



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:26 AM GMT

PDB ID : 3LUT
Title : A Structural Model for the Full-length Shaker Potassium Channel Kv1.2
Authors : Chen, X.; Ni, F.; Wang, Q.; Ma, J.
Deposited on : 2010-02-18
Resolution : 2.90 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

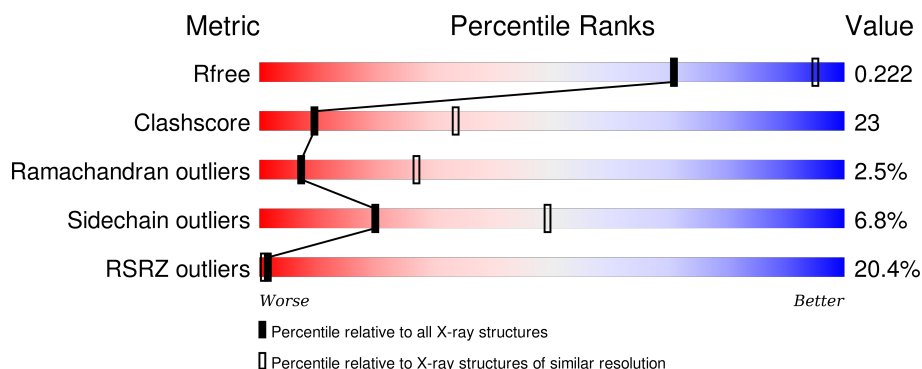
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	367	<div> <div>76%</div> <div>11% • 11%</div> </div>
2	B	499	<div> <div>29%</div> <div>42%</div> <div>29%</div> <div>6%</div> <div>22%</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5848 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			

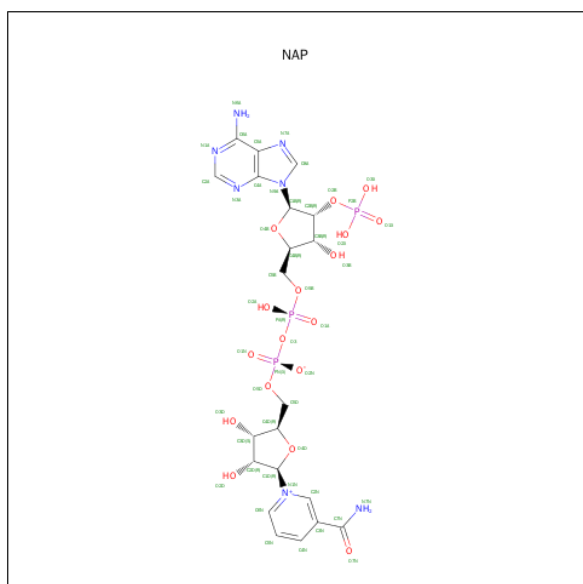
- Molecule 2 is a protein called Potassium voltage-gated channel subfamily A member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	390	Total	C	N	O	S	0	0	0
			3152	2060	509	568	15			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	207	GLN	ASN	ENGINEERED	UNP P63142

- Molecule 3 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
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	6	Total	K	0	0
			6	6		

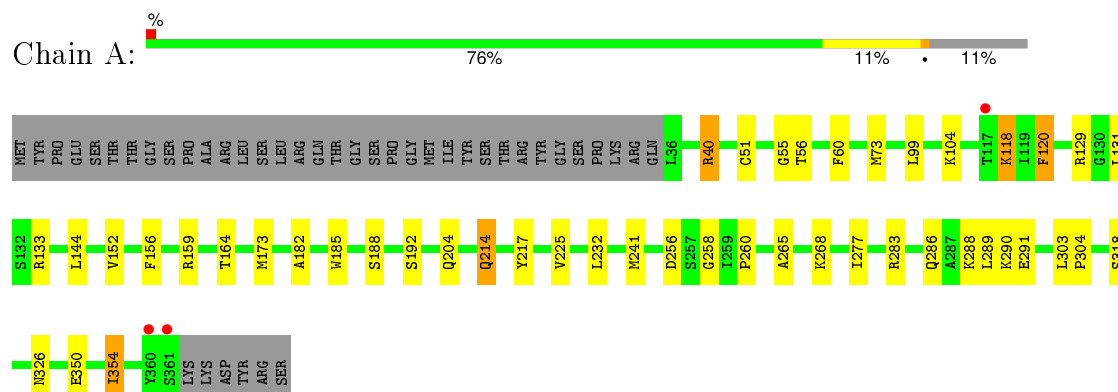
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	72	Total	O	0	0
			72	72		
5	B	14	Total	O	0	0
			14	14		

