Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:53 PM GMT

PDB ID	:	4JTA
Title	:	Crystal structure of Kv1.2-2.1 paddle chimera channel in complex with Charybdotoxin
Authors	:	MacKinnon, R.; Banerjee, A.; Lee, A.; Campbell, E.
Deposited on	:	2013-03-23
Resolution	:	2.50 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 ①) were used in the production of this report:

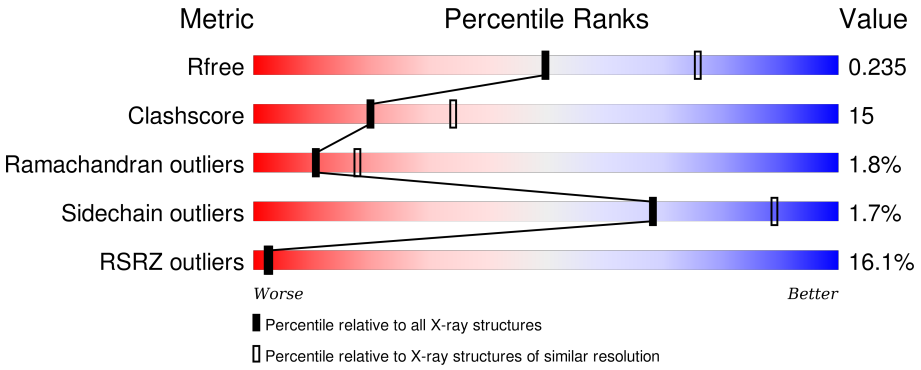
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 <=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%, 81%, 16%
1	P	333	3%, 81%, 15%
2	B	514	10%, 51%, 24%, 25%
2	Q	514	26%, 40%, 29%, 29%
3	Y	37	84%, 49%, 43%, 8%

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
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	514	-	-	-	X
6	PGW	B	515	-	-	-	X
6	PGW	B	516	-	-	-	X
6	PGW	B	518	-	-	-	X
6	PGW	Q	504	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12106 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	P	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
P	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	Q	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
Q	-18	MET	-	EXPRESSION TAG	UNP P63142
Q	-17	ALA	-	EXPRESSION TAG	UNP P63142
Q	-16	HIS	-	EXPRESSION TAG	UNP P63142
Q	-15	HIS	-	EXPRESSION TAG	UNP P63142
Q	-14	HIS	-	EXPRESSION TAG	UNP P63142
Q	-13	HIS	-	EXPRESSION TAG	UNP P63142
Q	-12	HIS	-	EXPRESSION TAG	UNP P63142
Q	-11	HIS	-	EXPRESSION TAG	UNP P63142
Q	-10	HIS	-	EXPRESSION TAG	UNP P63142
Q	-9	HIS	-	EXPRESSION TAG	UNP P63142
Q	-8	HIS	-	EXPRESSION TAG	UNP P63142
Q	-7	HIS	-	EXPRESSION TAG	UNP P63142
Q	-6	GLY	-	EXPRESSION TAG	UNP P63142
Q	-5	LEU	-	EXPRESSION TAG	UNP P63142
Q	-4	VAL	-	EXPRESSION TAG	UNP P63142
Q	-3	PRO	-	EXPRESSION TAG	UNP P63142
Q	-2	ARG	-	EXPRESSION TAG	UNP P63142
Q	-1	GLY	-	EXPRESSION TAG	UNP P63142
Q	0	SER	-	EXPRESSION TAG	UNP P63142
Q	31	SER	CYS	ENGINEERED MUTATION	UNP P63142
Q	32	SER	CYS	ENGINEERED MUTATION	UNP P63142
Q	207	GLN	ASN	ENGINEERED MUTATION	UNP P63142
Q	431	SER	CYS	ENGINEERED MUTATION	UNP P63142
Q	478	SER	CYS	ENGINEERED MUTATION	UNP P63142

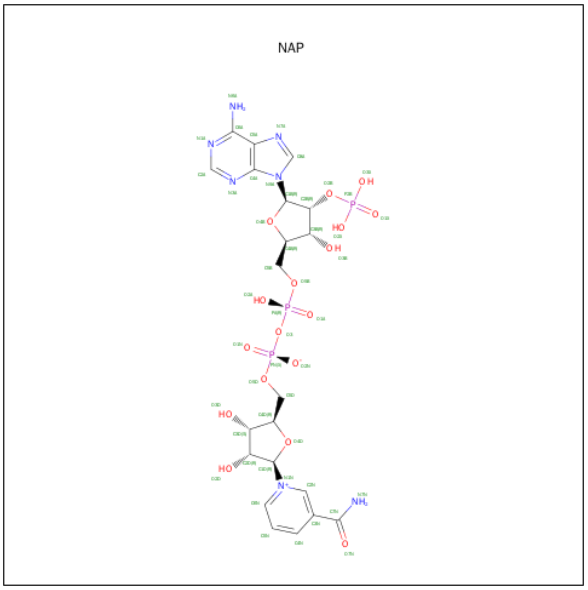
- Molecule 3 is a protein called Potassium channel toxin alpha-KTx 1.1.

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: $C_{21}H_{28}N_7O_{17}P_3$).



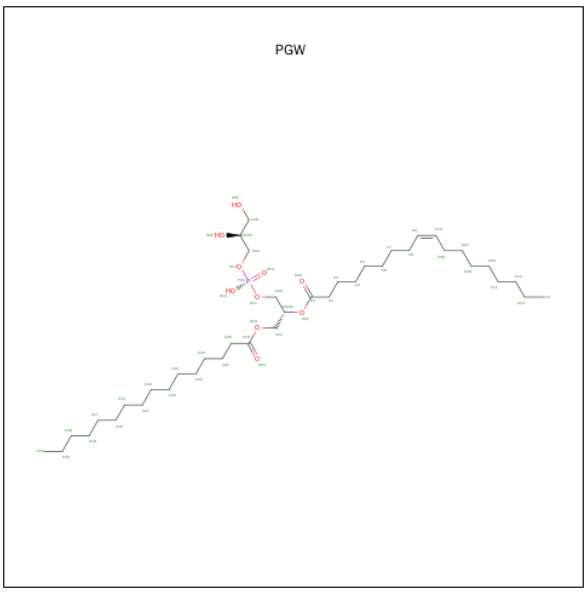
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	P	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	3	Total	K	0	0
			3	3		
5	Q	3	Total	K	0	0
			3	3		

- Molecule 6 is (1R)-2-{[(S)-{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(HEXADECANOYLOXY)METHYL]ETHYL (9Z)-OCTADEC-9-ENOA

TE (three-letter code: PGW) (formula: $C_{40}H_{77}O_{10}P$).



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 12 12	0	0
6	B	1	Total C O P 23 14 8 1	0	0
6	B	1	Total C 12 12	0	0
6	B	1	Total C O P 37 26 10 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C 10 10	0	0
6	B	1	Total C 12 12	0	0
6	B	1	Total C 12 12	0	0
6	Q	1	Total C O 22 17 5	0	0

- Molecule 7 is water.

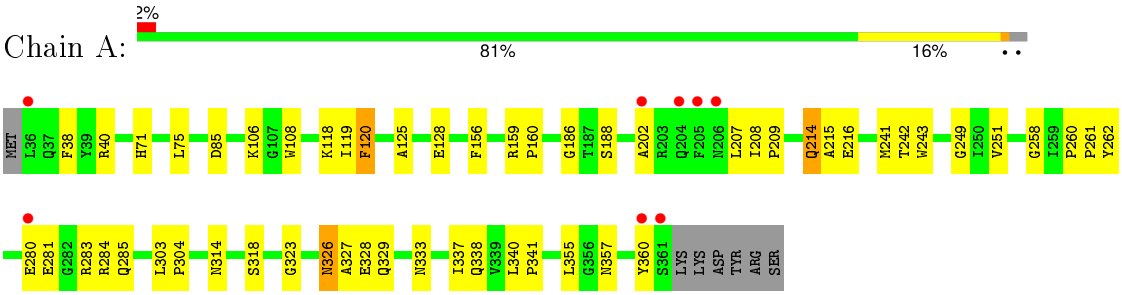
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	140	Total O 140 140	0	0
7	B	53	Total O 53 53	0	0
7	P	102	Total O 102 102	0	0
7	Q	23	Total O 23 23	0	0

3 Residue-property plots (i)

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.

