



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:34 AM GMT

PDB ID : 2R9R
Title : Shaker family voltage dependent potassium channel (kv1.2-kv2.1 paddle chimera channel) in association with beta subunit
Authors : Long, S.B.; Tao, X.; Campbell, E.B.; Mackinnon, R.
Deposited on : 2007-09-13
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<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

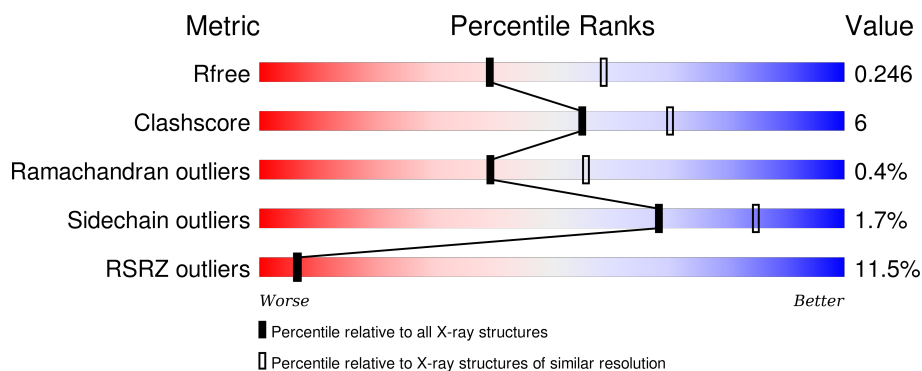
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	<div> <div>88%</div> <div>9% ..</div> </div>
1	G	333	<div> <div>86%</div> <div>11% ..</div> </div>
2	B	514	<div> <div>5%</div> <div>61%</div> <div>13%</div> <div>25%</div> </div>
2	H	514	<div> <div>25%</div> <div>55%</div> <div>15%</div> <div>29%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PGW	B	500	-	-	-	X
5	PGW	B	501	-	-	-	X
5	PGW	B	505	-	-	-	X
5	PGW	B	506	-	-	-	X
5	PGW	B	509	-	-	-	X
5	PGW	B	510	-	-	-	X
5	PGW	B	511	-	-	-	X
5	PGW	B	512	-	-	-	X
5	PGW	B	514	-	-	-	X
5	PGW	B	515	-	-	-	X
5	PGW	H	500	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11814 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 Paddle chimera voltage gated potassium channel Kv1.2-Kv2.1.

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			

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

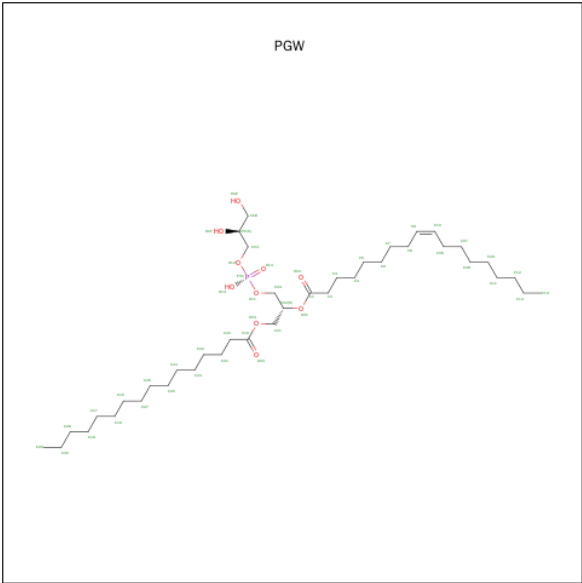
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	4	Total	K	0	0
			4	4		
3	B	4	Total	K	0	0
			4	4		

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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 (1R)-2-{[(S)-{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSP HORYL]OXY}-1-[(HEXADECANOYLOXY)METHYL]ETHYL (9Z)-OCTADEC-9-ENOA TE (three-letter code: PGW) (formula: C₄₀H₇₇O₁₀P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			22	17	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C 9 9	0	0
5	B	1	Total C 9 9	0	0
5	B	1	Total C 9 9	0	0
5	B	1	Total C 9 9	0	0
5	B	1	Total C 9 9	0	0
5	B	1	Total C 9 9	0	0
5	B	1	Total C 7 7	0	0
5	B	1	Total C 9 9	0	0
5	B	1	Total C 12 12	0	0
5	B	1	Total C O P 23 14 8 1	0	0
5	B	1	Total C 12 12	0	0
5	B	1	Total C O P 37 26 10 1	0	0
5	B	1	Total C 10 10	0	0
5	B	1	Total C 12 12	0	0
5	B	1	Total C 12 12	0	0
5	H	1	Total C O 22 17 5	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	141	Total O 141 141	0	0
6	B	52	Total O 52 52	0	0
6	G	102	Total O 102 102	0	0