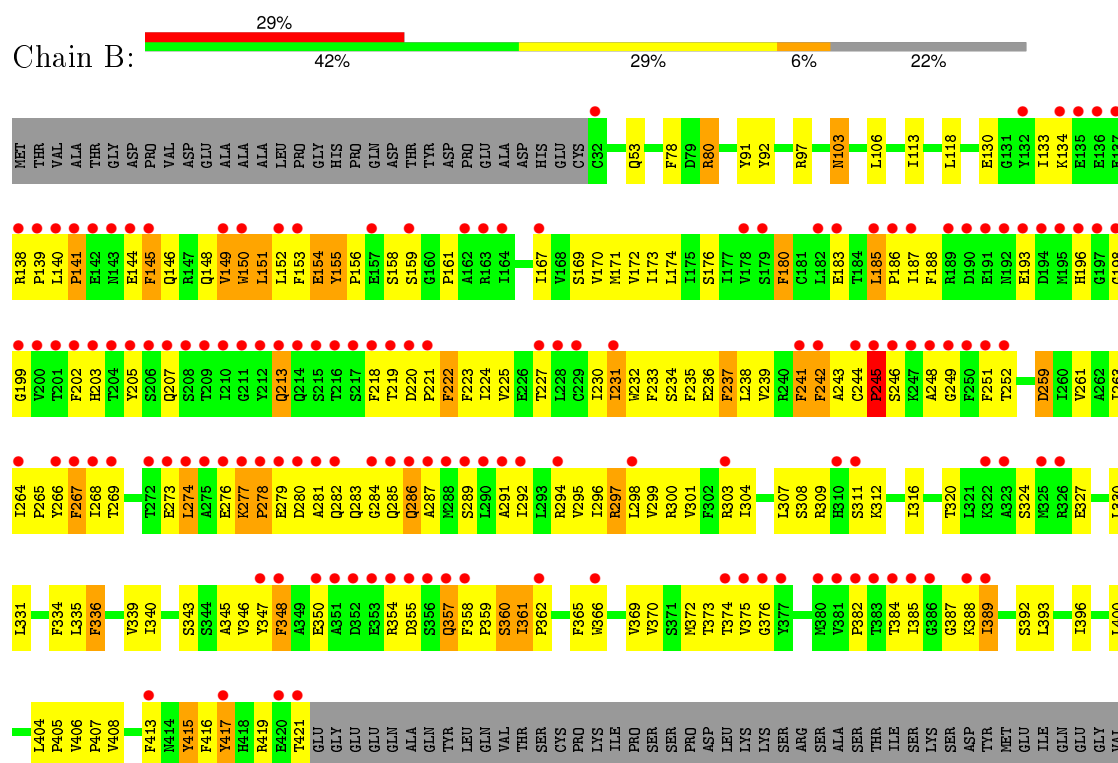
3 Residue-property plots

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 2: Potassium voltage-gated channel subfamily A member 2



ASN	ASN	SER	ASN	GLU	ASP	PHE	ARG	GLU	GLU	ASN	LEU	LYS	THR	ALA	ASN	CYS	THR	LEU	ALA	ASN	THR	ASN	TYR	VAL	ASN	ILE	THR	LYS	MET	LEU	THR	ASP	VAL
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	113.61Å 113.61Å 260.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.48 – 2.90 30.63 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.48-2.90) 89.9 (30.63-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.211 , 0.221 0.209 , 0.222	Depositor DCC
R_{free} test set	1777 reflections (5.63%)	DCC
Wilson B-factor (Å ²)	51.5	Xtriage
Anisotropy	0.711	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 94.7	EDS
Estimated twinning fraction	0.035 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 36329 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5848	wwPDB-VP
Average B, all atoms (Å ²)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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: 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	0.38	0/2608	0.51	0/3524
2	B	0.50	2/3234 (0.1%)	0.62	0/4385
All	All	0.45	2/5842 (0.0%)	0.57	0/7909

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	245	PRO	N-CD	8.41	1.59	1.47
2	B	289	SER	CB-OG	5.22	1.49	1.42

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	27	0
2	B	3152	0	3116	234	1
3	A	48	0	25	1	0
4	B	6	0	0	0	0
5	A	72	0	0	2	0
5	B	14	0	0	0	0
All	All	5848	0	5723	261	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 23.