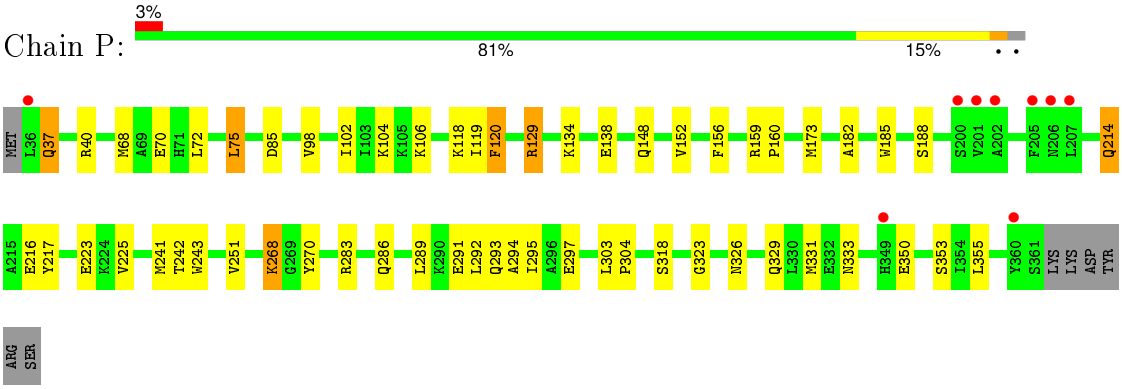
• Molecule 1: Voltage-gated potassium channel subunit beta-2

Chain A:



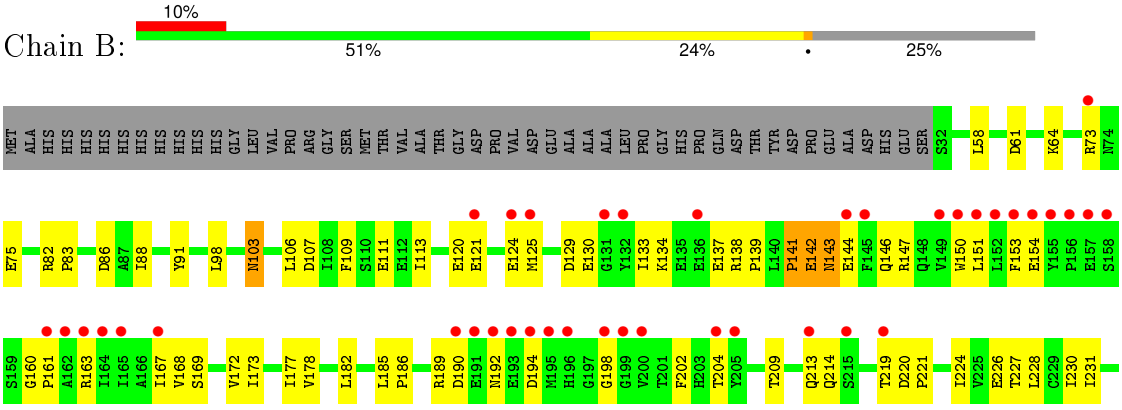
• Molecule 1: Voltage-gated potassium channel subunit beta-2

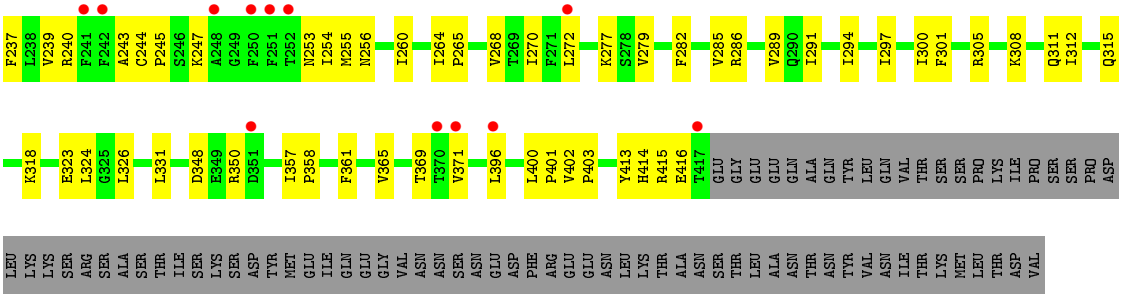
Chain P:



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

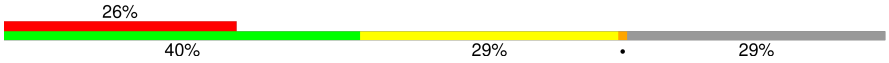
Chain B:

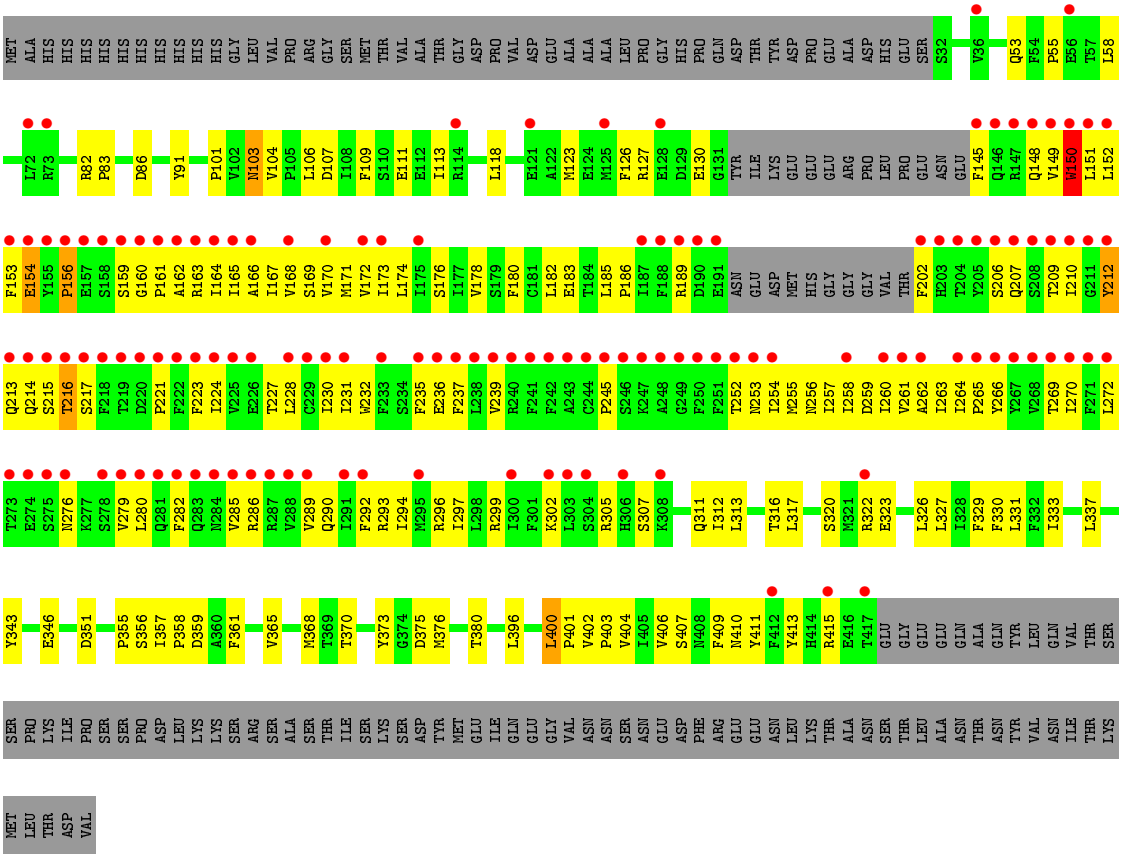




• Molecule 2: Potassium voltage-gated channel subfamily A member 2, Potassium voltage-gated channel subfamily B member 1

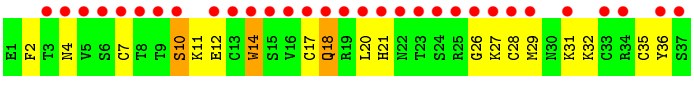
Chain Q:





• Molecule 3: Potassium channel toxin alpha-KTx 1.1

Chain Y:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α, β, γ	144.40Å 144.40Å 284.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 49.65 – 2.40	Depositor EDS
% Data completeness (in resolution range)	92.6 (50.00-2.50) 86.0 (49.65-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.210 , 0.236 0.212 , 0.235	Depositor DCC
R_{free} test set	4605 reflections (4.76%)	DCC
Wilson B-factor (Å^2)	46.8	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 64.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	2 of 112421 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12106	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.36	0/2608	0.58	0/3524
1	P	0.36	0/2608	0.56	0/3524
2	B	0.35	0/3169	0.53	0/4292
2	Q	0.32	0/3036	0.50	0/4114
3	Y	0.26	0/292	0.46	0/389
All	All	0.35	0/11713	0.54	0/15843

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	P	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	270	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2556	0	2582	42	0
1	P	2556	0	2582	46	0
2	B	3088	0	3034	91	0
2	Q	2959	0	2956	142	0
3	Y	295	0	282	19	0
4	A	48	0	25	3	0
4	P	48	0	25	3	0
5	B	3	0	0	0	0
5	Q	3	0	0	0	0
6	B	210	0	291	19	0
6	Q	22	0	25	7	0
7	A	140	0	0	2	0
7	B	53	0	0	1	0
7	P	102	0	0	0	0
7	Q	23	0	0	1	0
All	All	12106	0	11802	349	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 15.

