	1.90	0.53
2:B:294:ILE:O	2:B:297:ILE:HG22	2.09	0.53
2:B:36:VAL:HG22	2:B:45:GLU:HG2	1.92	0.52
2:H:224:ILE:O	2:H:228:LEU:HG	2.09	0.52
2:B:88:ILE:O	2:B:91:TYR:HB3	2.10	0.52
2:H:287:ARG:HG2	2:H:290:GLN:OE1	2.10	0.52
2:H:361:PHE:HB3	6:H:504:PGW:H4	1.91	0.52
2:H:303:LEU:O	2:H:310:LEU:HD23	2.10	0.52
1:G:247:ALA:O	1:G:248:CYS:HB2	2.10	0.52
2:H:210:ILE:HG21	2:H:269:THR:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:120:PHE:O	1:G:129:ARG:HA	2.10	0.52
2:H:230:ILE:H	2:H:230:ILE:HD12	1.73	0.51
2:B:110:SER:O	2:B:114:ARG:HG3	2.10	0.51
2:B:153:PHE:CE1	2:B:165:ILE:HD13	2.45	0.51
6:H:504:PGW:H01	6:H:504:PGW:O02	2.09	0.51
2:H:268:VAL:HG12	2:H:268:VAL:O	2.10	0.51
1:G:291:GLU:O	1:G:294:ALA:HB3	2.10	0.51
3:Y:29:MET:C	3:Y:31:LYS:H	2.13	0.51
1:A:302:THR:OG1	1:A:305:GLN:HG3	2.10	0.51
2:B:178:VAL:O	2:B:182:LEU:HG	2.10	0.51
1:G:37:GLN:HA	1:G:37:GLN:NE2	2.25	0.51
2:H:279:VAL:HG12	2:H:279:VAL:O	2.11	0.51
1:G:331:MET:HE2	1:G:334:ILE:HD12	1.93	0.51
2:H:381:ILE:CD1	2:H:381:ILE:H	2.24	0.51
2:H:168:VAL:O	2:H:172:VAL:HG23	2.11	0.51
6:B:510:PGW:H2	6:B:515:PGW:H16	1.93	0.51
2:H:210:ILE:HD12	2:H:212:TYR:CE1	2.46	0.50
2:B:414:HIS:O	2:B:416:GLU:N	2.39	0.50
2:B:203:HIS:HE1	2:B:277:LYS:NZ	2.09	0.50
1:A:303:LEU:HB3	1:A:304:PRO:HD3	1.94	0.50
1:G:217:TYR:HB3	1:G:242:THR:HB	1.93	0.50
2:H:205:TYR:CE2	2:H:279:VAL:HG13	2.47	0.50
2:B:107:ASP:O	2:B:111:GLU:HG3	2.12	0.50
1:A:216:GLU:HB2	1:A:243:TRP:CH2	2.45	0.50
1:G:189:ARG:NH2	4:G:1001:NAP:H71N	2.04	0.50
2:H:213:GLN:HG2	2:H:215:SER:HB3	1.94	0.50
2:H:368:MET:C	2:H:370:THR:H	2.15	0.50
6:B:504:PGW:H01	6:B:504:PGW:O02	2.12	0.50
2:B:253:ASN:HB3	2:B:256:ASN:HD22	1.76	0.50
2:H:152:LEU:HD22	2:H:161:PRO:CG	2.42	0.50
2:H:353:GLN:O	2:H:355:PRO:HD3	2.10	0.50
2:H:150:TRP:HB2	2:H:243:ALA:HB1	1.93	0.49
2:B:402:VAL:HB	2:B:403:PRO:HD3	1.94	0.49
2:H:322:ARG:HG3	2:H:322:ARG:HH11	1.77	0.49
1:A:144:LEU:HD21	1:A:152:VAL:HG13	1.93	0.49
1:A:217:TYR:HB3	1:A:242:THR:HB	1.95	0.49
1:G:55:GLY:CA	4:G:1001:NAP:O3D	2.50	0.49
1:A:120:PHE:O	1:A:129:ARG:HA	2.13	0.49
6:B:510:PGW:C2	6:B:515:PGW:H16	2.42	0.49
1:A:55:GLY:CA	4:A:1001:NAP:O3D	2.52	0.49
2:H:177:ILE:O	2:H:180:PHE:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:152:LEU:HA	2:B:162:ALA:CB	2.42	0.49
2:H:176:SER:HB2	2:H:299:ARG:NH1	2.27	0.49
3:Y:20:LEU:HD12	3:Y:20:LEU:N	2.28	0.49
2:H:106:LEU:HD11	2:H:130:GLU:HG2	1.92	0.49
2:H:212:TYR:CE2	2:H:226:GLU:HG2	2.46	0.49
2:H:146:GLN:HG3	2:H:242:PHE:O	2.12	0.49
2:B:145:PHE:O	2:B:148:GLN:HB3	2.13	0.49
2:B:213:GLN:HB3	2:B:220:ASP:HB2	1.93	0.49
2:B:299:ARG:O	2:B:302:LYS:HB2	2.12	0.49
2:B:320:SER:O	2:B:324:LEU:HB2	2.12	0.49
2:B:369:THR:HA	2:B:398:ILE:HD11	1.94	0.49
2:B:361:PHE:HB2	6:B:504:PGW:H2	1.94	0.49
2:B:150:TRP:CE2	2:B:154:GLU:HG2	2.48	0.49
1:A:57:TRP:HB3	4:A:1001:NAP:H3D	1.93	0.49
6:H:504:PGW:H03A	6:H:504:PGW:O02	2.12	0.49
2:B:109:PHE:CE2	2:B:113:ILE:HD11	2.48	0.49
2:H:267:TYR:C	2:H:269:THR:H	2.16	0.48
2:H:187:ILE:O	2:H:187:ILE:HG22	2.13	0.48
2:H:224:ILE:N	2:H:224:ILE:HD12	2.27	0.48
2:H:127:ARG:HH11	2:H:127:ARG:HG2	1.78	0.48
1:A:326:ASN:HD22	1:A:328:GLU:H	1.61	0.48
2:H:287:ARG:HH11	2:H:287:ARG:HB3	1.79	0.48
2:B:260:ILE:O	2:B:264:ILE:HG13	2.14	0.48
2:B:246:SER:C	2:B:248:ALA:H	2.17	0.48
2:B:318:LYS:HD2	6:B:516:PGW:H22	1.95	0.48
1:G:333:ASN:ND2	4:G:1001:NAP:H61A	2.01	0.48
6:B:510:PGW:C1	6:B:515:PGW:H16	2.43	0.48
2:H:171:MET:HB3	2:H:175:ILE:HD12	1.96	0.48
1:G:52:LEU:HD13	1:G:322:LEU:HD11	1.95	0.48
2:B:235:PHE:O	2:B:239:VAL:HG23	2.13	0.48
2:H:123:MET:O	2:H:127:ARG:HG3	2.13	0.48
2:B:153:PHE:CE2	2:B:239:VAL:HG11	2.48	0.48
1:G:156:PHE:HA	1:G:186:GLY:O	2.13	0.48
2:H:234:SER:HA	2:H:237:PHE:HB2	1.96	0.48
2:H:210:ILE:HD11	2:H:213:GLN:C	2.35	0.48