All (261) 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:199:GLY:O	2:B:205:TYR:HB2	1.52	1.10
2:B:277:LYS:HB2	2:B:278:PRO:HD3	1.31	1.06
2:B:145:PHE:CZ	2:B:155:TYR:HE1	1.75	1.05
2:B:185:LEU:HB2	2:B:186:PRO:CD	1.89	1.01
2:B:278:PRO:HG2	2:B:281:ALA:HB3	1.42	1.00
2:B:185:LEU:HB2	2:B:186:PRO:HD3	1.03	0.99
2:B:266:TYR:CE2	2:B:300:ARG:HG2	2.01	0.96
1:A:129:ARG:HD3	5:A:438:HOH:O	1.66	0.94
2:B:415:TYR:OH	2:B:419:ARG:NH2	2.04	0.91
1:A:40:ARG:HD2	1:A:318:SER:O	1.70	0.91
2:B:219:THR:HB	2:B:222:PHE:CE2	2.06	0.91
2:B:221:PRO:HA	2:B:224:ILE:HD12	1.53	0.90
2:B:265:PRO:HB2	2:B:299:VAL:HG11	1.51	0.90
2:B:199:GLY:O	2:B:205:TYR:CB	2.18	0.90
2:B:277:LYS:HB2	2:B:278:PRO:CD	2.00	0.90
2:B:185:LEU:CB	2:B:186:PRO:HD3	1.97	0.90
2:B:198:GLY:HA2	2:B:205:TYR:CE1	2.06	0.90
2:B:277:LYS:CB	2:B:278:PRO:HD3	2.03	0.89
2:B:153:PHE:C	2:B:156:PRO:HD2	1.94	0.88
2:B:286:GLN:HG3	2:B:287:ALA:H	1.39	0.87
2:B:140:LEU:H	2:B:141:PRO:HD2	1.39	0.86
2:B:278:PRO:HG2	2:B:281:ALA:CB	2.05	0.86
2:B:266:TYR:HE2	2:B:300:ARG:HG2	1.36	0.86
2:B:138:ARG:HB3	2:B:141:PRO:CG	2.07	0.84
2:B:155:TYR:HA	2:B:158:SER:HB2	1.60	0.83
2:B:259:ASP:OD2	2:B:309:ARG:NH2	2.10	0.83
2:B:265:PRO:CB	2:B:299:VAL:HG11	2.09	0.83
2:B:219:THR:HB	2:B:222:PHE:CD2	2.14	0.83
2:B:146:GLN:HG2	2:B:151:LEU:HB3	1.61	0.82
2:B:140:LEU:N	2:B:141:PRO:HD2	1.93	0.82
2:B:278:PRO:CG	2:B:281:ALA:HB3	2.10	0.81
1:A:118:LYS:HG3	1:A:156:PHE:HB2	1.63	0.80
2:B:234:SER:O	2:B:238:LEU:HB2	1.81	0.80
2:B:145:PHE:CZ	2:B:155:TYR:CE1	2.67	0.79
2:B:277:LYS:HE2	2:B:291:ALA:HB2	1.65	0.79
2:B:292:ILE:HG23	2:B:296:ILE:HG21	1.63	0.78
2:B:263:ILE:HG13	2:B:264:ILE:N	1.99	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:220:ASP:O	2:B:224:ILE:HG13	1.85	0.77
2:B:320:THR:HG22	2:B:416:PHE:HD1	1.49	0.77
2:B:144:GLU:OE1	2:B:144:GLU:HA	1.85	0.76
2:B:153:PHE:HA	2:B:156:PRO:HG2	1.67	0.76
2:B:266:TYR:O	2:B:269:THR:HG22	1.86	0.75
2:B:308:SER:HA	2:B:311:SER:HB3	1.67	0.75
2:B:292:ILE:O	2:B:296:ILE:HG12	1.87	0.74
2:B:146:GLN:HE21	2:B:151:LEU:HD13	1.52	0.74
2:B:146:GLN:HG2	2:B:151:LEU:CB	2.18	0.74
2:B:138:ARG:HB3	2:B:141:PRO:HG3	1.69	0.73
2:B:372:MET:C	2:B:374:THR:H	1.87	0.73
2:B:286:GLN:HG3	2:B:287:ALA:N	2.02	0.73
2:B:404:LEU:HB2	2:B:405:PRO:HD3	1.68	0.73
2:B:138:ARG:HB3	2:B:141:PRO:HG2	1.70	0.72
2:B:266:TYR:HE2	2:B:300:ARG:CG	2.03	0.72
2:B:370:VAL:HG12	2:B:376:GLY:H	1.55	0.72
2:B:331:LEU:HB2	2:B:405:PRO:HG2	1.72	0.71
2:B:372:MET:C	2:B:374:THR:N	2.44	0.71
1:A:133:ARG:HD2	5:A:372:HOH:O	1.89	0.71
2:B:156:PRO:HA	2:B:161:PRO:HG2	1.73	0.71
2:B:330:LEU:HG	2:B:334:PHE:HE1	1.55	0.69
2:B:366:TRP:O	2:B:370:VAL:HG23	1.91	0.69
1:A:291:GLU:HB2	1:A:354:ILE:HD13	1.73	0.69
2:B:297:ARG:O	2:B:301:VAL:HG23	1.93	0.69
2:B:202:PHE:CE2	2:B:203:HIS:HD2	2.11	0.68
2:B:330:LEU:HG	2:B:334:PHE:CE1	2.28	0.68
2:B:265:PRO:HG2	2:B:299:VAL:CG1	2.24	0.68
2:B:219:THR:HB	2:B:222:PHE:HE2	1.57	0.68