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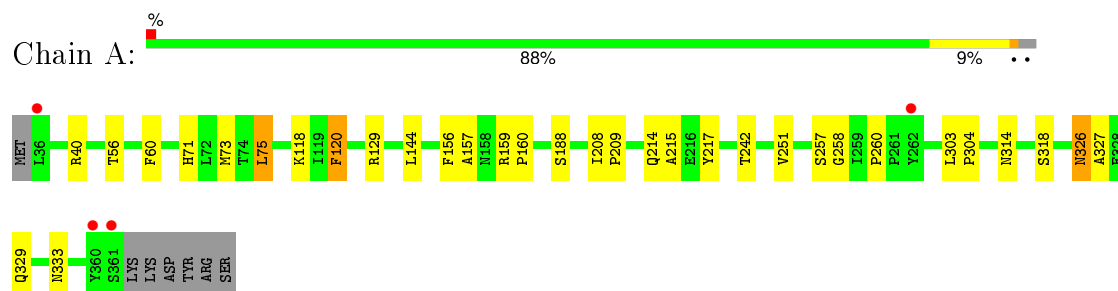
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	24	Total	O	0	0
			24	24		

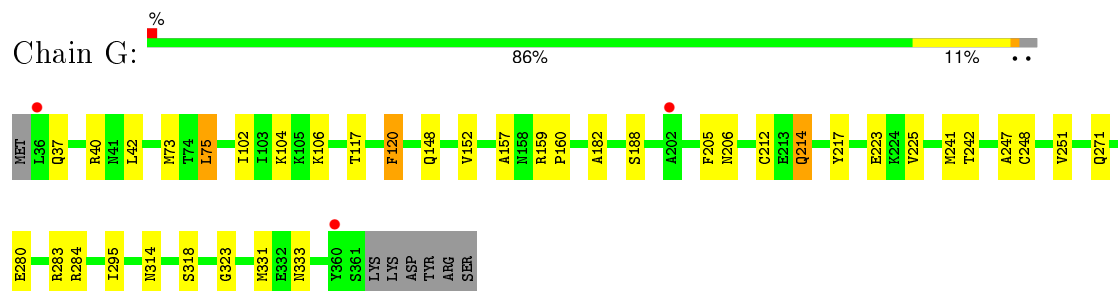
3 Residue-property plots

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.

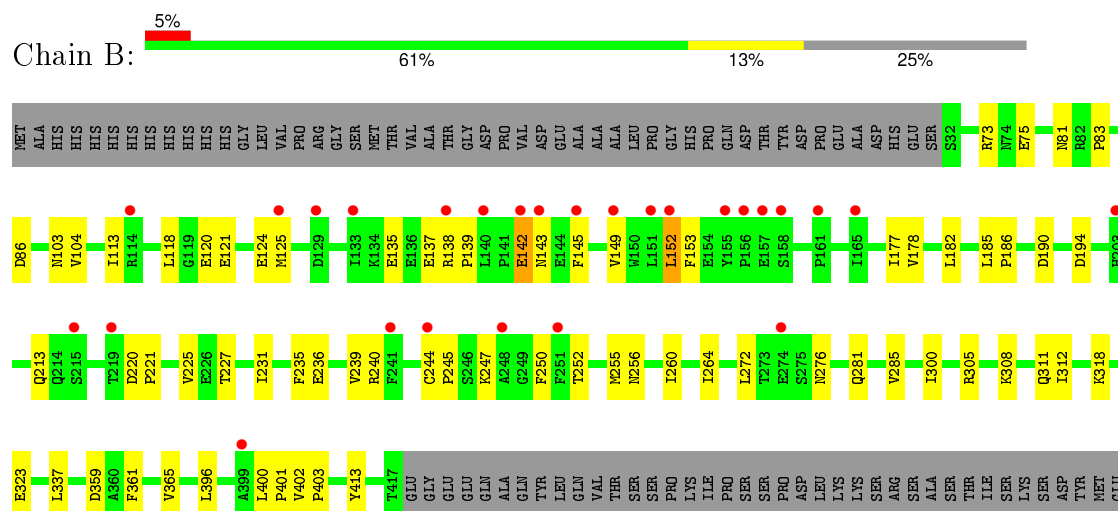
- Molecule 1: Voltage-gated potassium channel subunit beta-2



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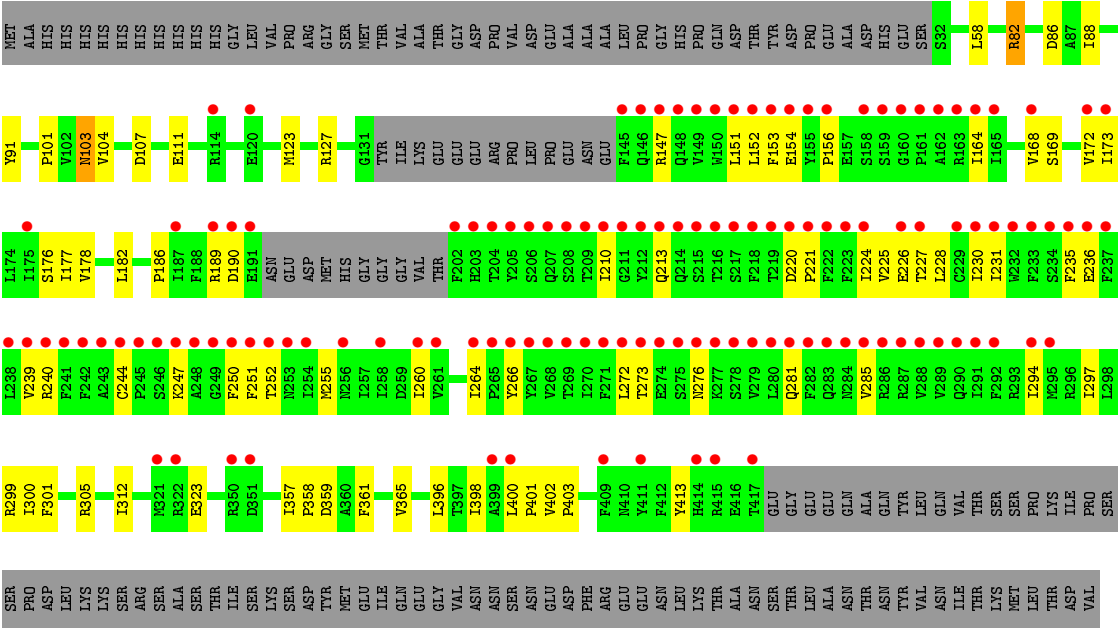