2:H:152:LEU:HA	2:H:158:SER:OG	2.14	0.48
3:Y:17:CYS:O	3:Y:21:HIS:HB2	2.14	0.48
2:H:253:ASN:HD21	2:H:255:MET:HE3	1.78	0.47
2:H:204:THR:HG23	2:H:208:SER:OG	2.13	0.47
2:B:127:ARG:CG	2:B:132:TYR:HB2	2.43	0.47
2:H:358:PRO:HB3	6:H:504:PGW:H20	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:240:ARG:NH2	2:B:305:ARG:HD3	2.29	0.47
2:H:374:GLY:C	2:H:376:MET:H	2.18	0.47
2:H:231:ILE:HG22	2:H:231:ILE:O	2.13	0.47
2:H:280:LEU:HD12	2:H:280:LEU:N	2.30	0.47
1:A:229:LEU:N	1:A:230:PRO:CD	2.77	0.47
2:H:180:PHE:HE2	2:H:297:ILE:HD13	1.77	0.47
2:B:309:GLY:HA2	2:B:312:ILE:HD12	1.94	0.47
2:B:311:GLN:HA	6:B:516:PGW:H5	1.96	0.47
1:G:329:GLN:OE1	4:G:1001:NAP:H2B	2.14	0.47
4:A:1001:NAP:H52N	4:A:1001:NAP:H6N	1.97	0.47
2:H:127:ARG:NH1	2:H:127:ARG:HG2	2.30	0.47
2:B:368:MET:C	2:B:370:THR:H	2.18	0.47
2:H:327:LEU:HD11	2:H:398:ILE:HG23	1.97	0.47
2:B:366:VAL:CG1	2:B:372:GLY:HA2	2.44	0.47
2:B:264:ILE:O	2:B:268:VAL:HG23	2.15	0.47
2:B:174:LEU:O	2:B:178:VAL:HG23	2.15	0.46
2:H:175:ILE:O	2:H:175:ILE:HG22	2.14	0.46
2:H:366:VAL:O	2:H:372:GLY:N	2.45	0.46
2:H:369:THR:OG1	2:H:371:VAL:HG23	2.15	0.46
2:B:240:ARG:HH21	2:B:305:ARG:HD3	1.81	0.46
2:B:414:HIS:C	2:B:416:GLU:N	2.69	0.46
2:B:173:ILE:HD13	2:B:302:LYS:HB3	1.98	0.46
1:A:215:ALA:O	1:A:242:THR:HA	2.15	0.46
2:B:350:ARG:CB	2:B:350:ARG:NH1	2.79	0.46
1:G:37:GLN:HA	1:G:37:GLN:HE21	1.80	0.46
2:B:200:VAL:O	2:B:200:VAL:HG23	2.15	0.46
2:B:80:ARG:NH1	2:B:112:GLU:OE1	2.48	0.46
1:G:167:GLU:HA	1:G:201:VAL:HG11	1.97	0.46
2:H:53:GLN:HB3	2:H:54:PHE:CD1	2.51	0.46
1:A:188:SER:O	1:A:189:ARG:HB2	2.16	0.46
2:H:240:ARG:HH12	2:H:305:ARG:CD	2.29	0.46
2:B:320:SER:HA	2:B:323:GLU:OE2	2.16	0.46
2:B:202:PHE:HB2	2:B:279:VAL:HG22	1.98	0.46
1:G:37:GLN:HG3	1:G:39:TYR:O	2.16	0.46
2:H:312:ILE:HD13	2:H:413:TYR:HA	1.98	0.46
2:H:98:LEU:HD21	2:H:113:ILE:HD13	1.97	0.46
1:A:326:ASN:ND2	1:A:328:GLU:HB2	2.31	0.46
1:A:120:PHE:CD1	1:A:159:ARG:HG3	2.52	0.45
1:A:254:LYS:HE3	4:A:1001:NAP:N3A	2.32	0.45
2:B:212:TYR:CE2	2:B:226:GLU:HG2	2.51	0.45
2:B:207:GLN:O	2:B:207:GLN:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:173:MET:HG3	1:G:185:TRP:CE3	2.52	0.45
2:H:262:ALA:HB1	2:H:302:LYS:HD2	1.98	0.45
2:H:286:ARG:HG2	2:H:286:ARG:HH11	1.81	0.45
2:H:291:ILE:HG22	2:H:291:ILE:O	2.16	0.45
1:A:189:ARG:HH21	4:A:1001:NAP:H71N	1.64	0.45
2:B:168:VAL:O	2:B:172:VAL:HG23	2.17	0.45
1:A:252:SER:OG	1:A:254:LYS:HG2	2.16	0.45
2:H:415:ARG:C	2:H:417:THR:H	2.20	0.45
2:H:204:THR:O	2:H:204:THR:HG22	2.17	0.45
1:G:260:PRO:HG2	1:G:263:SER:HB3	1.98	0.45
2:H:276:ASN:HD21	2:H:285:VAL:HG11	1.81	0.45
1:G:251:VAL:CG1	1:G:251:VAL:O	2.65	0.45
2:B:189:ARG:HG3	2:B:189:ARG:HH11	1.82	0.45
2:H:230:ILE:HG23	2:H:263:ILE:HG22	1.99	0.45
2:H:288:VAL:O	2:H:288:VAL:HG12	2.17	0.45
3:Y:26:GLY:HA2	3:Y:36:TYR:HD1	1.82	0.45
2:H:302:LYS:C	2:H:304:SER:H	2.20	0.45
2:B:149:VAL:O	2:B:151:LEU:N	2.50	0.44
2:H:219:THR:O	2:H:219:THR:HG22	2.16	0.44
2:H:270:ILE:H	2:H:270:ILE:CD1	2.27	0.44
2:H:305:ARG:HG2	2:H:305:ARG:NH1	2.30	0.44
2:H:346:GLU:HG2	2:H:380:THR:HG23	2.00	0.44
1:A:340:LEU:HB3	1:A:341:PRO:HD3	1.98	0.44
2:B:350:ARG:HH11	2:B:350:ARG:CB	2.29	0.44
2:B:270:ILE:O	2:B:274:GLU:HG2	2.17	0.44
1:G:57:TRP:HB3	4:G:1001:NAP:H3D	1.99	0.44
2:H:276:ASN:ND2	2:H:285:VAL:HG11	2.33	0.44
1:G:189:ARG:NE	4:G:1001:NAP:N7N	2.66	0.44
2:H:285:VAL:HG23	2:H:288:VAL:HG21	1.99	0.44
1:A:40:ARG:HD2	1:A:318:SER:O	2.17	0.44
2:H:227:THR:HG23	2:H:231:ILE:HG13	1.99	0.44
2:B:411:TYR:CE1	2:B:415:ARG:HD3	2.53	0.44
2:H:287:ARG:NH1	2:H:287:ARG:HB3	2.32	0.44
2:H:106:LEU:CD1	2:H:130:GLU:HG2	2.48	0.44
2:B:357:ILE:HB	2:B:358:PRO:HD3	2.00	0.44
1:G:56:THR:HB	1:G:60:PHE:HB2	1.98	0.44
2:H:343:TYR:HE1	2:H:355:PRO:O	2.01	0.44