2:B:241:PHE:C	2:B:243:ALA:H	1.97	0.67
2:B:223:PHE:CZ	2:B:227:THR:HG21	2.30	0.67
2:B:286:GLN:CG	2:B:287:ALA:N	2.58	0.66
2:B:213:GLN:O	2:B:213:GLN:HG2	1.95	0.66
2:B:170:VAL:O	2:B:174:LEU:HG	1.94	0.66
2:B:372:MET:O	2:B:374:THR:HG23	1.94	0.66
2:B:148:GLN:HB3	2:B:151:LEU:HB2	1.77	0.65
2:B:346:VAL:O	2:B:350:GLU:HG2	1.96	0.65
1:A:40:ARG:HE	1:A:51:CYS:HB3	1.62	0.65
2:B:149:VAL:HG23	2:B:150:TRP:CE3	2.32	0.65
2:B:320:THR:HG22	2:B:416:PHE:CD1	2.32	0.64
2:B:274:LEU:O	2:B:274:LEU:HG	1.96	0.64
2:B:205:TYR:CD1	2:B:205:TYR:O	2.51	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:276:GLU:HB3	2:B:282:GLN:OE1	1.98	0.64
2:B:169:SER:O	2:B:172:VAL:HG22	1.98	0.64
2:B:361:ILE:HD13	2:B:361:ILE:H	1.62	0.63
2:B:304:ILE:O	2:B:307:LEU:HG	1.98	0.63
2:B:279:GLU:HG3	2:B:280:ASP:H	1.63	0.63
2:B:278:PRO:CD	2:B:281:ALA:HB3	2.29	0.62
2:B:264:ILE:O	2:B:268:ILE:HG13	1.99	0.62
2:B:279:GLU:HG3	2:B:280:ASP:N	2.15	0.61
2:B:266:TYR:CZ	2:B:300:ARG:HG2	2.35	0.61
2:B:370:VAL:HG12	2:B:376:GLY:N	2.15	0.61
2:B:202:PHE:CE2	2:B:203:HIS:CD2	2.88	0.61
2:B:149:VAL:C	2:B:150:TRP:HE3	2.05	0.60
2:B:146:GLN:NE2	2:B:151:LEU:HD13	2.17	0.59
2:B:336:PHE:O	2:B:340:ILE:HG12	2.02	0.59
2:B:145:PHE:CE2	2:B:155:TYR:HE1	2.19	0.59
2:B:140:LEU:N	2:B:141:PRO:CD	2.66	0.59
2:B:155:TYR:CD2	2:B:158:SER:HB2	2.37	0.59
2:B:198:GLY:CA	2:B:205:TYR:CE1	2.85	0.58
2:B:389:ILE:HG12	2:B:393:LEU:HD23	1.84	0.58
2:B:106:LEU:HD11	2:B:130:GLU:HG2	1.86	0.58
2:B:223:PHE:O	2:B:227:THR:HG23	2.04	0.58
2:B:171:MET:HE1	2:B:174:LEU:HD12	1.86	0.58
2:B:221:PRO:O	2:B:224:ILE:HB	2.04	0.58
2:B:284:GLY:C	2:B:286:GLN:H	2.06	0.57
2:B:155:TYR:CE2	2:B:159:SER:HB3	2.40	0.57
2:B:171:MET:CE	2:B:174:LEU:HD12	2.34	0.57
2:B:357:GLN:O	2:B:357:GLN:HG3	2.05	0.57
2:B:113:ILE:HG23	2:B:118:LEU:HD12	1.87	0.57
2:B:296:ILE:O	2:B:300:ARG:HG3	2.03	0.56
2:B:384:THR:O	2:B:388:LYS:HE2	2.06	0.56
2:B:278:PRO:HD2	2:B:281:ALA:HB3	1.86	0.56
2:B:284:GLY:C	2:B:286:GLN:N	2.58	0.56
2:B:155:TYR:HD2	2:B:158:SER:HB2	1.70	0.56
2:B:78:PHE:HB3	2:B:80:ARG:HG3	1.86	0.56
2:B:198:GLY:HA2	2:B:205:TYR:CD1	2.41	0.55
2:B:350:GLU:OE2	2:B:387:GLY:HA3	2.05	0.55
2:B:276:GLU:HA	2:B:276:GLU:OE1	2.07	0.54
2:B:167:ILE:O	2:B:171:MET:HG2	2.06	0.54
2:B:286:GLN:HE21	2:B:287:ALA:HB2	1.73	0.54
2:B:155:TYR:HE2	2:B:159:SER:HB3	1.72	0.53
2:B:267:PHE:HD2	2:B:267:PHE:C	2.12	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:232:TRP:HA	2:B:232:TRP:CE3	2.43	0.53
2:B:265:PRO:CG	2:B:299:VAL:HG11	2.39	0.53
2:B:180:PHE:C	2:B:180:PHE:CD1	2.81	0.53
2:B:263:ILE:HG13	2:B:264:ILE:H	1.72	0.53
2:B:343:SER:O	2:B:346:VAL:HG12	2.09	0.53
2:B:279:GLU:CG	2:B:280:ASP:H	2.21	0.52
2:B:316:ILE:O	2:B:320:THR:HG23	2.10	0.52
2:B:286:GLN:NE2	2:B:287:ALA:HB2	2.24	0.52
2:B:372:MET:O	2:B:374:THR:N	2.43	0.52
2:B:148:GLN:O	2:B:151:LEU:N	2.42	0.52
2:B:392:SER:O	2:B:396:ILE:HG12	2.10	0.52
2:B:180:PHE:HA	2:B:183:GLU:CG	2.40	0.52