All (349) 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)
6:B:510:PGW:H2A	6:B:515:PGW:H21A	1.42	0.98
2:Q:400:LEU:HB2	2:Q:401:PRO:HD3	1.52	0.89
1:P:333:ASN:HD21	4:P:1001:NAP:H61A	1.21	0.88
2:Q:312:ILE:HD13	2:Q:413:TYR:HA	1.59	0.83
2:Q:227:THR:HA	2:Q:230:ILE:HG22	1.61	0.82
2:Q:152:LEU:HD22	2:Q:161:PRO:HB2	1.62	0.81
2:Q:103:ASN:H	2:Q:103:ASN:HD22	1.29	0.80
3:Y:4:ASN:HA	3:Y:32:LYS:HD3	1.63	0.80
1:A:118:LYS:HG3	1:A:156:PHE:HB2	1.63	0.80
2:B:400:LEU:HB2	2:B:401:PRO:HD3	1.62	0.79
2:B:350:ARG:HH11	2:B:350:ARG:HB3	1.48	0.78
1:P:40:ARG:HD2	1:P:318:SER:O	1.85	0.76
2:B:311:GLN:HG2	6:B:516:PGW:H3	1.69	0.74
1:P:295:ILE:H	1:P:295:ILE:HD12	1.53	0.71
2:Q:103:ASN:H	2:Q:103:ASN:ND2	1.89	0.71
6:B:510:PGW:H4A	6:B:515:PGW:H23A	1.72	0.71
2:Q:103:ASN:HD22	2:Q:103:ASN:N	1.86	0.69
2:B:350:ARG:HB3	2:B:350:ARG:NH1	2.08	0.69
2:Q:260:ILE:HG22	2:Q:264:ILE:HD11	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:361:PHE:HB2	6:Q:504:PGW:H2	1.73	0.69
1:P:268:LYS:NZ	1:P:268:LYS:HB3	2.08	0.69
2:Q:264:ILE:HB	2:Q:265:PRO:HD3	1.75	0.68
2:B:361:PHE:HB2	6:B:504:PGW:H2	1.76	0.68
3:Y:26:GLY:HA3	3:Y:35:CYS:HA	1.77	0.67
2:Q:307:SER:O	2:Q:311:GLN:HG3	1.94	0.67
2:Q:262:ALA:HB1	2:Q:302:LYS:HE2	1.76	0.67
2:Q:361:PHE:CB	6:Q:504:PGW:H2	2.25	0.67
1:A:333:ASN:HD21	4:A:1001:NAP:H61A	1.43	0.66
1:A:280:GLU:HA	1:A:283:ARG:NH1	2.10	0.66
2:Q:167:ILE:O	2:Q:171:MET:HG2	1.96	0.66
2:Q:265:PRO:HA	2:Q:292:PHE:HD2	1.59	0.66
2:Q:293:ARG:HA	2:Q:296:ARG:HD3	1.78	0.66
1:P:104:LYS:NZ	1:P:148:GLN:HE22	1.93	0.65
2:B:294:ILE:O	2:B:297:ILE:HG22	1.97	0.65
2:Q:101:PRO:HB2	2:Q:104:VAL:HG23	1.79	0.65
1:A:258:GLY:O	1:A:260:PRO:HD3	1.97	0.64
2:B:103:ASN:H	2:B:103:ASN:HD22	1.44	0.64
2:B:213:GLN:HB3	2:B:220:ASP:HB2	1.78	0.63
1:P:293:GLN:HE21	1:P:297:GLU:HG3	1.64	0.63
2:Q:230:ILE:HG12	2:Q:266:TYR:CD2	2.34	0.63
2:Q:259:ASP:HA	2:Q:302:LYS:NZ	2.15	0.62
2:B:82:ARG:HB2	2:B:83:PRO:HD3	1.80	0.62
6:Q:504:PGW:O02	6:Q:504:PGW:H01	1.99	0.61
2:Q:262:ALA:CB	2:Q:302:LYS:HE2	2.31	0.61
2:B:226:GLU:O	2:B:230:ILE:HD13	2.01	0.61
1:A:326:ASN:ND2	1:A:329:GLN:H	1.98	0.61
2:B:147:ARG:O	2:B:151:LEU:HG	2.00	0.61
2:Q:316:THR:HG21	2:Q:409:PHE:HB2	1.83	0.60
2:Q:411:TYR:CZ	2:Q:415:ARG:HD3	2.36	0.60
1:A:251:VAL:HG12	1:A:251:VAL:O	2.01	0.60
2:Q:230:ILE:HG21	2:Q:266:TYR:CZ	2.36	0.60
2:Q:174:LEU:O	2:Q:178:VAL:HG23	2.02	0.60
1:A:280:GLU:HG2	1:A:284:ARG:HH12	1.65	0.60
1:A:159:ARG:HA	1:A:188:SER:O	2.02	0.60
2:Q:212:TYR:HB2	2:Q:223:PHE:HB2	1.84	0.60
2:B:227:THR:O	2:B:231:ILE:HG12	2.02	0.59
2:Q:227:THR:O	2:Q:231:ILE:HG12	2.01	0.59
2:Q:260:ILE:O	2:Q:264:ILE:HG13	2.01	0.59
2:B:120:GLU:O	2:B:124:GLU:HG3	2.03	0.59
2:Q:86:ASP:HB2	7:Q:616:HOH:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:LEU:C	2:B:58:LEU:HD23	2.23	0.59
2:B:221:PRO:HB2	6:B:513:PGW:H23	1.85	0.58
2:Q:357:ILE:HB	2:Q:358:PRO:HD3	1.86	0.58
3:Y:14:TRP:HA	3:Y:14:TRP:CE3	2.38	0.58
3:Y:14:TRP:HA	3:Y:14:TRP:HE3	1.68	0.58
2:Q:294:ILE:O	2:Q:297:ILE:HG22	2.04	0.58
2:Q:207:GLN:HE21	2:Q:213:GLN:HB2	1.68	0.58
2:Q:293:ARG:HA	2:Q:296:ARG:CD	2.34	0.58
2:B:121:GLU:O	2:B:125:MET:HG2	2.03	0.58
2:Q:163:ARG:O	2:Q:167:ILE:HG12	2.04	0.58
2:Q:113:ILE:HG23	2:Q:118:LEU:HD12	1.86	0.58
2:Q:148:GLN:NE2	2:Q:151:LEU:HD12	2.18	0.57
2:Q:82:ARG:HB2	2:Q:83:PRO:HD3	1.86	0.57
1:P:118:LYS:HG2	1:P:156:PHE:HB2	1.86	0.57
1:P:295:ILE:N	1:P:295:ILE:HD12	2.20	0.57
2:B:255:MET:CE	2:B:305:ARG:HA	2.35	0.57
2:Q:170:VAL:HB	2:Q:171:MET:HE2	1.86	0.57
2:Q:169:SER:O	2:Q:173:ILE:HG13	2.05	0.57
1:P:214:GLN:HA	1:P:241:MET:O	2.05	0.57
2:Q:402:VAL:O	2:Q:406:VAL:HG23	2.05	0.56
6:B:516:PGW:O02	6:B:516:PGW:H03A	2.05	0.56
2:Q:322:ARG:HG3	2:Q:322:ARG:HH11	1.68	0.56
2:B:365:VAL:HG21	6:B:504:PGW:H6A	1.87	0.56
6:B:504:PGW:H01	6:B:504:PGW:O02	2.05	0.56
1:A:303:LEU:HB3	1:A:304:PRO:HD3	1.88	0.56
2:B:255:MET:HE3	2:B:305:ARG:HA	1.87	0.56
2:B:103:ASN:H	2:B:103:ASN:ND2	2.03	0.56
2:Q:145:PHE:CZ	2:Q:149:VAL:HG21	2.41	0.56
2:Q:259:ASP:HA	2:Q:302:LYS:HZ3	1.70	0.55
2:Q:148:GLN:HE22	2:Q:151:LEU:HD12	1.71	0.55
2:Q:255:MET:CE	2:Q:305:ARG:HA	2.37	0.55
2:Q:235:PHE:O	2:Q:239:VAL:HG23	2.06	0.55
1:A:280:GLU:HG2	1:A:284:ARG:NH1	2.22	0.55
1:A:340:LEU:HB3	1:A:341:PRO:HD3	1.88	0.55
1:P:75:LEU:HG	1:P:331:MET:HE3	1.88	0.55
2:B:141:PRO:C	2:B:143:ASN:H	2.10	0.55
2:Q:400:LEU:O	2:Q:403:PRO:HD2	2.07	0.55
2:Q:168:VAL:O	2:Q:172:VAL:HG23	2.08	0.54
2:B:414:HIS:C	2:B:416:GLU:H	2.10	0.54
1:P:217:TYR:HB2	1:P:225:VAL:HG21	1.89	0.54
2:Q:282:PHE:CZ	2:Q:289:VAL:HG21	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:251:VAL:HG12	1:P:251:VAL:O	2.06	0.54
1:A:71:HIS:CD2	1:A:327:ALA:HB2	2.43	0.54
2:Q:227:THR:CA	2:Q:230:ILE:HG22	2.34	0.54
1:P:152:VAL:O	1:P:182:ALA:HA	2.07	0.54
3:Y:29:MET:C	3:Y:31:LYS:H	2.11	0.54
2:Q:232:TRP:O	2:Q:236:GLU:HG3	2.07	0.53
2:Q:221:PRO:HA	2:Q:224:ILE:HD12	1.90	0.53
1:P:173:MET:HG3	1:P:185:TRP:CE3	2.44	0.53
6:B:514:PGW:O02	6:B:514:PGW:O11	2.25	0.53
1:P:159:ARG:HB2	1:P:160:PRO:HD2	1.90	0.53
2:Q:272:LEU:HD13	2:Q:285:VAL:HG21	1.90	0.53
2:B:253:ASN:HB3	2:B:256:ASN:ND2	2.24	0.53
2:B:177:ILE:HD13	2:B:300:ILE:HD12	1.89	0.53
2:Q:355:PRO:HB2	2:Q:359:ASP:OD2	2.09	0.53
2:B:318:LYS:HD2	6:B:516:PGW:H21A	1.91	0.52
2:B:357:ILE:HB	2:B:358:PRO:HD3	1.91	0.52
2:B:214:GLN:HE22	2:B:270:ILE:HA	1.75	0.52