1:G:202:ALA:HA	1:G:207:LEU:HB2	1.99	0.44
2:H:102:VAL:HG23	2:H:102:VAL:O	2.17	0.44
2:H:258:ILE:O	2:H:258:ILE:HG22	2.18	0.44
3:Y:10:SER:C	3:Y:12:GLU:H	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ARG:NH2	4:A:1001:NAP:H4B	2.33	0.43
2:H:152:LEU:HB3	2:H:159:SER:OG	2.17	0.43
2:B:296:ARG:HE	2:B:299:ARG:NH2	2.16	0.43
2:H:174:LEU:O	2:H:178:VAL:HG23	2.18	0.43
2:H:343:TYR:CE1	2:H:356:SER:HA	2.53	0.43
2:H:368:MET:C	2:H:370:THR:N	2.71	0.43
1:G:152:VAL:O	1:G:182:ALA:HA	2.18	0.43
2:B:297:ILE:C	2:B:299:ARG:H	2.20	0.43
2:B:214:GLN:O	2:B:215:SER:HB2	2.18	0.43
2:H:259:ASP:CG	2:H:305:ARG:HH21	2.21	0.43
2:H:322:ARG:HG3	2:H:322:ARG:NH1	2.33	0.43
2:H:189:ARG:HH11	2:H:189:ARG:HG3	1.84	0.43
2:B:152:LEU:HB3	2:B:165:ILE:HD12	2.01	0.43
1:A:125:ALA:HB3	1:A:128:GLU:CG	2.48	0.43
2:B:81:ASN:OD1	2:B:83:PRO:HD2	2.19	0.43
2:B:106:LEU:CD1	2:B:130:GLU:HG2	2.49	0.43
2:B:149:VAL:HA	2:B:152:LEU:HD13	2.00	0.43
2:H:172:VAL:HG12	2:H:233:PHE:CZ	2.54	0.43
2:B:308:LYS:O	2:B:312:ILE:HG13	2.19	0.42
2:B:215:SER:C	2:B:217:SER:H	2.22	0.42
2:H:271:PHE:O	2:H:271:PHE:CG	2.72	0.42
2:H:212:TYR:OH	2:H:269:THR:HG21	2.19	0.42
2:B:415:ARG:O	6:B:516:PGW:HADA	2.19	0.42
2:H:230:ILE:H	2:H:230:ILE:CD1	2.32	0.42
2:H:329:PHE:O	2:H:333:ILE:HG12	2.19	0.42
2:B:149:VAL:C	2:B:151:LEU:N	2.73	0.42
1:A:173:MET:HG3	1:A:185:TRP:CE3	2.54	0.42
2:H:379:THR:HA	2:H:384:LYS:HE3	2.01	0.42
1:A:244:SER:HA	4:A:1001:NAP:O3	2.19	0.42
2:H:261:VAL:HA	2:H:264:ILE:CD1	2.50	0.42
2:B:246:SER:C	2:B:248:ALA:N	2.73	0.42
2:H:338:PHE:CE2	2:H:390:CYS:HA	2.55	0.42
2:B:100:ARG:HG3	2:B:109:PHE:CG	2.55	0.42
2:B:106:LEU:HD13	2:B:130:GLU:HG2	2.01	0.42
2:B:350:ARG:CZ	2:B:350:ARG:HB3	2.50	0.42
2:H:230:ILE:HG21	2:H:266:TYR:HB3	2.02	0.42
6:B:504:PGW:H03A	6:B:504:PGW:O02	2.20	0.42
2:B:80:ARG:NH1	2:B:112:GLU:OE2	2.52	0.42
1:G:347:ILE:O	1:G:351:ILE:HG13	2.20	0.42
1:G:276:LYS:O	1:G:282:GLY:HA3	2.19	0.41
2:H:100:ARG:HB2	2:H:126:PHE:HE1	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:318:LYS:CD	6:B:516:PGW:H22	2.50	0.41
2:B:311:GLN:CG	6:B:516:PGW:H3	2.43	0.41
2:H:312:ILE:CD1	2:H:413:TYR:HD1	2.32	0.41
2:H:254:ILE:C	2:H:256:ASN:H	2.23	0.41
1:A:208:ILE:HA	1:A:209:PRO:HD3	1.83	0.41
2:H:272:LEU:CD2	2:H:289:VAL:HG22	2.50	0.41
2:H:49:LYS:HG3	2:H:50:THR:N	2.36	0.41
2:H:166:ALA:O	2:H:170:VAL:HG23	2.20	0.41
2:B:109:PHE:O	2:B:113:ILE:HG13	2.21	0.41
2:H:236:GLU:HA	2:H:239:VAL:HG23	2.02	0.41
2:B:342:VAL:CG1	2:B:343:TYR:N	2.84	0.41
1:A:333:ASN:ND2	4:A:1001:NAP:H61A	2.09	0.41
2:H:264:ILE:O	2:H:268:VAL:HG23	2.21	0.41
2:B:202:PHE:HB2	2:B:279:VAL:CG2	2.51	0.41
2:H:171:MET:HE2	2:H:174:LEU:HD12	2.03	0.41
1:A:261:PRO:O	1:A:262:TYR:HB2	2.20	0.41
2:B:150:TRP:CG	2:B:150:TRP:O	2.73	0.41
2:B:83:PRO:HB2	2:B:104:VAL:HG22	2.03	0.41
2:B:346:GLU:OE2	2:B:380:THR:HG23	2.21	0.41
1:G:174:THR:HG22	1:G:178:ASN:ND2	2.36	0.41
2:H:400:LEU:C	2:H:403:PRO:HD2	2.40	0.40
2:B:368:MET:C	2:B:370:THR:N	2.73	0.40
1:A:236:ILE:HG13	1:A:238:VAL:HG23	2.02	0.40
2:B:187:ILE:HG21	6:B:512:PGW:C2	2.49	0.40
2:H:261:VAL:HA	2:H:264:ILE:HD12	2.02	0.40
1:A:167:GLU:HA	1:A:201:VAL:HG11	2.03	0.40
1:G:326:ASN:OD1	1:G:329:GLN:HG3	2.21	0.40
2:H:51:LEU:C	2:H:53:GLN:H	2.25	0.40
1:G:102:ILE:O	1:G:106:LYS:HG2	2.22	0.40
3:Y:26:GLY:HA2	3:Y:36:TYR:CD1	2.56	0.40
1:A:68:MET:O	1:A:72:LEU:HG	2.20	0.40
2:B:244:CYS:HA	2:B:245:PRO:HD3	1.90	0.40
2:H:172:VAL:O	2:H:176:SER:HB3	2.21	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%)	308 (95%)	14 (4%)	2 (1%)	30	52
1	G	324/333 (97%)	313 (97%)	10 (3%)	1 (0%)	46	68
2	B	384/514 (75%)	344 (90%)	27 (7%)	13 (3%)	5	6
2	H	357/514 (70%)	280 (78%)	60 (17%)	17 (5%)	3	3
3	Y	35/37 (95%)	17 (49%)	17 (49%)	1 (3%)	6	8
All	All	1424/1731 (82%)	1262 (89%)	128 (9%)	34 (2%)	7	12