2:B:176:SER:HB3	2:B:303:ARG:NH1	2.25	0.52
2:B:265:PRO:HG2	2:B:299:VAL:HG13	1.92	0.52
2:B:292:ILE:HG23	2:B:296:ILE:CG2	2.39	0.51
2:B:145:PHE:HD2	2:B:146:GLN:H	1.58	0.51
2:B:400:LEU:O	2:B:404:LEU:HG	2.10	0.51
2:B:232:TRP:CZ3	2:B:235:PHE:CD2	2.98	0.51
2:B:327:GLU:HG2	2:B:408:VAL:HG11	1.92	0.51
2:B:276:GLU:HB3	2:B:282:GLN:CD	2.31	0.51
2:B:233:PHE:O	2:B:237:PHE:HB3	2.11	0.51
2:B:345:ALA:HA	2:B:348:PHE:HD2	1.74	0.51
2:B:180:PHE:O	2:B:183:GLU:HG3	2.11	0.51
2:B:267:PHE:C	2:B:267:PHE:CD2	2.84	0.51
2:B:265:PRO:CG	2:B:299:VAL:HG21	2.41	0.51
1:A:56:THR:HB	1:A:60:PHE:HB2	1.93	0.51
2:B:346:VAL:HG22	2:B:350:GLU:HG3	1.93	0.50
1:A:288:LYS:HG2	1:A:354:ILE:HD12	1.94	0.50
1:A:214:GLN:HA	1:A:241:MET:O	2.12	0.50
2:B:339:VAL:HG21	2:B:369:VAL:HG22	1.94	0.50
2:B:171:MET:HA	2:B:171:MET:HE2	1.94	0.50
2:B:220:ASP:HB2	2:B:221:PRO:HD3	1.94	0.49
2:B:155:TYR:N	2:B:156:PRO:CD	2.75	0.49
2:B:350:GLU:OE1	2:B:384:THR:OG1	2.22	0.49
1:A:256:ASP:OD2	1:A:290:LYS:HD3	2.11	0.49
2:B:185:LEU:CB	2:B:186:PRO:CD	2.71	0.49
2:B:279:GLU:CG	2:B:280:ASP:N	2.75	0.49
2:B:180:PHE:HA	2:B:183:GLU:HG3	1.94	0.49
1:A:217:TYR:HB2	1:A:225:VAL:HG21	1.94	0.48
2:B:154:GLU:OE2	2:B:239:VAL:CG1	2.60	0.48
2:B:265:PRO:HG2	2:B:299:VAL:CG2	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:266:TYR:OH	2:B:300:ARG:HG2	2.12	0.48
2:B:219:THR:HB	2:B:222:PHE:HD2	1.75	0.48
2:B:264:ILE:HG13	2:B:265:PRO:HD3	1.96	0.48
2:B:264:ILE:N	2:B:265:PRO:CD	2.76	0.48
2:B:145:PHE:CD2	2:B:146:GLN:N	2.81	0.48
2:B:357:GLN:O	2:B:357:GLN:CG	2.61	0.48
2:B:264:ILE:CG1	2:B:265:PRO:HD3	2.44	0.48
2:B:406:VAL:HB	2:B:407:PRO:HD3	1.96	0.47
2:B:358:PHE:N	2:B:358:PHE:CD1	2.82	0.47
2:B:230:ILE:HA	2:B:233:PHE:HD2	1.80	0.47
2:B:145:PHE:HD2	2:B:146:GLN:N	2.12	0.47
2:B:385:ILE:O	2:B:388:LYS:HG2	2.15	0.47
2:B:267:PHE:HD2	2:B:267:PHE:O	1.97	0.47
2:B:103:ASN:H	2:B:103:ASN:HD22	1.63	0.47
2:B:180:PHE:HB2	2:B:300:ARG:NH2	2.30	0.46
2:B:296:ILE:HG13	2:B:297:ARG:N	2.29	0.46
2:B:372:MET:O	2:B:374:THR:CG2	2.63	0.46
2:B:350:GLU:OE2	2:B:387:GLY:CA	2.62	0.46
2:B:359:PRO:O	2:B:360:SER:C	2.53	0.46
2:B:148:GLN:C	2:B:150:TRP:N	2.69	0.46
2:B:222:PHE:HA	2:B:225:VAL:HG23	1.98	0.46
2:B:295:VAL:HG13	2:B:299:VAL:CG2	2.45	0.46
2:B:320:THR:CG2	2:B:416:PHE:HD1	2.24	0.46
2:B:265:PRO:HB3	2:B:299:VAL:HG21	1.98	0.46
2:B:134:LYS:HG3	2:B:134:LYS:O	2.15	0.46
2:B:224:ILE:HA	2:B:227:THR:HG1	1.81	0.46
2:B:320:THR:O	2:B:324:SER:N	2.49	0.46
2:B:236:GLU:OE1	2:B:236:GLU:HA	2.15	0.46
2:B:237:PHE:CD1	2:B:237:PHE:O	2.69	0.46
2:B:241:PHE:O	2:B:243:ALA:N	2.50	0.45
1:A:159:ARG:HA	1:A:188:SER:O	2.16	0.45
2:B:148:GLN:CB	2:B:151:LEU:HD12	2.47	0.45
2:B:241:PHE:C	2:B:243:ALA:N	2.66	0.45
2:B:417:TYR:CD1	2:B:417:TYR:C	2.90	0.45
2:B:106:LEU:CD1	2:B:130:GLU:HG2	2.46	0.45
2:B:294:ARG:O	2:B:298:LEU:HG	2.17	0.45
1:A:258:GLY:O	1:A:260:PRO:HD3	2.17	0.45
2:B:173:ILE:HG21	2:B:307:LEU:CD2	2.47	0.45