2:Q:227:THR:HA	2:Q:230:ILE:CG2	2.36	0.52
2:Q:280:LEU:HD12	2:Q:280:LEU:H	1.73	0.52
2:B:254:ILE:HD12	6:B:516:PGW:H24A	1.92	0.52
1:P:37:GLN:HE21	1:P:37:GLN:N	2.07	0.52
2:Q:53:GLN:O	2:Q:55:PRO:HD3	2.10	0.52
2:Q:375:ASP:O	2:Q:376:MET:HG3	2.10	0.52
2:Q:178:VAL:O	2:Q:182:LEU:HG	2.10	0.52
3:Y:17:CYS:O	3:Y:21:HIS:HB2	2.09	0.52
2:Q:285:VAL:HG13	2:Q:285:VAL:O	2.10	0.52
2:Q:224:ILE:O	2:Q:228:LEU:HG	2.11	0.51
2:B:277:LYS:O	2:B:277:LYS:HG3	2.10	0.51
2:Q:150:TRP:CE3	2:Q:150:TRP:HA	2.44	0.51
2:Q:152:LEU:O	2:Q:165:ILE:HD12	2.10	0.51
1:P:120:PHE:CD1	1:P:159:ARG:HG3	2.46	0.51
2:Q:152:LEU:HD13	2:Q:165:ILE:CD1	2.41	0.51
2:Q:166:ALA:O	2:Q:170:VAL:HG23	2.10	0.51
2:B:177:ILE:CD1	2:B:300:ILE:HD12	2.41	0.51
2:Q:53:GLN:C	2:Q:55:PRO:HD3	2.31	0.51
2:B:150:TRP:O	2:B:154:GLU:HB3	2.10	0.51
2:Q:402:VAL:HB	2:Q:403:PRO:HD3	1.94	0.50
3:Y:10:SER:C	3:Y:12:GLU:H	2.15	0.50
3:Y:27:LYS:CG	3:Y:28:CYS:N	2.72	0.50
2:Q:150:TRP:HE3	2:Q:150:TRP:HA	1.76	0.50
1:P:333:ASN:ND2	4:P:1001:NAP:H61A	2.01	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:161:PRO:O	2:Q:165:ILE:HG13	2.10	0.50
1:P:326:ASN:OD1	1:P:329:GLN:HG3	2.12	0.50
2:Q:206:SER:O	2:Q:210:ILE:HD12	2.11	0.50
2:Q:237:PHE:CE1	2:Q:260:ILE:HG12	2.45	0.50
2:Q:254:ILE:O	2:Q:258:ILE:HG13	2.12	0.50
1:P:286:GLN:NE2	1:P:289:LEU:HD12	2.27	0.49
1:P:134:LYS:O	1:P:138:GLU:HG3	2.12	0.49
2:B:189:ARG:HG3	2:B:189:ARG:HH11	1.77	0.49
2:B:312:ILE:HD13	2:B:413:TYR:HA	1.94	0.49
2:B:106:LEU:HD13	2:B:130:GLU:HG2	1.93	0.49
1:P:303:LEU:HB3	1:P:304:PRO:HD3	1.94	0.49
2:Q:411:TYR:CE2	2:Q:415:ARG:HD3	2.48	0.49
2:Q:186:PRO:HB3	2:Q:189:ARG:NH2	2.27	0.49
1:P:295:ILE:H	1:P:295:ILE:CD1	2.24	0.49
2:B:202:PHE:HB2	2:B:279:VAL:CG2	2.42	0.49
3:Y:27:LYS:HG3	3:Y:28:CYS:N	2.28	0.49
3:Y:29:MET:HG3	3:Y:31:LYS:HB3	1.94	0.49
2:B:308:LYS:O	2:B:312:ILE:HG13	2.12	0.49
1:A:281:GLU:O	1:A:285:GLN:HG3	2.11	0.49
2:Q:106:LEU:CD1	2:Q:130:GLU:HG2	2.42	0.49
2:Q:176:SER:HB2	2:Q:299:ARG:HH11	1.78	0.49
2:B:178:VAL:O	2:B:182:LEU:HG	2.13	0.49
2:B:186:PRO:O	2:B:190:ASP:HB2	2.13	0.49
1:P:333:ASN:HD22	1:P:333:ASN:N	2.10	0.49
2:Q:327:LEU:O	2:Q:331:LEU:HD13	2.12	0.49
2:Q:323:GLU:OE1	2:Q:404:VAL:HG11	2.14	0.48
2:B:260:ILE:O	2:B:264:ILE:HG13	2.13	0.48
2:Q:280:LEU:HD12	2:Q:280:LEU:N	2.28	0.48
2:B:323:GLU:CD	2:B:323:GLU:H	2.16	0.48
2:B:348:ASP:HB2	7:B:646:HOH:O	2.13	0.48
2:B:214:GLN:NE2	2:B:270:ILE:HG12	2.28	0.48
2:B:107:ASP:O	2:B:111:GLU:HG3	2.13	0.48
2:Q:326:LEU:HG	2:Q:330:PHE:CE2	2.49	0.48
2:B:415:ARG:HH11	2:B:415:ARG:HG2	1.76	0.48
2:Q:91:TYR:CE2	2:Q:118:LEU:HD22	2.48	0.48
2:Q:107:ASP:O	2:Q:111:GLU:HG3	2.14	0.48
1:P:268:LYS:HB3	1:P:268:LYS:HZ3	1.77	0.47
2:B:285:VAL:O	2:B:285:VAL:HG22	2.14	0.47
2:Q:253:ASN:HB3	2:Q:256:ASN:ND2	2.29	0.47
2:Q:368:MET:C	2:Q:370:THR:H	2.17	0.47
2:Q:396:LEU:O	2:Q:400:LEU:HG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:SER:O	2:B:173:ILE:HG13	2.15	0.47
1:A:355:LEU:HB3	1:A:357:ASN:OD1	2.14	0.47
2:B:291:ILE:HG23	6:B:507:PGW:H5	1.95	0.47
2:Q:101:PRO:HB2	2:Q:104:VAL:CG2	2.44	0.47
6:Q:504:PGW:O02	6:Q:504:PGW:C01	2.60	0.47
1:A:326:ASN:ND2	1:A:328:GLU:HB2	2.29	0.47
2:B:109:PHE:O	2:B:113:ILE:HG13	2.13	0.47
3:Y:20:LEU:N	3:Y:20:LEU:HD12	2.30	0.47
2:Q:346:GLU:OE2	2:Q:380:THR:HG23	2.15	0.47
2:Q:365:VAL:HG21	6:Q:504:PGW:H6A	1.96	0.47
2:B:305:ARG:HG3	2:B:305:ARG:HH11	1.80	0.46
1:P:104:LYS:HZ3	1:P:148:GLN:HE22	1.61	0.46
1:P:102:ILE:O	1:P:106:LYS:HG2	2.15	0.46
1:P:68:MET:O	1:P:72:LEU:HG	2.15	0.46
3:Y:26:GLY:HA2	3:Y:36:TYR:HD1	1.80	0.46
2:Q:320:SER:HA	2:Q:323:GLU:HG2	1.96	0.46
2:Q:58:LEU:HD23	2:Q:58:LEU:C	2.36	0.46
1:P:119:ILE:O	1:P:120:PHE:HB2	2.15	0.46
2:Q:123:MET:O	2:Q:126:PHE:HB3	2.15	0.46
1:A:214:GLN:HA	1:A:241:MET:O	2.15	0.46
2:Q:152:LEU:HA	2:Q:162:ALA:HB2	1.98	0.46
6:B:504:PGW:H03A	6:B:504:PGW:O02	2.16	0.46
2:B:264:ILE:O	2:B:268:VAL:HG23	2.16	0.46
1:P:75:LEU:HG	1:P:331:MET:CE	2.46	0.46
2:B:168:VAL:O	2:B:172:VAL:HG23	2.16	0.46
2:Q:407:SER:O	2:Q:410:ASN:HB3	2.16	0.46
1:P:291:GLU:O	1:P:294:ALA:HB3	2.16	0.46
2:Q:152:LEU:CD2	2:Q:161:PRO:HB2	2.41	0.46
2:Q:361:PHE:HB3	6:Q:504:PGW:H2	1.97	0.46
2:Q:185:LEU:O	2:Q:189:ARG:HG2	2.16	0.46
1:P:350:GLU:O	1:P:353:SER:HB2	2.16	0.46
2:B:402:VAL:HB	2:B:403:PRO:HD3	1.97	0.46
2:B:264:ILE:HB	2:B:265:PRO:HD3	1.98	0.45
1:A:106:LYS:HG3	1:A:108:TRP:CH2	2.51	0.45
2:Q:127:ARG:HG2	2:Q:127:ARG:HH11	1.81	0.45
1:A:326:ASN:HD22	1:A:328:GLU:N	2.15	0.45
2:Q:257:ILE:HD13	2:Q:260:ILE:HD12	1.98	0.45
2:Q:272:LEU:HD13	2:Q:285:VAL:CG2	2.46	0.45
2:Q:152:LEU:CB	2:Q:162:ALA:HB2	2.47	0.45
2:Q:153:PHE:O	2:Q:154:GLU:HB2	2.16	0.45
2:Q:227:THR:O	2:Q:230:ILE:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:PHE:CD1	1:A:159:ARG:HG3	2.52	0.45
3:Y:28:CYS:SG	3:Y:29:MET:N	2.90	0.45
1:A:85:ASP:OD1	1:A:118:LYS:NZ	2.47	0.45
2:Q:254:ILE:HG23	2:Q:255:MET:N	2.32	0.45
2:B:178:VAL:HG22	6:B:509:PGW:H8	1.99	0.45
1:A:314:ASN:HB2	7:A:1166:HOH:O	2.16	0.45
2:B:153:PHE:CD2	2:B:239:VAL:HG11	2.52	0.45
1:A:360:TYR:HD1	1:A:360:TYR:H	1.65	0.44
2:Q:400:LEU:CB	2:Q:401:PRO:HD3	2.35	0.44
2:Q:156:PRO:HA	2:Q:162:ALA:HB1	1.99	0.44
2:B:318:LYS:HD2	6:B:516:PGW:C22	2.47	0.44
2:Q:253:ASN:HB3	2:Q:256:ASN:HD22	1.82	0.44
1:A:326:ASN:HD21	1:A:329:GLN:H	1.63	0.44
2:Q:260:ILE:HG22	2:Q:264:ILE:CD1	2.45	0.44