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	132	TYR
2	B	133	ILE
2	B	134	LYS
2	B	135	GLU
2	B	137	GLU
2	H	275	SER
2	H	285	VAL
1	A	120	PHE
2	B	150	TRP
2	B	372	GLY
1	G	120	PHE
2	H	102	VAL
2	H	213	GLN
2	H	243	ALA
2	H	245	PRO
2	H	268	VAL
2	H	372	GLY
2	H	103	ASN
2	H	217	SER
1	A	219	MET
2	B	138	ARG

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Mol	Chain	Res	Type
2	B	141	PRO
2	B	143	ASN
2	B	298	LEU
2	B	415	ARG
2	H	218	PHE
2	H	373	TYR
3	Y	24	SER
2	B	245	PRO
2	H	209	THR
2	H	352	SER
2	H	187	ILE
2	H	265	PRO
2	H	406	VAL

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%)	267 (98%)	6 (2%)	60	82
1	G	273/280 (98%)	266 (97%)	7 (3%)	54	77
2	B	332/459 (72%)	325 (98%)	7 (2%)	61	83
2	H	324/459 (71%)	319 (98%)	5 (2%)	72	88
3	Y	35/35 (100%)	33 (94%)	2 (6%)	25	46
All	All	1237/1513 (82%)	1210 (98%)	27 (2%)	60	82