2:B:173:ILE:HG21	2:B:307:LEU:HD21	1.98	0.45
2:B:230:ILE:HG13	2:B:231:ILE:N	2.32	0.45
2:B:145:PHE:CE2	2:B:155:TYR:CE1	3.01	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:PHE:N	2:B:242:PHE:CD1	2.85	0.44
2:B:148:GLN:HG2	2:B:151:LEU:HD12	1.98	0.44
2:B:350:GLU:OE1	2:B:350:GLU:HA	2.18	0.44
2:B:343:SER:OG	2:B:365:PHE:HD2	2.01	0.44
2:B:265:PRO:CG	2:B:299:VAL:CG1	2.94	0.44
2:B:297:ARG:HD2	2:B:297:ARG:HA	1.78	0.44
2:B:148:GLN:O	2:B:150:TRP:N	2.51	0.44
2:B:145:PHE:CE1	2:B:155:TYR:HE1	2.30	0.44
2:B:292:ILE:O	2:B:296:ILE:HG23	2.18	0.44
1:A:256:ASP:HA	1:A:286:GLN:HG2	1.99	0.44
2:B:295:VAL:HG13	2:B:299:VAL:HG21	2.00	0.44
2:B:139:PRO:HB2	2:B:140:LEU:HD23	2.00	0.44
2:B:370:VAL:HG13	2:B:375:VAL:HB	2.00	0.44
1:A:350:GLU:O	1:A:354:ILE:HG23	2.18	0.43
2:B:207:GLN:O	2:B:207:GLN:HG3	2.18	0.43
1:A:144:LEU:HA	1:A:144:LEU:HD23	1.85	0.43
2:B:278:PRO:O	2:B:282:GLN:N	2.34	0.43
2:B:154:GLU:N	2:B:156:PRO:HD2	2.32	0.43
1:A:192:SER:HA	1:A:232:LEU:HD11	2.01	0.43
2:B:316:ILE:HG21	2:B:417:TYR:HB2	2.00	0.43
2:B:360:SER:C	2:B:362:PRO:HD2	2.38	0.43
2:B:223:PHE:CE1	2:B:227:THR:CG2	3.02	0.43
1:A:73:MET:SD	1:A:99:LEU:HD12	2.59	0.43
2:B:282:GLN:O	2:B:283:GLN:C	2.58	0.42
2:B:237:PHE:C	2:B:237:PHE:CD1	2.91	0.42
1:A:289:LEU:HD22	1:A:303:LEU:HD21	2.00	0.42
1:A:55:GLY:HA3	3:A:368:NAP:O3D	2.19	0.42
2:B:91:TYR:HA	2:B:97:ARG:O	2.19	0.42
2:B:296:ILE:HG13	2:B:297:ARG:HD3	2.00	0.42
2:B:242:PHE:HD1	2:B:242:PHE:N	2.17	0.42
1:A:131:LEU:O	1:A:164:THR:HG21	2.20	0.42
2:B:264:ILE:HG13	2:B:265:PRO:CD	2.50	0.42
2:B:336:PHE:CE1	2:B:340:ILE:HD11	2.55	0.42
2:B:354:ARG:HG2	2:B:355:ASP:N	2.35	0.42
2:B:148:GLN:C	2:B:150:TRP:H	2.23	0.42
2:B:264:ILE:O	2:B:268:ILE:CG1	2.67	0.42
2:B:265:PRO:CB	2:B:299:VAL:HG21	2.50	0.42
2:B:146:GLN:HG2	2:B:151:LEU:HB2	2.00	0.42
2:B:316:ILE:HG22	2:B:413:PHE:CD1	2.55	0.41
1:A:144:LEU:HD21	1:A:152:VAL:HG13	2.02	0.41
2:B:198:GLY:HA2	2:B:205:TYR:HE1	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:138:ARG:O	2:B:141:PRO:HG2	2.20	0.41
1:A:265:ALA:HB2	1:A:277:ILE:HD12	2.01	0.41
2:B:312:LYS:HG2	2:B:312:LYS:H	1.58	0.41
2:B:261:VAL:CG1	2:B:261:VAL:O	2.69	0.41
1:A:120:PHE:O	1:A:129:ARG:HA	2.21	0.41
2:B:265:PRO:CG	2:B:299:VAL:CG2	2.97	0.41
2:B:155:TYR:N	2:B:156:PRO:HD2	2.35	0.41
1:A:152:VAL:O	1:A:182:ALA:HA	2.21	0.41
1:A:303:LEU:HB3	1:A:304:PRO:HD3	2.02	0.41
2:B:53:GLN:NE2	2:B:92:TYR:O	2.53	0.41
2:B:154:GLU:O	2:B:158:SER:N	2.53	0.40
2:B:172:VAL:O	2:B:176:SER:CB	2.69	0.40
2:B:176:SER:HB3	2:B:303:ARG:CZ	2.51	0.40
1:A:173:MET:HG3	1:A:185:TRP:CE3	2.56	0.40
2:B:276:GLU:OE1	2:B:282:GLN:HG3	2.21	0.40
2:B:244:CYS:HA	2:B:245:PRO:HD3	1.92	0.40
2:B:278:PRO:HG2	2:B:281:ALA:HB2	1.97	0.40
2:B:419:ARG:C	2:B:421:THR:H	2.24	0.40
2:B:348:PHE:CD1	2:B:348:PHE:C	2.95	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:297:ARG:NH2	2:B:347:TYR:OH[3_755]	2.18	0.02