- Molecule 2: Paddle chimera voltage gated potassium channel Kv1.2-Kv2.1



ILE	GLN	GLY	GLY	VAL	ASN	ASN	SER	ASN	ASN	GLU	ASP	PHE	ARG	GLU	GLU	GLU	ASN	PRO	LEU	LYS	THR	ALA	ASN	SER	SER	THR	THR	LEU	ALA	ASN	THR	ASN	THR	TYR	VAL	VAL	ASN	ILE	THR	LYS	MET	MET	LEU	THR	ASP	VAL
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- Molecule 2: Paddle chimera voltage gated potassium channel Kv1.2-Kv2.1



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	144.05Å 144.05Å 284.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.66 – 2.40 49.66 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.4 (49.66-2.40) 85.3 (49.66-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.212 , 0.244 0.216 , 0.246	Depositor DCC
R_{free} test set	5319 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 113410 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11814	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGW, K, 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	0.69	0/2608	0.73	1/3524 (0.0%)
1	G	0.68	0/2608	0.70	1/3524 (0.0%)
2	B	0.57	0/3169	0.66	0/4292
2	H	0.49	0/3036	0.60	2/4114 (0.0%)
All	All	0.61	0/11421	0.67	4/15454 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	82	ARG	NE-CZ-NH2	-7.47	116.56	120.30
2	H	82	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	G	157	ALA	N-CA-C	-5.08	97.28	111.00
1	A	157	ALA	N-CA-C	-5.07	97.31	111.00

There are no chirality outliers.

There are no planarity outliers.

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	21	0
1	G	2556	0	2582	23	0
2	B	3088	0	3033	44	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	2959	0	2955	53	0
3	B	4	0	0	0	0
3	H	4	0	0	0	0
4	A	48	0	25	1	0
4	G	48	0	25	3	0
5	B	210	0	291	9	0
5	H	22	0	25	6	0
6	A	141	0	0	1	0
6	B	52	0	0	0	0
6	G	102	0	0	0	0
6	H	24	0	0	1	0
All	All	11814	0	11518	144	1

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 6.