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

Mol	Chain	Res	Type
1	A	94	LYS
1	A	214	GLN
1	A	280	GLU
1	A	314	ASN
1	A	326	ASN
1	A	338	GLN

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Mol	Chain	Res	Type
2	B	34	ARG
2	B	82	ARG
2	B	103	ASN
2	B	121	GLU
2	B	190	ASP
2	B	207	GLN
2	B	302	LYS
1	G	73	MET
1	G	75	LEU
1	G	129	ARG
1	G	212	CYS
1	G	214	GLN
1	G	271	GLN
1	G	283	ARG
2	H	34	ARG
2	H	214	GLN
2	H	223	PHE
2	H	292	PHE
2	H	350	ARG
3	Y	14	TRP
3	Y	18	GLN

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

Mol	Chain	Res	Type
1	A	71	HIS
1	A	204	GLN
1	A	286	GLN
1	A	314	ASN
1	A	326	ASN
1	A	333	ASN
1	A	338	GLN
2	B	53	GLN
2	B	103	ASN
2	B	203	HIS
2	B	207	GLN
2	B	213	GLN
2	B	253	ASN
2	B	256	ASN
1	G	37	GLN
1	G	148	GLN
1	G	178	ASN

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Mol	Chain	Res	Type
1	G	333	ASN
2	H	53	GLN
2	H	207	GLN
2	H	213	GLN
2	H	284	ASN
3	Y	18	GLN

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	7,8,9	0.57	0	9,10,12	1.02	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	-	42,52,52	1.72	3 (7%)	54,80,80	2.57	14 (25%)
6	PGW	B	504	-	21,21,50	0.60	0	23,23,56	1.25	4 (17%)
6	PGW	B	505	-	8,8,50	0.34	0	7,7,56	0.52	0
6	PGW	B	506	-	8,8,50	0.34	0	7,7,56	0.50	0
6	PGW	B	507	-	8,8,50	0.34	0	7,7,56	0.54	0
6	PGW	B	508	-	8,8,50	0.34	0	7,7,56	0.53	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	-	6,6,50	0.35	0	5,5,56	0.45	0
6	PGW	B	512	-	8,8,50	0.34	0	7,7,56	0.51	0
6	PGW	B	513	-	7,7,50	0.35	0	6,6,56	0.50	0
6	PGW	B	514	-	22,22,50	0.82	0	25,27,56	1.29	5 (20%)
6	PGW	B	515	-	7,7,50	0.34	0	6,6,56	0.49	0
6	PGW	B	516	-	35,35,50	0.66	0	36,41,56	0.94	3 (8%)
6	PGW	B	517	-	6,6,50	0.35	0	5,5,56	0.42	0
6	PGW	B	518	-	7,7,50	0.34	0	6,6,56	0.49	0
6	PGW	B	519	-	7,7,50	0.35	0	6,6,56	0.49	0
4	NAP	G	1001	-	42,52,52	1.67	7 (16%)	54,80,80	2.60	16 (29%)
6	PGW	H	504	-	21,21,50	0.60	0	23,23,56	1.31	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	504	-	-	0/23/23/55	0/0/0/0
6	PGW	B	505	-	-	0/6/6/55	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	-	-	0/4/4/55	0/0/0/0
6	PGW	B	512	-	-	0/6/6/55	0/0/0/0
6	PGW	B	513	-	-	0/5/5/55	0/0/0/0
6	PGW	B	514	-	-	0/24/24/55	0/0/0/0
6	PGW	B	515	-	-	0/5/5/55	0/0/0/0
6	PGW	B	516	-	-	0/40/40/55	0/0/0/0
6	PGW	B	517	-	-	0/4/4/55	0/0/0/0
6	PGW	B	518	-	-	0/5/5/55	0/0/0/0
6	PGW	B	519	-	-	0/5/5/55	0/0/0/0
4	NAP	G	1001	-	-	0/27/67/67	0/5/5/5
6	PGW	H	504	-	-	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	O3D-C3D	-2.29	1.37	1.43
4	G	1001	NAP	C8A-N7A	-2.28	1.30	1.34
4	G	1001	NAP	P2B-O3X	2.06	1.62	1.54
4	G	1001	NAP	C4N-C3N	2.33	1.43	1.39
4	G	1001	NAP	C2N-C3N	2.78	1.43	1.39
4	A	1001	NAP	C2N-C3N	3.52	1.44	1.39
4	G	1001	NAP	O4D-C1D	4.02	1.46	1.41
4	A	1001	NAP	O4D-C1D	4.90	1.47	1.41
4	G	1001	NAP	O4B-C1B	6.35	1.49	1.41
4	A	1001	NAP	O4B-C1B	6.40	1.49	1.41