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	324/367 (88%)	316 (98%)	7 (2%)	1 (0%)	46 79

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	388/499 (78%)	325 (84%)	46 (12%)	17 (4%)	3	12
All	All	712/866 (82%)	641 (90%)	53 (7%)	18 (2%)	7	27

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	193	GLU
2	B	252	THR
2	B	286	GLN
1	A	120	PHE
2	B	242	PHE
2	B	245	PRO
2	B	248	ALA
2	B	373	THR
2	B	278	PRO
2	B	360	SER
2	B	141	PRO
2	B	149	VAL
2	B	249	GLY
2	B	357	GLN
2	B	274	LEU
2	B	277	LYS
2	B	185	LEU
2	B	382	PRO

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	273/309 (88%)	264 (97%)	9 (3%)	45	80
2	B	342/441 (78%)	309 (90%)	33 (10%)	10	31
All	All	615/750 (82%)	573 (93%)	42 (7%)	20	49

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	104	LYS
1	A	118	LYS
1	A	204	GLN
1	A	214	GLN
1	A	268	LYS
1	A	283	ARG
1	A	326	ASN
1	A	354	ILE
2	B	80	ARG
2	B	103	ASN
2	B	133	ILE
2	B	145	PHE
2	B	150	TRP
2	B	151	LEU
2	B	152	LEU
2	B	154	GLU
2	B	155	TYR
2	B	180	PHE
2	B	187	ILE
2	B	188	PHE
2	B	196	HIS
2	B	213	GLN
2	B	218	PHE
2	B	222	PHE
2	B	231	ILE
2	B	237	PHE
2	B	241	PHE
2	B	246	SER
2	B	251	PHE
2	B	259	ASP
2	B	267	PHE
2	B	273	GLU
2	B	285	GLN
2	B	297	ARG
2	B	335	LEU
2	B	336	PHE
2	B	348	PHE
2	B	361	ILE
2	B	389	ILE
2	B	415	TYR
2	B	417	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	163	ASN
1	A	333	ASN
2	B	47	GLN
2	B	103	ASN
2	B	146	GLN
2	B	203	HIS
2	B	286	GLN
2	B	357	GLN
2	B	412	ASN
2	B	414	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 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 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	$\# Z > 2$
3	NAP	A	368	-	42,52,52	1.61	3 (7%)	54,80,80	1.99	7 (12%)

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	NAP	A	368	-	-	1/27/67/67	0/5/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	368	NAP	C2A-N1A	2.58	1.38	1.33
3	A	368	NAP	C2A-N3A	3.66	1.38	1.32
3	A	368	NAP	O7N-C7N	8.20	1.41	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	368	NAP	N3A-C2A-N1A	-11.23	120.29	128.89
3	A	368	NAP	C4D-O4D-C1D	2.01	111.92	109.72
3	A	368	NAP	O4B-C1B-N9A	2.05	112.39	108.10
3	A	368	NAP	O4D-C1D-N1N	2.30	110.66	108.13
3	A	368	NAP	C4B-O4B-C1B	2.47	112.44	109.72
3	A	368	NAP	O2B-C2B-C1B	2.54	119.91	110.02
3	A	368	NAP	P2B-O2B-C2B	4.86	133.21	121.56

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	368	NAP	P2B-O2B-C2B-C1B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	368	NAP	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	326/367 (88%)	-0.05	3 (0%) 85 84	34, 56, 98, 117	0
2	B	390/499 (78%)	1.91	143 (36%) 0 0	49, 187, 273, 349	0
All	All	716/866 (82%)	1.01	146 (20%) 1 1	34, 89, 262, 349	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	212	TYR	18.3
2	B	245	PRO	12.6
2	B	216	THR	10.2
2	B	217	SER	9.5
2	B	246	SER	9.4
2	B	355	ASP	9.4
2	B	194	ASP	9.3
2	B	144	GLU	8.8
2	B	182	LEU	8.8
2	B	221	PRO	8.6
2	B	356	SER	8.5
2	B	354	ARG	8.1
2	B	249	GLY	8.0
2	B	211	GLY	8.0
2	B	381	VAL	7.8
2	B	241	PHE	7.7
2	B	210	ILE	7.7
2	B	140	LEU	7.7
2	B	193	GLU	7.7
2	B	421	THR	7.7
2	B	201	THR	7.3
2	B	203	HIS	7.2
2	B	197	GLY	7.1
2	B	383	THR	7.1