All (144) 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:H:103:ASN:HD22	2:H:103:ASN:H	1.16	0.93
1:G:333:ASN:HD21	4:G:1001:NAP:H61A	1.29	0.79
1:A:118:LYS:HG3	1:A:156:PHE:HB2	1.72	0.71
2:B:177:ILE:HD13	2:B:300:ILE:HD12	1.73	0.70
2:H:400:LEU:HB2	2:H:401:PRO:HD3	1.72	0.70
2:B:359:ASP:HA	5:B:500:PGW:H02	1.74	0.69
2:B:318:LYS:HD2	5:B:512:PGW:H23A	1.74	0.68
2:H:177:ILE:HD13	2:H:300:ILE:HD12	1.76	0.67
1:A:326:ASN:ND2	1:A:329:GLN:H	1.93	0.66
1:G:295:ILE:HD12	1:G:295:ILE:H	1.62	0.65
1:G:40:ARG:HD2	1:G:318:SER:O	1.98	0.64
2:H:227:THR:O	2:H:231:ILE:HG12	1.98	0.63
2:H:103:ASN:ND2	2:H:103:ASN:H	1.92	0.63
2:B:143:ASN:C	2:B:145:PHE:H	2.01	0.63
2:H:359:ASP:HA	5:H:500:PGW:H02	1.80	0.63
1:A:40:ARG:HD2	1:A:318:SER:O	2.00	0.62
1:A:333:ASN:HD21	4:A:1001:NAP:H61A	1.49	0.59
2:H:236:GLU:HB3	2:H:240:ARG:NH1	2.19	0.58
2:B:400:LEU:HB2	2:B:401:PRO:HD3	1.85	0.57
2:B:177:ILE:CD1	2:B:300:ILE:HD12	2.35	0.57
2:H:236:GLU:HB3	2:H:240:ARG:HH12	1.70	0.56
2:B:227:THR:O	2:B:231:ILE:HG12	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:ASN:H	2:B:103:ASN:HD22	1.54	0.56
2:B:323:GLU:CD	2:B:323:GLU:H	2.09	0.56
2:H:361:PHE:HB2	5:H:500:PGW:H2	1.88	0.55
2:H:186:PRO:O	2:H:190:ASP:HB2	2.07	0.55
1:G:159:ARG:HB2	1:G:160:PRO:HD2	1.89	0.54
2:B:236:GLU:HB3	2:B:240:ARG:NH1	2.22	0.54
2:B:244:CYS:SG	2:B:247:LYS:HD3	2.47	0.54
5:B:500:PGW:H01	5:B:500:PGW:O02	2.06	0.54
2:B:361:PHE:HB2	5:B:500:PGW:H2	1.89	0.54
2:B:103:ASN:H	2:B:103:ASN:ND2	2.05	0.53
2:B:186:PRO:O	2:B:190:ASP:HB2	2.08	0.53
2:H:86:ASP:HB2	6:H:516:HOH:O	2.09	0.53
2:B:121:GLU:O	2:B:125:MET:HG2	2.08	0.53
2:H:153:PHE:CE2	2:H:239:VAL:HG11	2.44	0.52
1:A:258:GLY:O	1:A:260:PRO:HD3	2.09	0.52
1:G:214:GLN:HA	1:G:241:MET:O	2.10	0.52
2:H:177:ILE:CD1	2:H:300:ILE:HD12	2.40	0.51
2:B:139:PRO:O	2:B:245:PRO:CG	2.59	0.51
1:A:159:ARG:HA	1:A:188:SER:O	2.11	0.51
2:H:244:CYS:SG	2:H:247:LYS:HD3	2.50	0.51
2:B:236:GLU:HB3	2:B:240:ARG:HH12	1.75	0.51
2:H:235:PHE:O	2:H:239:VAL:HG23	2.11	0.50
1:G:333:ASN:ND2	4:G:1001:NAP:H61A	2.05	0.50
1:G:280:GLU:O	1:G:284:ARG:HG3	2.12	0.49
1:G:251:VAL:O	1:G:251:VAL:HG12	2.12	0.49
2:B:311:GLN:HG2	5:B:512:PGW:H3	1.93	0.49
2:B:113:ILE:HG23	2:B:118:LEU:HD12	1.95	0.49
1:A:251:VAL:O	1:A:251:VAL:HG12	2.13	0.49
2:H:312:ILE:HD13	2:H:413:TYR:HA	1.95	0.49
2:H:169:SER:O	2:H:173:ILE:HG13	2.12	0.49
1:G:247:ALA:O	1:G:248:CYS:HB2	2.13	0.49
2:H:272:LEU:HD22	2:H:285:VAL:HG21	1.95	0.49
2:H:396:LEU:O	2:H:400:LEU:HG	2.13	0.48
2:B:276:ASN:HB3	2:B:281:GLN:HB3	1.94	0.48
2:B:221:PRO:O	2:B:225:VAL:HG23	2.13	0.48
1:A:326:ASN:HD21	1:A:329:GLN:H	1.58	0.48
2:B:396:LEU:O	2:B:400:LEU:HG	2.12	0.48
1:A:303:LEU:HB3	1:A:304:PRO:HD3	1.96	0.48
5:H:500:PGW:O02	5:H:500:PGW:H01	2.13	0.48
2:H:276:ASN:HB3	2:H:281:GLN:HB3	1.96	0.47
2:B:143:ASN:C	2:B:145:PHE:N	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:217:TYR:HB3	1:G:242:THR:HB	1.96	0.47
2:B:250:PHE:C	2:B:252:THR:H	2.18	0.47
1:A:314:ASN:HB2	6:A:1068:HOH:O	2.15	0.47
1:A:120:PHE:O	1:A:129:ARG:HA	2.15	0.46
2:H:213:GLN:HB3	2:H:220:ASP:HB2	1.96	0.46
2:H:226:GLU:O	2:H:230:ILE:HD13	2.16	0.46
2:H:365:VAL:HG21	5:H:500:PGW:H6A	1.97	0.46
1:G:217:TYR:HB2	1:G:225:VAL:HG21	1.96	0.46