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1001	NAP	N3A-C2A-N1A	-9.23	121.83	128.89
4	A	1001	NAP	N3A-C2A-N1A	-8.88	122.10	128.89
4	G	1001	NAP	PN-O3-PA	-8.23	109.62	132.73
4	A	1001	NAP	PN-O3-PA	-8.00	110.26	132.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	NAP	O3-PA-O5B	-6.89	84.66	102.94
4	G	1001	NAP	O3-PA-O5B	-6.60	85.43	102.94
4	A	1001	NAP	O2A-PA-O3	-3.44	89.48	105.09
4	G	1001	NAP	O2A-PA-O3	-3.24	90.39	105.09
6	B	514	PGW	C03-C02-C01	-2.82	105.47	112.07
4	A	1001	NAP	O4B-C4B-C5B	-2.65	99.86	109.32
4	G	1001	NAP	O4B-C4B-C5B	-2.63	99.92	109.32
4	A	1001	NAP	C4A-C5A-N7A	-2.47	107.21	109.48
4	G	1001	NAP	C4A-C5A-N7A	-2.42	107.25	109.48
6	H	504	PGW	C01-O03-C19	-2.40	110.13	116.85
6	B	514	PGW	C01-O03-C19	-2.39	110.16	116.85
4	A	1001	NAP	O7N-C7N-N7N	-2.25	119.43	122.59
6	B	504	PGW	C01-O03-C19	-2.24	110.58	116.85
4	G	1001	NAP	O7N-C7N-N7N	-2.16	119.56	122.59
6	B	516	PGW	O01-C02-C01	-2.14	100.81	108.36
6	H	504	PGW	C02-O01-C1	-2.14	112.76	117.89
6	B	504	PGW	C02-O01-C1	-2.09	112.87	117.89
6	B	516	PGW	O03-C01-C02	-2.07	103.12	108.69
4	G	1001	NAP	C5D-C4D-C3D	-2.05	107.08	115.21
4	A	1001	NAP	O4D-C4D-C3D	2.02	109.22	105.15
4	G	1001	NAP	O5B-PA-O1A	2.10	117.76	109.62
6	B	514	PGW	O11-P-O14	2.19	112.72	107.14
4	G	1001	NAP	O2B-P2B-O1X	2.23	112.68	107.11
6	B	516	PGW	O01-C1-C2	2.43	116.81	111.53
6	B	514	PGW	O03-C19-C20	2.43	119.31	111.90
6	B	504	PGW	O03-C19-C20	2.44	119.33	111.90
6	H	504	PGW	O03-C19-C20	2.53	119.61	111.90
6	B	514	PGW	O01-C1-C2	2.75	117.50	111.53
4	A	1001	NAP	C4B-O4B-C1B	2.91	112.91	109.72
4	G	1001	NAP	O2B-C2B-C3B	3.09	123.51	111.51
4	A	1001	NAP	O3-PN-O5D	3.18	111.39	102.94
4	G	1001	NAP	C4B-O4B-C1B	3.28	113.33	109.72
6	B	504	PGW	O01-C1-C2	3.30	118.70	111.53
6	H	504	PGW	O01-C1-C2	3.51	119.17	111.53
4	A	1001	NAP	O2B-C2B-C3B	3.53	125.22	111.51
4	G	1001	NAP	O3-PN-O5D	3.53	112.30	102.94
4	G	1001	NAP	C2B-C3B-C4B	3.56	110.28	101.85
4	A	1001	NAP	C2B-C3B-C4B	3.58	110.34	101.85
4	G	1001	NAP	O4D-C1D-N1N	3.96	112.48	108.13
4	A	1001	NAP	O4D-C1D-N1N	4.03	112.56	108.13
4	G	1001	NAP	O4B-C1B-N9A	5.29	119.17	108.10
4	A	1001	NAP	O4B-C1B-N9A	5.37	119.35	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1001	NAP	11	0
6	B	504	PGW	3	0
6	B	510	PGW	3	0
6	B	512	PGW	2	0
6	B	513	PGW	1	0
6	B	514	PGW	1	0
6	B	515	PGW	3	0
6	B	516	PGW	8	0
4	G	1001	NAP	12	0
6	H	504	PGW	7	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	326/333 (97%)	0.28	8 (2%) 61 59	17, 33, 60, 83	0
1	G	326/333 (97%)	0.20	8 (2%) 61 59	21, 39, 72, 96	0
2	B	386/514 (75%)	0.96	68 (17%) 2 1	25, 66, 110, 125	0
2	H	363/514 (70%)	3.17	163 (44%) 0 0	38, 115, 185, 204	0
3	Y	36/37 (97%)	6.99	36 (100%) 0 0	102, 107, 122, 126	36 (100%)
All	All	1437/1731 (83%)	1.34	283 (19%) 1 1	17, 56, 176, 204	36 (2%)

All (283) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	272	LEU	22.1
2	H	218	PHE	19.6
2	H	280	LEU	17.6
2	H	248	ALA	17.4
2	H	214	GLN	16.6
2	H	217	SER	13.9
2	H	211	GLY	12.9
2	H	205	TYR	12.8
3	Y	5	VAL	12.7
2	H	241	PHE	12.5
2	H	288	VAL	12.5
2	H	212	TYR	12.3
2	H	246	SER	12.2
2	H	206	SER	12.1
2	H	279	VAL	11.6
3	Y	6	SER	11.5
2	H	281	GLN	11.5
3	Y	17	CYS	11.4
2	H	270	ILE	11.2
2	H	244	CYS	11.1