2:Q:322:ARG:HG3	2:Q:322:ARG:NH1	2.33	0.44
2:Q:270:ILE:O	2:Q:270:ILE:HG22	2.17	0.44
2:Q:337:LEU:HD23	2:Q:337:LEU:O	2.18	0.44
2:Q:286:ARG:HH12	2:Q:290:GLN:NE2	2.16	0.44
2:B:244:CYS:SG	2:B:247:LYS:HG2	2.58	0.44
3:Y:2:PHE:HZ	3:Y:31:LYS:HE2	1.83	0.44
2:Q:202:PHE:HB2	2:Q:279:VAL:CG2	2.47	0.44
2:B:318:LYS:HD2	6:B:516:PGW:C21	2.48	0.44
6:Q:504:PGW:O02	6:Q:504:PGW:H03A	2.17	0.44
2:Q:255:MET:HE1	2:Q:305:ARG:HA	2.00	0.44
1:P:251:VAL:CG1	1:P:251:VAL:O	2.65	0.44
1:P:120:PHE:O	1:P:129:ARG:HA	2.18	0.44
3:Y:7:CYS:HA	3:Y:12:GLU:OE1	2.18	0.44
2:B:192:ASN:ND2	2:B:194:ASP:H	2.16	0.44
2:B:163:ARG:O	2:B:167:ILE:HG12	2.18	0.44
1:P:323:GLY:HA3	4:P:1001:NAP:H51A	2.00	0.43
2:Q:176:SER:HB2	2:Q:299:ARG:NH1	2.33	0.43
2:B:192:ASN:HD22	2:B:204:THR:HG21	1.81	0.43
2:Q:214:GLN:NE2	2:Q:269:THR:HG22	2.33	0.43
2:B:237:PHE:CE1	2:B:260:ILE:HG12	2.53	0.43
1:A:280:GLU:HA	1:A:283:ARG:HH11	1.80	0.43
1:A:159:ARG:HB2	1:A:160:PRO:HD2	1.99	0.43
1:P:104:LYS:HZ2	1:P:148:GLN:HE22	1.64	0.43
2:Q:154:GLU:O	2:Q:156:PRO:HD3	2.19	0.43
2:Q:313:LEU:O	2:Q:317:LEU:HG	2.19	0.43
2:Q:329:PHE:O	2:Q:333:ILE:HG12	2.18	0.43
3:Y:2:PHE:CZ	3:Y:31:LYS:HE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:276:ASN:ND2	2:Q:285:VAL:HG11	2.34	0.43
2:B:318:LYS:HB2	6:B:516:PGW:H23A	2.01	0.43
1:P:217:TYR:HB3	1:P:242:THR:HB	2.00	0.43
1:A:156:PHE:HA	1:A:186:GLY:O	2.19	0.42
2:B:350:ARG:HH11	2:B:350:ARG:CB	2.24	0.42
2:B:240:ARG:HG3	2:B:240:ARG:HH11	1.84	0.42
3:Y:18:GLN:NE2	3:Y:18:GLN:C	2.72	0.42
1:P:70:GLU:HA	1:P:102:ILE:HD13	2.02	0.42
1:A:202:ALA:HA	1:A:207:LEU:HB2	2.00	0.42
2:Q:109:PHE:CE2	2:Q:113:ILE:HD11	2.54	0.42
3:Y:11:LYS:HA	3:Y:14:TRP:CD1	2.54	0.42
1:P:85:ASP:OD1	1:P:118:LYS:NZ	2.50	0.42
2:Q:368:MET:C	2:Q:370:THR:N	2.73	0.42
2:B:240:ARG:O	2:B:244:CYS:HB3	2.19	0.42
2:Q:316:THR:CG2	2:Q:409:PHE:HB2	2.49	0.42
2:Q:236:GLU:HA	2:Q:239:VAL:CG2	2.49	0.42
2:Q:261:VAL:HG12	2:Q:261:VAL:O	2.20	0.42
1:P:292:LEU:HD11	1:P:355:LEU:HD21	2.02	0.42
1:P:104:LYS:HB3	1:P:104:LYS:HE2	1.86	0.42
2:B:331:LEU:HD12	2:B:331:LEU:HA	1.83	0.42
1:P:216:GLU:HB2	1:P:243:TRP:CH2	2.54	0.42
1:P:216:GLU:HB2	1:P:243:TRP:CZ2	2.55	0.42
2:B:255:MET:SD	6:B:516:PGW:H2A	2.60	0.42
2:Q:172:VAL:HG12	2:Q:172:VAL:O	2.20	0.42
1:A:38:PHE:HE1	1:A:337:ILE:CD1	2.33	0.42
2:Q:160:GLY:H	2:Q:161:PRO:CD	2.32	0.42
1:A:333:ASN:ND2	4:A:1001:NAP:H61A	2.15	0.42
2:B:272:LEU:HD22	2:B:285:VAL:HG21	2.01	0.42
2:B:98:LEU:HD21	2:B:113:ILE:HD13	2.01	0.42
1:A:261:PRO:O	1:A:262:TYR:HB2	2.19	0.42
2:B:256:ASN:O	2:B:260:ILE:HG13	2.19	0.42
1:A:40:ARG:HD2	1:A:318:SER:O	2.20	0.42
2:B:396:LEU:O	2:B:400:LEU:HG	2.20	0.41
2:B:369:THR:OG1	2:B:371:VAL:HG23	2.20	0.41
2:Q:230:ILE:HD11	2:Q:263:ILE:HG22	2.01	0.41
2:Q:160:GLY:N	2:Q:161:PRO:CD	2.83	0.41
1:A:208:ILE:HA	1:A:209:PRO:HD3	1.92	0.41
1:A:323:GLY:HA3	4:A:1001:NAP:H51A	2.02	0.41
1:A:119:ILE:O	1:A:120:PHE:HB2	2.20	0.41
2:Q:202:PHE:CD1	2:Q:279:VAL:HG22	2.55	0.41
2:Q:215:SER:O	2:Q:216:THR:C	2.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:159:ARG:HA	1:P:188:SER:O	2.21	0.41
2:B:253:ASN:HB3	2:B:256:ASN:HD22	1.85	0.41
2:B:300:ILE:HG23	2:B:301:PHE:N	2.34	0.41
1:A:38:PHE:CD1	1:A:337:ILE:HD13	2.56	0.41
2:B:326:LEU:HD12	2:B:326:LEU:HA	1.83	0.41
2:Q:305:ARG:HG3	2:Q:305:ARG:HH11	1.86	0.41
2:Q:164:ILE:O	2:Q:168:VAL:HG23	2.20	0.41
2:B:202:PHE:HB2	2:B:279:VAL:HG22	2.03	0.41
2:B:282:PHE:HA	2:B:285:VAL:HG12	2.03	0.41
1:A:75:LEU:HD12	1:A:75:LEU:HA	1.79	0.41
2:Q:297:ILE:C	2:Q:299:ARG:N	2.74	0.41
2:Q:209:THR:HG22	2:Q:209:THR:O	2.21	0.41
2:B:73:ARG:HB2	2:B:75:GLU:HG2	2.03	0.41
2:B:160:GLY:N	2:B:161:PRO:CD	2.83	0.41
2:B:318:LYS:HD2	6:B:516:PGW:H22	2.01	0.41
2:B:213:GLN:HE22	2:B:219:THR:HB	1.86	0.41
2:Q:236:GLU:HA	2:Q:239:VAL:HG23	2.02	0.41
2:B:189:ARG:NH1	2:B:189:ARG:HG3	2.36	0.41
2:B:415:ARG:NH1	2:B:415:ARG:HG2	2.36	0.41
2:Q:337:LEU:HD23	2:Q:337:LEU:C	2.42	0.41
2:B:209:THR:HG21	2:B:286:ARG:HG3	2.03	0.41
1:A:125:ALA:HB3	1:A:128:GLU:HG3	2.01	0.41
2:B:61:ASP:OD2	2:B:64:LYS:HG3	2.20	0.41
2:Q:252:THR:HG22	2:Q:252:THR:O	2.21	0.41
1:A:249:GLY:HA3	7:A:1140:HOH:O	2.21	0.41
2:B:88:ILE:O	2:B:91:TYR:HB3	2.21	0.41
1:A:251:VAL:CG1	1:A:251:VAL:O	2.68	0.41
1:P:98:VAL:O	1:P:102:ILE:HG13	2.21	0.41
1:A:360:TYR:CD1	1:A:360:TYR:N	2.89	0.41
3:Y:26:GLY:HA2	3:Y:36:TYR:CD1	2.56	0.40
2:Q:170:VAL:O	2:Q:173:ILE:HB	2.21	0.40
2:B:224:ILE:O	2:B:228:LEU:HG	2.20	0.40
2:Q:255:MET:HE3	2:Q:305:ARG:HG3	2.03	0.40
1:P:292:LEU:HA	1:P:295:ILE:HD13	2.02	0.40
2:Q:343:TYR:CE1	2:Q:356:SER:HA	2.56	0.40
1:A:216:GLU:HB2	1:A:243:TRP:CZ2	2.56	0.40
2:B:311:GLN:O	2:B:315:GLN:HG3	2.21	0.40
2:Q:106:LEU:HD11	2:Q:130:GLU:HG2	2.03	0.40
2:Q:180:PHE:HA	2:Q:183:GLU:OE2	2.21	0.40
2:Q:171:MET:N	2:Q:171:MET:HE2	2.37	0.40
2:B:142:GLU:O	2:B:143:ASN:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:285:VAL:O	2:B:289:VAL:HG23	2.21	0.40
1:A:215:ALA:O	1:A:242:THR:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	324/333 (97%)	313 (97%)	10 (3%)	1 (0%)	46 68
1	P	324/333 (97%)	313 (97%)	10 (3%)	1 (0%)	46 68
2	B	384/514 (75%)	350 (91%)	21 (6%)	13 (3%)	5 6
2	Q	357/514 (70%)	311 (87%)	37 (10%)	9 (2%)	7 10
3	Y	35/37 (95%)	19 (54%)	15 (43%)	1 (3%)	6 8
All	All	1424/1731 (82%)	1306 (92%)	93 (6%)	25 (2%)	11 18