2:B:138:ARG:O	2:B:245:PRO:HG2	2.16	0.46
2:H:221:PRO:O	2:H:225:VAL:HG23	2.16	0.46
5:B:500:PGW:C01	5:B:500:PGW:O02	2.64	0.46
2:B:153:PHE:CE2	2:B:239:VAL:HG11	2.51	0.45
2:H:250:PHE:C	2:H:252:THR:H	2.19	0.45
2:H:255:MET:CE	2:H:305:ARG:HA	2.47	0.45
2:B:260:ILE:O	2:B:264:ILE:HG13	2.16	0.45
2:B:312:ILE:HD13	2:B:413:TYR:HA	1.98	0.45
1:G:120:PHE:CD1	1:G:159:ARG:HG3	2.51	0.45
2:B:402:VAL:HB	2:B:403:PRO:HD3	1.99	0.45
2:H:107:ASP:O	2:H:111:GLU:HG3	2.17	0.45
2:B:73:ARG:HB2	2:B:75:GLU:HG2	1.98	0.45
1:G:75:LEU:HG	1:G:331:MET:HE3	1.98	0.45
2:H:361:PHE:CB	5:H:500:PGW:H2	2.47	0.45
2:H:323:GLU:CD	2:H:323:GLU:H	2.19	0.45
2:B:235:PHE:O	2:B:239:VAL:HG23	2.16	0.45
1:A:71:HIS:CD2	1:A:327:ALA:HB2	2.52	0.45
2:H:88:ILE:O	2:H:91:TYR:HB3	2.17	0.45
2:B:149:VAL:O	2:B:152:LEU:HD12	2.17	0.45
2:H:357:ILE:HB	2:H:358:PRO:HD3	1.98	0.45
1:G:102:ILE:O	1:G:106:LYS:HG2	2.16	0.45
1:G:42:LEU:HD11	1:G:212:CYS:SG	2.56	0.44
2:B:255:MET:CE	2:B:305:ARG:HA	2.47	0.44
2:H:154:GLU:C	2:H:156:PRO:HD3	2.37	0.44
1:G:152:VAL:O	1:G:182:ALA:HA	2.17	0.44
1:A:144:LEU:HD23	1:A:144:LEU:HA	1.87	0.44
2:B:120:GLU:O	2:B:124:GLU:HG3	2.17	0.44
2:B:178:VAL:HG22	5:B:505:PGW:H8	1.99	0.44
1:G:295:ILE:N	1:G:295:ILE:HD12	2.28	0.44
2:B:365:VAL:HG21	5:B:500:PGW:H6A	1.99	0.44
2:H:224:ILE:O	2:H:228:LEU:HG	2.18	0.44
2:H:260:ILE:O	2:H:264:ILE:HG13	2.18	0.43
2:B:256:ASN:O	2:B:260:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:168:VAL:O	2:H:172:VAL:HG23	2.18	0.43
1:A:215:ALA:O	1:A:242:THR:HA	2.19	0.43
1:G:323:GLY:HA3	4:G:1001:NAP:H51A	2.01	0.43
2:H:210:ILE:HD11	2:H:273:THR:HG21	2.00	0.43
2:H:402:VAL:HB	2:H:403:PRO:HD3	2.01	0.43
2:H:178:VAL:O	2:H:182:LEU:HG	2.19	0.42
2:H:294:ILE:O	2:H:297:ILE:HG22	2.19	0.42
1:A:208:ILE:HA	1:A:209:PRO:HD3	1.92	0.42
2:H:361:PHE:HD2	5:H:500:PGW:H20A	1.85	0.42
2:H:58:LEU:HD23	2:H:58:LEU:C	2.40	0.42
2:H:398:ILE:O	2:H:402:VAL:HG23	2.19	0.42
1:A:75:LEU:HD12	1:A:75:LEU:HA	1.93	0.42
1:A:159:ARG:HB2	1:A:160:PRO:HD2	2.00	0.42
2:B:308:LYS:N	5:B:510:PGW:O13	2.53	0.42
2:H:123:MET:O	2:H:127:ARG:HG3	2.20	0.42
1:A:120:PHE:CD1	1:A:159:ARG:HG3	2.55	0.41
2:B:308:LYS:O	2:B:312:ILE:HG13	2.20	0.41
2:B:178:VAL:O	2:B:182:LEU:HG	2.19	0.41
1:A:217:TYR:HB3	1:A:242:THR:HB	2.01	0.41
2:H:101:PRO:HB2	2:H:104:VAL:HG23	2.02	0.41
1:G:251:VAL:CG1	1:G:251:VAL:O	2.68	0.41
2:H:164:ILE:O	2:H:168:VAL:HG23	2.20	0.41
2:H:189:ARG:HG3	2:H:189:ARG:HH11	1.84	0.41
2:H:300:ILE:HG23	2:H:301:PHE:N	2.35	0.41
2:B:83:PRO:HB2	2:B:104:VAL:HG22	2.01	0.41
1:A:56:THR:HB	1:A:60:PHE:HB2	2.02	0.41
2:H:154:GLU:O	2:H:156:PRO:HD3	2.20	0.41
2:H:260:ILE:HG22	2:H:264:ILE:HD11	2.03	0.41
1:G:117:THR:HG22	1:G:152:VAL:HG11	2.02	0.41
2:B:81:ASN:OD1	2:B:83:PRO:HD2	2.21	0.41
2:B:213:GLN:HB3	2:B:220:ASP:HB2	2.03	0.41
1:G:104:LYS:NZ	1:G:148:GLN:HE22	2.19	0.41
2:H:255:MET:HB3	2:H:305:ARG:NH2	2.36	0.40
2:H:176:SER:HB2	2:H:299:ARG:NH1	2.35	0.40
2:B:272:LEU:HD22	2:B:285:VAL:HG21	2.02	0.40
1:A:326:ASN:HD21	1:A:329:GLN:HG3	1.87	0.40
2:H:147:ARG:O	2:H:151:LEU:HG	2.22	0.40
2:H:230:ILE:HG21	2:H:266:TYR:CD2	2.56	0.40
1:G:205:PHE:O	1:G:206:ASN:HB3	2.21	0.40
1:G:159:ARG:HA	1:G:188:SER:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:GLU:O	2:B:142:GLU:O[8_556]	1.43	0.77