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Mol	Chain	Res	Type	RSRZ
2	H	269	THR	11.0
3	Y	3	THR	11.0
2	H	254	ILE	10.9
3	Y	28	CYS	10.9
2	H	242	PHE	10.8
2	H	224	ILE	10.6
3	Y	29	MET	10.5
2	H	225	VAL	10.2
2	H	250	PHE	9.9
2	H	282	PHE	9.8
2	H	210	ILE	9.6
2	H	251	PHE	9.6
2	H	229	CYS	9.5
2	H	153	PHE	9.4
2	H	289	VAL	9.3
3	Y	8	THR	9.3
2	H	283	GLN	9.1
2	H	168	VAL	9.1
2	H	235	PHE	9.0
2	H	247	LYS	8.9
3	Y	36	TYR	8.9
2	H	271	PHE	8.8
2	H	245	PRO	8.7
3	Y	16	VAL	8.7
2	H	149	VAL	8.5
2	H	240	ARG	8.5
3	Y	27	LYS	8.5
2	H	172	VAL	8.5
2	H	228	LEU	8.4
3	Y	14	TRP	8.4
3	Y	7	CYS	8.3
2	H	164	ILE	8.2
2	H	183	GLU	8.2
2	H	215	SER	8.2
3	Y	9	THR	8.2
3	Y	12	GLU	8.0
2	H	238	LEU	8.0
2	H	188	PHE	8.0
2	H	216	THR	8.0
2	H	221	PRO	8.0
2	H	249	GLY	7.9
3	Y	24	SER	7.9

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Mol	Chain	Res	Type	RSRZ
2	H	222	PHE	7.9
2	H	231	ILE	7.8
3	Y	2	PHE	7.6
3	Y	21	HIS	7.6
2	H	220	ASP	7.4
2	H	302	LYS	7.1
2	H	252	THR	7.1
2	H	273	THR	7.1
2	H	262	ALA	7.0
2	H	167	ILE	7.0
2	H	267	TYR	6.9
2	H	284	ASN	6.9
2	H	230	ILE	6.9
2	H	151	LEU	6.7
3	Y	4	ASN	6.7
2	H	219	THR	6.7
2	H	285	VAL	6.7
2	H	286	ARG	6.6
3	Y	10	SER	6.6
3	Y	30	ASN	6.5
3	Y	13	CYS	6.5
2	H	209	THR	6.5
2	B	161	PRO	6.5
3	Y	33	CYS	6.4
2	H	260	ILE	6.4
2	B	193	GLU	6.4
2	H	233	PHE	6.3
2	H	409	PHE	6.2
3	Y	35	CYS	6.2
2	H	207	GLN	6.1
2	H	165	ILE	6.1
3	Y	23	THR	6.1
2	H	257	ILE	6.0
2	H	161	PRO	6.0
2	H	146	GLN	6.0
2	H	415	ARG	6.0
2	H	303	LEU	6.0
2	H	203	HIS	5.9
3	Y	34	ARG	5.9
2	H	417	THR	5.8
2	H	414	HIS	5.8
3	Y	37	SER	5.8