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	134	LYS
2	B	137	GLU
2	B	138	ARG
2	B	139	PRO
2	B	143	ASN
2	Q	154	GLU
1	A	120	PHE
2	B	133	ILE
2	B	144	GLU
1	P	120	PHE
2	Q	150	TRP
2	Q	159	SER

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Mol	Chain	Res	Type
2	Q	216	THR
2	Q	217	SER
2	B	245	PRO
2	B	142	GLU
2	B	146	GLN
2	B	243	ALA
2	Q	373	TYR
3	Y	10	SER
2	Q	245	PRO
2	B	141	PRO
2	B	198	GLY
2	Q	156	PRO
2	Q	400	LEU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	273/280 (98%)	270 (99%)	3 (1%)	80 94
1	P	273/280 (98%)	266 (97%)	7 (3%)	54 81
2	B	332/459 (72%)	327 (98%)	5 (2%)	72 91
2	Q	324/459 (71%)	320 (99%)	4 (1%)	78 93
3	Y	35/35 (100%)	33 (94%)	2 (6%)	25 46
All	All	1237/1513 (82%)	1216 (98%)	21 (2%)	68 89

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	214	GLN
1	A	326	ASN
1	A	338	GLN
2	B	86	ASP
2	B	103	ASN
2	B	129	ASP

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Mol	Chain	Res	Type
2	B	185	LEU
2	B	324	LEU
1	P	37	GLN
1	P	75	LEU
1	P	129	ARG
1	P	214	GLN
1	P	223	GLU
1	P	268	LYS
1	P	283	ARG
2	Q	103	ASN
2	Q	150	TRP
2	Q	212	TYR
2	Q	351	ASP
3	Y	14	TRP
3	Y	18	GLN

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	148	GLN
1	A	286	GLN
1	A	326	ASN
1	A	333	ASN
1	A	338	GLN
2	B	53	GLN
2	B	103	ASN
2	B	192	ASN
2	B	213	GLN
2	B	214	GLN
2	B	414	HIS
1	P	37	GLN
1	P	148	GLN
1	P	163	ASN
1	P	204	GLN
1	P	271	GLN
1	P	286	GLN
1	P	293	GLN
1	P	333	ASN
2	Q	53	GLN
2	Q	103	ASN
2	Q	148	GLN