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Mol	Chain	Res	Type	RSRZ
2	B	139	PRO	7.0
2	B	275	ALA	6.9
2	B	248	ALA	6.8
2	B	352	ASP	6.6
2	B	287	ALA	6.5
2	B	192	ASN	6.5
2	B	145	PHE	6.4
2	B	202	PHE	6.3
2	B	215	SER	6.2
2	B	213	GLN	6.1
2	B	285	GLN	6.1
2	B	200	VAL	6.0
2	B	136	GLU	6.0
2	B	286	GLN	6.0
2	B	179	SER	5.9
2	B	153	PHE	5.9
2	B	291	ALA	5.9
2	B	279	GLU	5.7
2	B	420	GLU	5.6
2	B	195	MET	5.6
2	B	135	GLU	5.6
2	B	218	PHE	5.5
2	B	290	LEU	5.5
2	B	196	HIS	5.5
2	B	247	LYS	5.4
2	B	353	GLU	5.3
2	B	244	CYS	5.3
2	B	138	ARG	5.2
2	B	162	ALA	5.2
2	B	199	GLY	5.2
2	B	150	TRP	5.2
2	B	164	ILE	5.1
2	B	351	ALA	4.9
2	B	294	ARG	4.9
2	B	198	GLY	4.9
2	B	205	TYR	4.9
2	B	417	TYR	4.8
2	B	274	LEU	4.8
2	B	242	PHE	4.8
2	B	357	GLN	4.6
2	B	382	PRO	4.6
2	B	141	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
2	B	280	ASP	4.4
2	B	204	THR	4.4
2	B	322	LYS	4.3
2	B	348	PHE	4.3
2	B	292	ILE	4.3
2	B	143	ASN	4.3
2	B	187	ILE	4.3
2	B	358	PHE	4.3
2	B	264	ILE	4.2
2	B	289	SER	4.2
2	B	149	VAL	4.1
2	B	284	GLY	4.1
2	B	132	TYR	4.1
2	B	278	PRO	4.1
2	B	219	THR	4.1
2	B	277	LYS	4.0
2	B	273	GLU	4.0
2	B	251	PHE	3.9
2	B	267	PHE	3.9
2	B	157	GLU	3.8
2	B	178	VAL	3.8
2	B	281	ALA	3.8
2	B	269	THR	3.8
2	B	214	GLN	3.7
2	B	220	ASP	3.7
2	B	266	TYR	3.6
2	B	250	PHE	3.5
2	B	288	MET	3.5
2	B	252	THR	3.5
2	B	209	THR	3.5
2	B	350	GLU	3.3
2	B	191	GLU	3.3
2	B	311	SER	3.2
2	B	208	SER	3.2
2	B	272	THR	3.2
2	B	268	ILE	3.2
2	B	388	LYS	3.2
2	B	207	GLN	3.2
2	B	374	THR	3.1
2	B	186	PRO	3.1
2	B	227	THR	3.1
2	B	380	MET	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	276	GLU	3.0
2	B	389	ILE	3.0
2	B	206	SER	3.0
2	B	142	GLU	2.9
2	B	310	HIS	2.9
2	B	32	CYS	2.9
2	B	163	ARG	2.9
2	B	385	ILE	2.9
2	B	384	THR	2.8
2	B	282	GLN	2.8
2	B	303	ARG	2.7
1	A	360	TYR	2.7
2	B	190	ASP	2.7
2	B	377	TYR	2.6
2	B	185	LEU	2.6
2	B	137	GLU	2.6
2	B	159	SER	2.5
2	B	386	GLY	2.5
2	B	134	LYS	2.5
2	B	229	CYS	2.5
2	B	326	ARG	2.4
2	B	323	ALA	2.4
2	B	376	GLY	2.4
2	B	298	LEU	2.4
2	B	167	ILE	2.4
2	B	152	LEU	2.3
2	B	183	GLU	2.3
2	B	347	TYR	2.3
2	B	413	PHE	2.3
2	B	228	LEU	2.2
2	B	189	ARG	2.2
2	B	362	PRO	2.1
2	B	366	TRP	2.1
2	B	231	ILE	2.1
2	B	325	MET	2.1
1	A	361	SER	2.1
2	B	375	VAL	2.1
1	A	117	THR	2.1

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

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(Å ²)	Q<0.9
3	NAP	A	368	48/48	0.95	0.19	-0.49	37,42,50,51	0
4	K	B	501	1/1	0.65	0.49	-	192,192,192,192	1
4	K	B	500	1/1	0.98	0.61	-	173,173,173,173	1
4	K	B	504	1/1	-0.40	1.24	-	258,258,258,258	1
4	K	B	503	1/1	0.81	0.63	-	226,226,226,226	1
4	K	B	505	1/1	0.31	4.43	-	165,165,165,165	1
4	K	B	502	1/1	0.86	0.50	-	209,209,209,209	1

6.5 Other polymers [i](#)

There are no such residues in this entry.