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Mol	Chain	Res	Type	RSRZ
2	H	213	GLN	5.8
2	B	153	PHE	5.7
2	H	263	ILE	5.6
2	H	145	PHE	5.6
2	H	276	ASN	5.5
2	H	232	TRP	5.5
2	H	266	TYR	5.5
2	H	277	LYS	5.4
3	Y	15	SER	5.2
2	H	290	GLN	5.2
2	H	416	GLU	5.1
2	H	261	VAL	5.0
2	H	255	MET	4.9
2	H	173	ILE	4.9
2	H	413	TYR	4.9
2	H	410	ASN	4.9
3	Y	26	GLY	4.8
2	H	265	PRO	4.8
2	H	295	MET	4.8
2	H	237	PHE	4.8
2	H	150	TRP	4.8
2	H	170	VAL	4.8
2	H	152	LEU	4.7
2	B	151	LEU	4.7
2	B	219	THR	4.7
2	H	253	ASN	4.6
2	H	155	TYR	4.5
2	H	190	ASP	4.5
2	H	157	GLU	4.5
2	H	275	SER	4.5
1	G	36	LEU	4.4
2	H	187	ILE	4.3
2	H	159	SER	4.3
2	H	171	MET	4.3
2	B	132	TYR	4.3
2	H	202	PHE	4.2
2	H	223	PHE	4.2
2	H	125	MET	4.2
2	B	192	ASN	4.1
3	Y	31	LYS	4.1
2	H	182	LEU	4.1
1	G	360	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
3	Y	32	LYS	4.0
2	H	306	HIS	4.0
2	H	236	GLU	4.0
2	H	226	GLU	4.0
3	Y	20	LEU	4.0
2	H	208	SER	4.0
2	H	350	ARG	3.9
1	A	360	TYR	3.9
2	B	149	VAL	3.9
2	H	63	LYS	3.9
2	B	157	GLU	3.8
2	H	156	PRO	3.8
2	H	308	LYS	3.7
2	B	164	ILE	3.7
2	H	381	ILE	3.7
2	H	287	ARG	3.7
2	H	204	THR	3.7
2	B	162	ALA	3.7
2	H	106	LEU	3.7
2	H	181	CYS	3.7
2	H	278	SER	3.6
2	H	158	SER	3.6
3	Y	18	GLN	3.6
2	H	177	ILE	3.5
2	H	128	GLU	3.5
2	H	163	ARG	3.5
2	B	213	GLN	3.4
2	B	125	MET	3.4
2	B	218	PHE	3.4
2	B	286	ARG	3.4
2	H	299	ARG	3.3
2	B	216	THR	3.3
2	H	162	ALA	3.2
2	B	163	ARG	3.2
2	H	154	GLU	3.2
2	H	114	ARG	3.2
2	H	234	SER	3.2
3	Y	25	ARG	3.2
2	H	179	SER	3.2
2	H	239	VAL	3.2
2	B	152	LEU	3.1
2	B	241	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	36	LEU	3.1
2	H	243	ALA	3.1
1	A	262	TYR	3.1
2	B	145	PHE	3.1
2	H	227	THR	3.1
2	B	197	GLY	3.1
2	B	344	PHE	3.0
2	H	174	LEU	3.0
2	H	119	GLY	3.0
2	B	201	THR	2.9
2	B	251	PHE	2.9
2	H	258	ILE	2.9
2	B	249	GLY	2.9
2	H	310	LEU	2.9
1	A	250	ILE	2.9
2	B	188	PHE	2.8
2	H	148	GLN	2.8
2	H	160	GLY	2.8
2	H	175	ILE	2.8
2	H	274	GLU	2.8
2	B	140	LEU	2.8
2	B	168	VAL	2.8
1	A	265	ALA	2.8
2	B	415	ARG	2.8
2	H	264	ILE	2.7
2	B	120	GLU	2.7
2	B	195	MET	2.7
2	B	160	GLY	2.7
2	B	150	TRP	2.7
1	G	349	HIS	2.6
2	B	252	THR	2.6
2	B	158	SER	2.6
1	G	300	GLY	2.6
2	B	190	ASP	2.6
2	H	121	GLU	2.6
2	B	308	LYS	2.6
2	B	397	THR	2.6
3	Y	22	ASN	2.6
2	B	282	PHE	2.6
2	H	312	ILE	2.5
2	B	196	HIS	2.5
2	B	285	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	400	LEU	2.5
2	H	147	ARG	2.5
2	H	124	GLU	2.5
2	H	307	SER	2.5
2	B	396	LEU	2.5
2	B	398	ILE	2.5
2	B	399	ALA	2.5
2	B	159	SER	2.5
2	B	250	PHE	2.5
1	A	205	PHE	2.5
1	G	361	SER	2.5
2	H	412	PHE	2.4
2	B	231	ILE	2.4
1	G	299	LEU	2.4
2	B	198	GLY	2.4
2	H	405	ILE	2.4
2	B	411	TYR	2.3
2	H	191	GLU	2.3
2	B	215	SER	2.3
2	H	111	GLU	2.3
2	H	109	PHE	2.3
2	B	124	GLU	2.3
2	B	155	TYR	2.3
2	H	36	VAL	2.2
2	H	411	TYR	2.2
2	B	191	GLU	2.2
2	B	413	TYR	2.2
2	H	305	ARG	2.2
3	Y	11	LYS	2.2
2	B	271	PHE	2.2
2	B	106	LEU	2.2
2	B	232	TRP	2.2
2	B	141	PRO	2.2
2	B	136	GLU	2.1
2	B	129	ASP	2.1
2	B	337	LEU	2.1
2	H	322	ARG	2.1
3	Y	19	ARG	2.1
2	H	376	MET	2.1
2	B	412	PHE	2.1
2	H	296	ARG	2.1
2	B	371	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	363	TRP	2.1
2	B	127	ARG	2.1
1	A	267	LEU	2.0
2	H	185	LEU	2.0
1	G	67	GLU	2.0
1	G	343	LEU	2.0
2	B	401	PRO	2.0
2	H	396	LEU	2.0
2	B	393	ALA	2.0
2	B	194	ASP	2.0
1	A	273	LEU	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	0.71	0.42	-	125,126,126,126	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	504	22/51	0.48	0.68	15.87	85,102,113,114	0
6	PGW	B	518	8/51	0.44	0.86	12.43	102,105,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	PGW	B	509	9/51	0.81	0.52	8.23	82,86,89,89	0
6	PGW	H	504	22/51	0.42	0.84	7.35	142,147,149,149	0
6	PGW	B	515	8/51	0.53	0.53	5.97	81,87,91,91	0
6	PGW	B	513	8/51	0.65	0.46	4.62	74,78,79,79	0
6	PGW	B	510	9/51	0.79	0.44	4.07	106,107,109,109	0
6	PGW	B	517	7/51	0.56	0.48	3.69	63,66,68,69	0
4	NAP	G	1001	48/48	0.95	0.20	2.64	25,39,51,51	0
6	PGW	B	505	9/51	0.64	0.36	2.25	79,82,84,85	0
6	PGW	B	516	36/51	0.58	0.39	2.22	107,125,141,141	0
6	PGW	B	514	23/51	0.70	0.31	1.48	109,119,123,124	0
4	NAP	A	1001	48/48	0.96	0.18	0.41	23,33,43,47	0
6	PGW	B	512	9/51	0.22	1.17	-	126,128,128,128	0
6	PGW	B	508	9/51	0.56	0.47	-	100,102,102,102	0
6	PGW	B	519	8/51	0.64	0.39	-	97,99,100,100	0
5	CS	H	505	1/1	0.92	0.39	-	126,126,126,126	1
5	CS	H	501	1/1	0.97	0.22	-	85,85,85,85	1
6	PGW	B	511	7/51	0.85	0.20	-	70,73,73,73	0
5	CS	B	503	1/1	0.93	0.14	-	101,101,101,101	1
5	CS	B	501	1/1	0.95	0.19	-	45,45,45,45	1
5	CS	B	520	1/1	1.00	0.21	-	61,61,61,61	1
5	CS	B	502	1/1	0.88	0.12	-	43,43,43,43	1
6	PGW	B	507	9/51	0.62	0.58	-	94,96,98,98	0
6	PGW	B	506	9/51	0.62	0.41	-	87,90,91,91	0
5	CS	H	503	1/1	0.94	0.24	-	75,75,75,75	1
5	CS	H	502	1/1	0.98	0.22	-	74,74,74,74	1

6.5 Other polymers

There are no such residues in this entry.