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%)	316 (98%)	7 (2%)	1 (0%)	46	63
1	G	324/333 (97%)	317 (98%)	6 (2%)	1 (0%)	46	63
2	B	384/514 (75%)	365 (95%)	16 (4%)	3 (1%)	24	35
2	H	357/514 (70%)	345 (97%)	11 (3%)	1 (0%)	46	63
All	All	1389/1694 (82%)	1343 (97%)	40 (3%)	6 (0%)	39	56

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	PHE
2	B	137	GLU
1	G	120	PHE
2	B	135	GLU
2	B	142	GLU
2	H	251	PHE

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%)	268 (98%)	5 (2%)	66	84
1	G	273/280 (98%)	265 (97%)	8 (3%)	50	71
2	B	332/459 (72%)	327 (98%)	5 (2%)	72	87
2	H	324/459 (71%)	321 (99%)	3 (1%)	84	93
All	All	1202/1478 (81%)	1181 (98%)	21 (2%)	68	85

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

Mol	Chain	Res	Type
1	A	73	MET
1	A	75	LEU
1	A	214	GLN
1	A	257	SER
1	A	326	ASN
2	B	86	ASP
2	B	152	LEU
2	B	185	LEU
2	B	194	ASP
2	B	337	LEU
1	G	37	GLN
1	G	73	MET
1	G	75	LEU
1	G	214	GLN
1	G	223	GLU
1	G	271	GLN
1	G	283	ARG
1	G	314	ASN
2	H	82	ARG
2	H	103	ASN
2	H	152	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) 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

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Mol	Chain	Res	Type
2	B	47	GLN
2	B	53	GLN
2	B	103	ASN
2	B	192	ASN
1	G	37	GLN
1	G	148	GLN
1	G	163	ASN
1	G	286	GLN
1	G	333	ASN
2	H	53	GLN
2	H	103	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	1.38	7 (16%)	54,80,80	1.33	5 (9%)
5	PGW	B	500	-	21,21,50	0.58	0	23,23,56	1.13	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PGW	B	501	-	8,8,50	0.35	0	7,7,56	0.50	0
5	PGW	B	502	-	8,8,50	0.35	0	7,7,56	0.49	0
5	PGW	B	503	-	8,8,50	0.35	0	7,7,56	0.50	0
5	PGW	B	504	-	8,8,50	0.35	0	7,7,56	0.49	0
5	PGW	B	505	-	8,8,50	0.34	0	7,7,56	0.53	0
5	PGW	B	506	-	8,8,50	0.33	0	7,7,56	0.57	0
5	PGW	B	507	-	6,6,50	0.35	0	5,5,56	0.46	0
5	PGW	B	508	-	8,8,50	0.34	0	7,7,56	0.51	0
5	PGW	B	509	-	11,11,50	0.35	0	10,10,56	0.58	0
5	PGW	B	510	-	22,22,50	0.82	0	25,27,56	1.31	5 (20%)
5	PGW	B	511	-	11,11,50	0.34	0	10,10,56	0.60	0
5	PGW	B	512	-	36,36,50	0.65	0	37,42,56	1.02	3 (8%)
5	PGW	B	513	-	9,9,50	0.35	0	8,8,56	0.58	0
5	PGW	B	514	-	11,11,50	0.35	0	10,10,56	0.54	0
5	PGW	B	515	-	11,11,50	0.34	0	10,10,56	0.58	0
4	NAP	G	1001	-	42,52,52	1.36	6 (14%)	54,80,80	1.23	4 (7%)
5	PGW	H	500	-	21,21,50	0.60	0	23,23,56	1.11	1 (4%)

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
5	PGW	B	500	-	-	0/23/23/55	0/0/0/0
5	PGW	B	501	-	-	0/6/6/55	0/0/0/0
5	PGW	B	502	-	-	0/6/6/55	0/0/0/0
5	PGW	B	503	-	-	0/6/6/55	0/0/0/0
5	PGW	B	504	-	-	0/6/6/55	0/0/0/0
5	PGW	B	505	-	-	0/6/6/55	0/0/0/0
5	PGW	B	506	-	-	0/6/6/55	0/0/0/0
5	PGW	B	507	-	-	0/4/4/55	0/0/0/0
5	PGW	B	508	-	-	0/6/6/55	0/0/0/0
5	PGW	B	509	-	-	0/9/9/55	0/0/0/0
5	PGW	B	510	-	-	0/24/24/55	0/0/0/0
5	PGW	B	511	-	-	0/9/9/55	0/0/0/0
5	PGW	B	512	-	-	0/41/41/55	0/0/0/0
5	PGW	B	513	-	-	0/7/7/55	0/0/0/0
5	PGW	B	514	-	-	0/9/9/55	0/0/0/0
5	PGW	B	515	-	-	0/9/9/55	0/0/0/0
4	NAP	G	1001	-	-	0/27/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PGW	H	500	-	-	0/23/23/55	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	NAP	O3D-C3D	-2.18	1.37	1.43
4	A	1001	NAP	C2A-N3A	2.39	1.36	1.32
4	G	1001	NAP	O4B-C4B	2.54	1.50	1.45
4	A	1001	NAP	O4B-C4B	2.72	1.51	1.45
4	A	1001	NAP	C4A-N3A	2.80	1.39	1.35
4	G	1001	NAP	C4N-C3N	2.81	1.44	1.39
4	A	1001	NAP	O4B-C1B	2.84	1.44	1.41
4	G	1001	NAP	C4A-N3A	2.91	1.39	1.35
4	G	1001	NAP	O4B-C1B	3.30	1.45	1.41
4	G	1001	NAP	C6N-N1N	3.40	1.44	1.35
4	A	1001	NAP	C4N-C3N	3.41	1.45	1.39
4	G	1001	NAP	C2A-N3A	3.58	1.38	1.32
4	A	1001	NAP	C6N-N1N	3.84	1.45	1.35