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Mol	Chain	Res	Type
2	Q	207	GLN
2	Q	213	GLN
2	Q	290	GLN
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	1.01	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 25 ligands modelled in this entry, 6 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	1.28	5 (11%)	54,80,80	1.18	4 (7%)
6	PGW	B	504	-	21,21,50	0.59	0	23,23,56	1.24	4 (17%)
6	PGW	B	505	-	8,8,50	0.34	0	7,7,56	0.53	0
6	PGW	B	506	-	8,8,50	0.34	0	7,7,56	0.53	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	0.52	0
6	PGW	B	509	-	8,8,50	0.34	0	7,7,56	0.54	0
6	PGW	B	510	-	8,8,50	0.34	0	7,7,56	0.54	0
6	PGW	B	511	-	6,6,50	0.34	0	5,5,56	0.46	0
6	PGW	B	512	-	8,8,50	0.34	0	7,7,56	0.52	0
6	PGW	B	513	-	11,11,50	0.34	0	10,10,56	0.59	0
6	PGW	B	514	-	22,22,50	0.82	0	25,27,56	1.30	5 (20%)
6	PGW	B	515	-	11,11,50	0.34	0	10,10,56	0.60	0
6	PGW	B	516	-	36,36,50	0.65	0	37,42,56	0.93	2 (5%)
6	PGW	B	517	-	9,9,50	0.34	0	8,8,56	0.56	0
6	PGW	B	518	-	11,11,50	0.34	0	10,10,56	0.57	0
6	PGW	B	519	-	11,11,50	0.34	0	10,10,56	0.57	0
4	NAP	P	1001	-	42,52,52	1.35	6 (14%)	54,80,80	1.19	4 (7%)
6	PGW	Q	504	-	21,21,50	0.60	0	23,23,56	1.24	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	-	-	0/9/9/55	0/0/0/0
6	PGW	B	514	-	-	0/24/24/55	0/0/0/0
6	PGW	B	515	-	-	0/9/9/55	0/0/0/0
6	PGW	B	516	-	-	0/41/41/55	0/0/0/0
6	PGW	B	517	-	-	0/7/7/55	0/0/0/0
6	PGW	B	518	-	-	0/9/9/55	0/0/0/0
6	PGW	B	519	-	-	0/9/9/55	0/0/0/0
4	NAP	P	1001	-	-	0/27/67/67	0/5/5/5
6	PGW	Q	504	-	-	0/23/23/55	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	1001	NAP	O4B-C4B	2.08	1.49	1.45
4	A	1001	NAP	C4A-N3A	2.47	1.39	1.35
4	A	1001	NAP	C2A-N3A	2.55	1.36	1.32
4	P	1001	NAP	C2A-N3A	2.94	1.37	1.32
4	P	1001	NAP	C4A-N3A	3.00	1.40	1.35
4	P	1001	NAP	O4B-C1B	3.30	1.45	1.41
4	A	1001	NAP	C4N-C3N	3.33	1.45	1.39
4	A	1001	NAP	C6N-N1N	3.37	1.44	1.35
4	P	1001	NAP	C4N-C3N	3.37	1.45	1.39
4	A	1001	NAP	O4B-C1B	3.48	1.45	1.41
4	P	1001	NAP	C6N-N1N	3.56	1.45	1.35

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1001	NAP	N3A-C2A-N1A	-3.70	126.06	128.89
4	P	1001	NAP	N3A-C2A-N1A	-3.62	126.13	128.89
6	B	514	PGW	C03-C02-C01	-3.03	104.99	112.07
6	B	504	PGW	C01-O03-C19	-2.55	109.72	116.85
6	Q	504	PGW	C01-O03-C19	-2.52	109.79	116.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	514	PGW	C01-O03-C19	-2.38	110.19	116.85
6	Q	504	PGW	C02-O01-C1	-2.08	112.89	117.89
6	B	516	PGW	O01-C02-C01	-2.05	101.13	108.36
6	B	504	PGW	C02-O01-C1	-2.02	113.04	117.89
4	A	1001	NAP	O4D-C1D-N1N	2.06	110.39	108.13
4	P	1001	NAP	C2A-N1A-C6A	2.09	122.49	118.77
6	B	514	PGW	O11-P-O14	2.21	112.76	107.14
4	A	1001	NAP	C2A-N1A-C6A	2.24	122.76	118.77
6	B	514	PGW	O03-C19-C20	2.29	118.89	111.90
6	Q	504	PGW	O03-C19-C20	2.32	118.95	111.90
6	B	516	PGW	O01-C1-C2	2.35	116.63	111.53
4	P	1001	NAP	P2B-O2B-C2B	2.36	127.21	121.56
6	B	504	PGW	O03-C19-C20	2.37	119.11	111.90
6	B	514	PGW	O01-C1-C2	2.94	117.92	111.53
4	A	1001	NAP	PN-O3-PA	3.23	141.79	132.73
6	B	504	PGW	O01-C1-C2	3.25	118.59	111.53
6	Q	504	PGW	O01-C1-C2	3.27	118.64	111.53
4	P	1001	NAP	PN-O3-PA	3.36	142.15	132.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1001	NAP	3	0
6	B	504	PGW	4	0
6	B	507	PGW	1	0
6	B	509	PGW	1	0
6	B	510	PGW	2	0
6	B	513	PGW	1	0
6	B	514	PGW	1	0
6	B	515	PGW	2	0
6	B	516	PGW	9	0
4	P	1001	NAP	3	0
6	Q	504	PGW	7	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, 95^{th} 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%)	0.10	8 (2%) 61 65	25, 41, 64, 92	0
1	P	326/333 (97%)	0.07	9 (2%) 56 61	26, 44, 77, 101	0
2	B	386/514 (75%)	0.74	52 (13%) 4 4	32, 67, 119, 128	0
2	Q	363/514 (70%)	2.45	132 (36%) 0 0	39, 102, 196, 208	0
3	Y	36/37 (97%)	4.83	31 (86%) 0 0	83, 90, 98, 98	36 (100%)
All	All	1437/1731 (83%)	0.98	232 (16%) 3 2	25, 59, 182, 208	36 (2%)

All (232) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Q	214	GLN	16.1
3	Y	20	LEU	14.3
2	Q	153	PHE	13.6
2	Q	210	ILE	13.4
2	Q	279	VAL	13.3
2	Q	280	LEU	13.3
2	Q	216	THR	13.1
2	Q	281	GLN	12.8
2	Q	218	PHE	12.6
2	Q	282	PHE	12.5
2	Q	250	PHE	12.4
3	Y	4	ASN	11.6
2	Q	272	LEU	11.1
2	Q	247	LYS	11.1
2	Q	242	PHE	11.0
2	Q	244	CYS	10.6
2	Q	206	SER	10.3
2	Q	205	TYR	10.2
2	Q	249	GLY	10.1
2	Q	161	PRO	10.0

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Mol	Chain	Res	Type	RSRZ
2	Q	240	ARG	10.0
2	Q	245	PRO	10.0
2	Q	150	TRP	9.8
2	Q	273	THR	9.8
2	Q	251	PHE	9.6
2	Q	248	ALA	9.6
2	Q	225	VAL	9.5
2	Q	246	SER	9.5
2	Q	215	SER	9.4
2	Q	212	TYR	9.4
2	Q	149	VAL	9.3
3	Y	21	HIS	9.2
2	Q	202	PHE	9.2
2	Q	164	ILE	9.1
2	Q	223	PHE	8.8
1	P	36	LEU	8.6
2	Q	288	VAL	8.5
2	Q	285	VAL	8.5
2	Q	208	SER	8.2
2	Q	283	GLN	7.9
2	Q	190	ASP	7.9
3	Y	28	CYS	7.8
2	B	152	LEU	7.7
2	Q	209	THR	7.6
2	Q	241	PHE	7.5
3	Y	16	VAL	7.3
2	Q	203	HIS	7.2
2	Q	284	ASN	7.2
2	Q	152	LEU	7.2
2	Q	165	ILE	7.1
2	Q	243	ALA	7.1
2	Q	156	PRO	7.1
3	Y	15	SER	6.8
2	Q	145	PHE	6.8
3	Y	17	CYS	6.7
2	Q	415	ARG	6.6
2	Q	252	THR	6.4
2	Q	217	SER	6.4
2	Q	275	SER	6.4
2	Q	158	SER	6.3
2	Q	238	LEU	6.3
1	A	360	TYR	6.3