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	NAP	N3A-C2A-N1A	-4.46	125.48	128.89
4	G	1001	NAP	N3A-C2A-N1A	-3.83	125.96	128.89
5	B	510	PGW	C03-C02-C01	-3.20	104.59	112.07
5	B	512	PGW	O03-C01-C02	-3.04	100.50	108.69
5	B	510	PGW	C01-O03-C19	-2.28	110.49	116.85
4	G	1001	NAP	C2A-N1A-C6A	2.03	122.39	118.77
4	A	1001	NAP	O7N-C7N-N7N	2.06	125.50	122.59
4	G	1001	NAP	P2B-O2B-C2B	2.12	126.64	121.56
5	B	510	PGW	O11-P-O14	2.22	112.80	107.14
5	B	510	PGW	O01-C1-C2	2.42	116.78	111.53
5	B	510	PGW	O03-C19-C20	2.42	119.27	111.90
5	B	512	PGW	O01-C02-C03	2.53	117.27	108.36
5	B	512	PGW	O01-C1-C2	2.60	117.17	111.53
4	A	1001	NAP	C2A-N1A-C6A	2.67	123.53	118.77
5	H	500	PGW	O01-C1-C2	2.91	117.86	111.53
4	A	1001	NAP	O4D-C1D-N1N	3.09	111.52	108.13
5	B	500	PGW	O01-C1-C2	3.22	118.53	111.53
4	A	1001	NAP	PN-O3-PA	3.27	141.91	132.73
4	G	1001	NAP	PN-O3-PA	3.39	142.24	132.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1001	NAP	1	0
5	B	500	PGW	5	0
5	B	505	PGW	1	0
5	B	510	PGW	1	0
5	B	512	PGW	2	0
4	G	1001	NAP	3	0
5	H	500	PGW	6	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	4 (1%) 81 81	18, 32, 54, 74	0
1	G	326/333 (97%)	-0.22	3 (0%) 85 85	19, 34, 63, 82	0
2	B	386/514 (75%)	0.26	27 (6%) 19 19	25, 53, 98, 113	0
2	H	363/514 (70%)	2.39	127 (34%) 0 0	30, 85, 176, 185	0
All	All	1401/1694 (82%)	0.57	161 (11%) 6 6	18, 46, 153, 185	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	205	TYR	23.0
2	H	149	VAL	17.1
2	H	214	GLN	16.8
2	H	244	CYS	16.0
2	H	269	THR	14.2
2	H	273	THR	13.6
2	H	282	PHE	13.1
2	H	150	TRP	12.7
2	H	241	PHE	12.6
2	H	204	THR	12.6
2	H	161	PRO	12.2
2	H	145	PHE	12.1
2	H	272	LEU	12.1
2	H	215	SER	12.1
2	H	242	PHE	11.8
2	H	251	PHE	11.4
2	H	164	ILE	11.0
2	H	249	GLY	10.9
2	H	240	ARG	10.7
2	H	218	PHE	10.4
2	H	279	VAL	10.2

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Mol	Chain	Res	Type	RSRZ
2	H	217	SER	10.1
2	H	153	PHE	10.0
2	H	271	PHE	9.9
2	H	203	HIS	9.7
2	H	280	LEU	9.7
2	H	219	THR	9.6
2	H	276	ASN	9.1
2	H	151	LEU	9.1
2	H	212	TYR	9.0
2	H	216	THR	9.0
2	H	152	LEU	8.8
2	H	248	ALA	8.6
2	H	286	ARG	8.5
2	H	190	ASP	8.3
2	H	168	VAL	8.2
2	H	283	GLN	8.2
2	H	288	VAL	8.0
2	H	252	THR	7.8
2	H	268	VAL	7.8
2	H	233	PHE	7.7
2	H	246	SER	7.6
2	H	208	SER	7.6
2	H	265	PRO	7.5
1	G	36	LEU	7.5
2	H	247	LYS	7.5
1	G	360	TYR	7.5
2	H	275	SER	7.3
2	H	165	ILE	7.3
2	H	209	THR	7.0
2	H	284	ASN	6.9
2	H	250	PHE	6.8
2	H	287	ARG	6.8
2	H	235	PHE	6.5
2	H	148	GLN	6.2
2	H	223	PHE	5.8
2	H	281	GLN	5.8
2	H	278	SER	5.7
2	H	159	SER	5.6
2	H	245	PRO	5.5
2	H	289	VAL	5.5
2	H	146	GLN	5.4
2	H	266	TYR	5.4