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Mol	Chain	Res	Type	RSRZ
2	Q	235	PHE	6.3
2	Q	271	PHE	6.3
2	Q	213	GLN	6.3
2	Q	151	LEU	6.2
2	Q	269	THR	6.1
2	Q	229	CYS	6.1
3	Y	8	THR	6.0
3	Y	23	THR	6.0
2	Q	155	TYR	5.9
2	Q	237	PHE	5.7
2	Q	168	VAL	5.7
2	Q	265	PRO	5.7
3	Y	22	ASN	5.7
3	Y	3	THR	5.7
3	Y	12	GLU	5.7
2	Q	219	THR	5.7
2	B	153	PHE	5.6
2	Q	160	GLY	5.6
3	Y	19	ARG	5.5
2	Q	286	ARG	5.5
2	Q	159	SER	5.5
2	Q	276	ASN	5.4
1	P	360	TYR	5.3
2	B	193	GLU	5.3
2	B	145	PHE	5.2
3	Y	24	SER	5.2
3	Y	18	GLN	5.2
2	Q	233	PHE	5.1
2	Q	268	VAL	5.1
3	Y	36	TYR	5.0
3	Y	6	SER	5.0
2	Q	154	GLU	5.0
2	Q	287	ARG	5.0
2	Q	146	GLN	4.9
2	B	156	PRO	4.9
2	Q	163	ARG	4.9
2	B	199	GLY	4.7
2	Q	224	ILE	4.6
3	Y	34	ARG	4.6
2	Q	222	PHE	4.6
2	Q	303	LEU	4.5
2	B	251	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
2	Q	231	ILE	4.4
2	Q	291	ILE	4.4
2	B	219	THR	4.4
2	B	136	GLU	4.4
2	Q	162	ALA	4.4
2	B	191	GLU	4.3
2	B	155	TYR	4.3
3	Y	9	THR	4.3
2	Q	258	ILE	4.2
2	Q	172	VAL	4.2
2	Q	261	VAL	4.2
3	Y	29	MET	4.1
2	Q	207	GLN	4.1
2	B	151	LEU	4.1
2	Q	166	ALA	4.1
3	Y	5	VAL	4.0
2	Q	221	PRO	4.0
3	Y	14	TRP	3.9
2	Q	204	THR	3.8
2	Q	226	GLU	3.8
1	A	36	LEU	3.8
2	Q	189	ARG	3.8
3	Y	26	GLY	3.7
2	B	190	ASP	3.7
2	B	158	SER	3.7
2	Q	147	ARG	3.6
2	Q	191	GLU	3.6
2	Q	289	VAL	3.6
2	Q	157	GLU	3.6
2	Q	220	ASP	3.5
2	B	165	ILE	3.5
2	Q	302	LYS	3.5
2	Q	267	TYR	3.5
2	Q	264	ILE	3.5
2	B	204	THR	3.5
2	B	194	ASP	3.5
3	Y	7	CYS	3.5
2	B	157	GLU	3.4
2	B	192	ASN	3.4
2	B	248	ALA	3.4
2	Q	253	ASN	3.3
2	B	161	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
2	Q	187	ILE	3.3
2	Q	266	TYR	3.3
2	Q	274	GLU	3.3
2	B	125	MET	3.2
2	Q	148	GLN	3.2
2	Q	306	HIS	3.2
2	B	150	TRP	3.2
2	B	252	THR	3.1
3	Y	25	ARG	3.1
2	B	205	TYR	3.0
2	Q	260	ILE	3.0
2	B	215	SER	3.0
2	Q	262	ALA	3.0
2	B	162	ALA	3.0
2	Q	170	VAL	3.0
3	Y	10	SER	2.9
2	Q	295	MET	2.9
2	B	241	PHE	2.9
3	Y	31	LYS	2.9
2	Q	173	ILE	2.9
1	A	280	GLU	2.9
2	Q	254	ILE	2.9
2	B	200	VAL	2.8
2	B	154	GLU	2.8
2	B	132	TYR	2.8
2	Q	322	ARG	2.8
2	Q	175	ILE	2.8
2	B	124	GLU	2.8
2	B	164	ILE	2.7
1	P	349	HIS	2.7
2	B	370	THR	2.7
2	B	351	ASP	2.7
2	B	213	GLN	2.7
2	Q	36	VAL	2.7
3	Y	13	CYS	2.7
2	Q	292	PHE	2.7
2	B	163	ARG	2.6
3	Y	33	CYS	2.6
2	Q	114	ARG	2.6
2	Q	188	PHE	2.6
2	B	149	VAL	2.6
2	Q	308	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	Q	417	THR	2.6
2	B	121	GLU	2.6
1	A	205	PHE	2.5
2	B	371	VAL	2.5
2	Q	304	SER	2.5
2	Q	73	ARG	2.5
1	P	207	LEU	2.5
2	B	144	GLU	2.5
2	B	242	PHE	2.4
2	Q	228	LEU	2.4
1	P	202	ALA	2.4
3	Y	37	SER	2.3
2	B	417	THR	2.3
2	B	272	LEU	2.3
1	P	201	VAL	2.3
2	B	73	ARG	2.3
2	Q	239	VAL	2.3
1	P	200	SER	2.3
3	Y	27	LYS	2.2
2	B	131	GLY	2.2
2	Q	72	LEU	2.2
2	Q	236	GLU	2.2
1	A	206	ASN	2.2
2	Q	270	ILE	2.2
2	Q	412	PHE	2.2
1	A	202	ALA	2.2
2	Q	211	GLY	2.2
1	A	361	SER	2.2
2	B	198	GLY	2.2
2	Q	121	GLU	2.2
2	Q	56	GLU	2.1
2	B	196	HIS	2.1
2	Q	125	MET	2.1
2	B	250	PHE	2.1
2	B	396	LEU	2.1
2	Q	278	SER	2.1
1	A	204	GLN	2.1
2	Q	300	ILE	2.1
1	P	205	PHE	2.1
2	B	167	ILE	2.0
2	Q	128	GLU	2.0
2	Q	230	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	P	206	ASN	2.0
2	B	195	MET	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, 95^{th} 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	0.84	0.22	-	88,88,89,89	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, 95^{th} 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	518	12/51	0.35	0.51	11.94	113,116,117,117	0
6	PGW	B	515	12/51	0.55	0.54	10.05	84,90,94,94	0
6	PGW	B	504	22/51	0.50	0.43	7.99	76,86,90,91	0
6	PGW	B	510	9/51	0.78	0.54	6.34	90,93,97,98	0
6	PGW	B	509	9/51	0.80	0.40	5.97	80,81,81,82	0
6	PGW	Q	504	22/51	0.51	0.34	4.03	100,113,118,119	0
6	PGW	B	514	23/51	0.56	0.40	3.47	136,139,148,149	0
6	PGW	B	516	37/51	0.37	0.38	3.42	108,129,144,145	0
6	PGW	B	513	12/51	0.66	0.35	3.25	74,80,83,84	0
6	PGW	B	505	9/51	0.69	0.29	2.70	98,99,102,102	0
6	PGW	B	517	10/51	0.73	0.31	1.64	77,78,80,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	NAP	P	1001	48/48	0.98	0.15	0.39	35,41,50,51	0
4	NAP	A	1001	48/48	0.99	0.14	-0.10	34,39,45,47	0
6	PGW	B	506	9/51	0.69	0.30	-	95,96,96,97	0
5	K	Q	502	1/1	0.99	0.24	-	62,62,62,62	1
6	PGW	B	507	9/51	0.65	0.28	-	100,101,102,103	0
5	K	B	501	1/1	1.00	0.31	-	23,23,23,23	1
6	PGW	B	511	7/51	0.81	0.23	-	86,87,87,87	0
5	K	B	502	1/1	0.99	0.20	-	27,27,27,27	1
6	PGW	B	512	9/51	0.73	0.25	-	91,91,92,93	0
5	K	Q	501	1/1	0.92	0.23	-	50,50,50,50	1
6	PGW	B	508	9/51	0.35	0.36	-	104,106,107,107	0
5	K	B	503	1/1	0.99	0.27	-	27,27,27,27	1
6	PGW	B	519	12/51	0.58	0.44	-	102,104,105,105	0
5	K	Q	503	1/1	0.97	0.34	-	38,38,38,38	1

6.5 Other polymers (i)

There are no such residues in this entry.