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Mol	Chain	Res	Type	RSRZ
2	H	213	GLN	5.4
2	H	206	SER	5.3
2	H	231	ILE	5.2
2	H	285	VAL	5.2
2	H	220	ASP	5.0
2	H	160	GLY	5.0
2	H	243	ALA	4.9
2	H	417	THR	4.9
2	H	227	THR	4.9
2	H	238	LEU	4.8
2	H	162	ALA	4.7
2	H	147	ARG	4.7
2	H	415	ARG	4.6
2	H	274	GLU	4.6
2	H	237	PHE	4.5
2	H	187	ILE	4.5
2	H	155	TYR	4.4
2	H	264	ILE	4.4
1	A	360	TYR	4.3
2	H	291	ILE	4.3
2	H	292	PHE	4.2
2	H	234	SER	4.2
1	A	36	LEU	4.1
2	H	172	VAL	4.1
2	H	290	GLN	4.1
2	H	260	ILE	4.0
2	B	244	CYS	3.9
2	H	202	PHE	3.9
2	B	251	PHE	3.8
2	H	226	GLU	3.7
2	H	221	PRO	3.7
2	H	229	CYS	3.7
2	H	191	GLU	3.7
2	H	224	ILE	3.6
2	H	163	ARG	3.6
2	H	210	ILE	3.6
2	H	158	SER	3.6
2	B	140	LEU	3.5
2	B	165	ILE	3.5
2	H	207	GLN	3.5
2	H	261	VAL	3.5
2	H	189	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	152	LEU	3.4
2	H	411	TYR	3.4
2	H	114	ARG	3.4
2	B	158	SER	3.2
2	H	230	ILE	3.2
2	H	350	ARG	3.2
2	H	277	LYS	3.2
2	H	270	ILE	3.2
2	H	254	ILE	3.1
2	H	232	TRP	3.0
2	H	154	GLU	3.0
2	B	114	ARG	3.0
2	B	248	ALA	2.9
2	H	253	ASN	2.9
2	B	133	ILE	2.9
2	B	145	PHE	2.8
2	H	222	PHE	2.8
2	H	175	ILE	2.8
2	H	211	GLY	2.8
2	B	142	GLU	2.8
2	B	125	MET	2.7
2	B	143	ASN	2.7
2	B	151	LEU	2.7
2	H	295	MET	2.7
2	H	256	ASN	2.6
2	B	161	PRO	2.6
2	B	156	PRO	2.6
2	H	258	ILE	2.6
2	H	267	TYR	2.6
2	H	236	GLU	2.6
2	B	149	VAL	2.5
2	H	351	ASP	2.4
2	H	239	VAL	2.4
2	H	294	ILE	2.4
2	H	321	MET	2.4
2	H	414	HIS	2.4
2	H	400	LEU	2.4
2	H	156	PRO	2.4
2	B	215	SER	2.4
2	H	120	GLU	2.3
2	B	155	TYR	2.3
1	G	202	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	361	SER	2.2
2	B	138	ARG	2.2
2	B	157	GLU	2.2
2	H	173	ILE	2.2
2	B	274	GLU	2.2
2	B	129	ASP	2.2
2	H	322	ARG	2.1
2	B	241	PHE	2.1
2	B	399	ALA	2.1
2	H	399	ALA	2.1
2	B	219	THR	2.1
2	B	203	HIS	2.0
1	A	262	TYR	2.0
2	H	409	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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(\AA^2)	Q<0.9
5	PGW	B	511	12/51	0.51	0.45	11.74	76,79,80,80	0
5	PGW	B	500	22/51	0.50	0.34	6.60	61,65,68,69	0
5	PGW	B	506	9/51	0.77	0.39	5.59	74,76,79,79	0
5	PGW	B	515	12/51	0.64	0.51	5.27	88,89,89,89	0
5	PGW	B	501	9/51	0.72	0.22	4.78	82,84,86,86	0
5	PGW	B	505	9/51	0.80	0.27	4.21	65,66,67,67	0
5	PGW	H	500	22/51	0.62	0.26	3.29	82,90,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	PGW	B	509	12/51	0.78	0.22	2.85	67,67,68,68	0
5	PGW	B	510	23/51	0.59	0.29	2.37	100,103,111,111	0
5	PGW	B	512	37/51	0.51	0.28	2.26	81,99,121,123	0
5	PGW	B	514	12/51	0.45	0.34	2.17	87,88,89,89	0
5	PGW	B	513	10/51	0.76	0.22	0.28	63,64,66,66	0
4	NAP	A	1001	48/48	0.99	0.13	0.24	26,30,34,34	0
4	NAP	G	1001	48/48	0.98	0.12	0.02	27,30,37,37	0
5	PGW	B	508	9/51	0.79	0.28	-	76,77,77,77	0
3	K	B	497	1/1	0.98	0.20	-	35,35,35,35	1
3	K	H	498	1/1	0.92	0.11	-	51,51,51,51	1
5	PGW	B	503	9/51	0.53	0.34	-	90,91,91,91	0
5	PGW	B	507	7/51	0.78	0.21	-	72,73,74,74	0
3	K	H	499	1/1	0.99	0.16	-	51,51,51,51	1
3	K	B	499	1/1	1.00	0.23	-	35,35,35,35	1
3	K	H	496	1/1	0.94	0.17	-	49,49,49,49	1
3	K	H	497	1/1	0.96	0.17	-	51,51,51,51	1
3	K	B	496	1/1	0.97	0.13	-	38,38,38,38	1
3	K	B	498	1/1	0.99	0.22	-	29,29,29,29	1
5	PGW	B	502	9/51	0.74	0.24	-	83,84,84,84	0
5	PGW	B	504	9/51	0.58	0.27	-	83,84,85,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.