



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:41 PM GMT

PDB ID : 4PNK
Title : G protein-coupled receptor kinase 2 in complex with GSK180736A
Authors : Homan, K.T.; Larimore, K.M.; Elkins, J.; Knapp, S.; Tesmer, J.J.G.
Deposited on : 2014-05-23
Resolution : 2.56 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

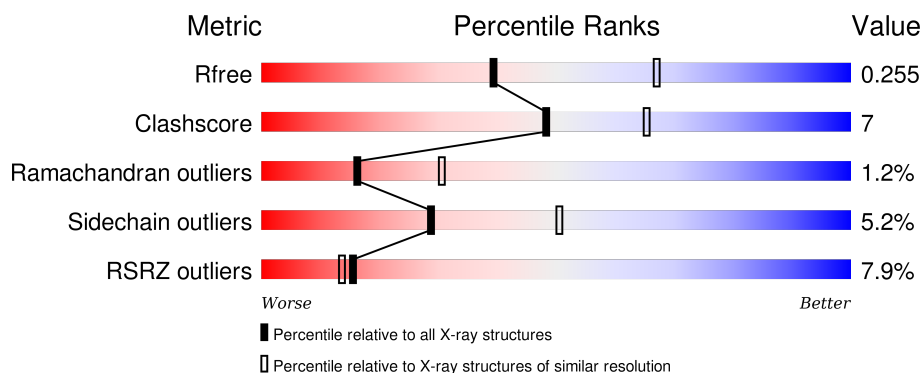
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3324 (2.60-2.52)
Clashscore	102246	3729 (2.60-2.52)
Ramachandran outliers	100387	3673 (2.60-2.52)
Sidechain outliers	100360	3673 (2.60-2.52)
RSRZ outliers	91569	3333 (2.60-2.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	689	<div> <div>10%</div> <div>70%</div> <div>18%</div> <div>9%</div> </div>
2	B	340	<div> <div>%</div> <div>80%</div> <div>18%</div> <div>.</div> </div>
3	G	71	<div> <div>10%</div> <div>79%</div> <div>7%</div> <div>13%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8322 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 Beta-adrenergic receptor kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	625	Total	C	N	O	S	0	0	0
			5123	3265	896	927	35			

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	339	Total	C	N	O	S	0	2	0
			2619	1613	470	513	23			

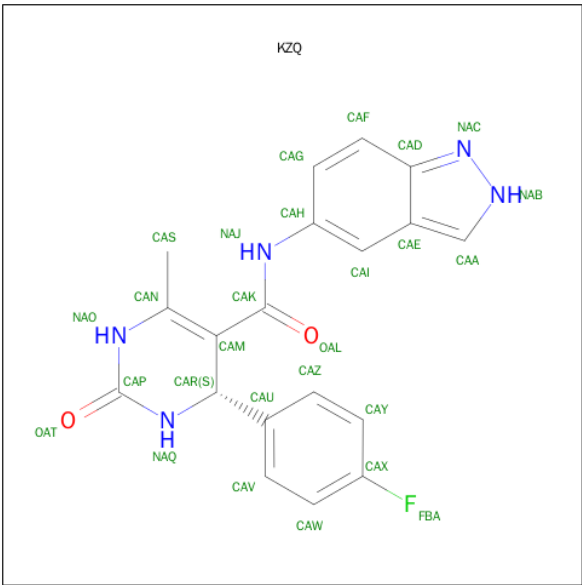
- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	62	Total	C	N	O	S	0	0	0
			484	307	84	90	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	68	SER	CYS	engineered mutation	UNP P63212

- Molecule 4 is (4S)-4-(4-fluorophenyl)-N-(2H-indazol-5-yl)-6-methyl-2-oxo-1,2,3,4-tetrahydro pyrimidine-5-carboxamide (three-letter code: KZQ) (formula: C₁₉H₁₆FN₅O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			27	19	1	5	2		

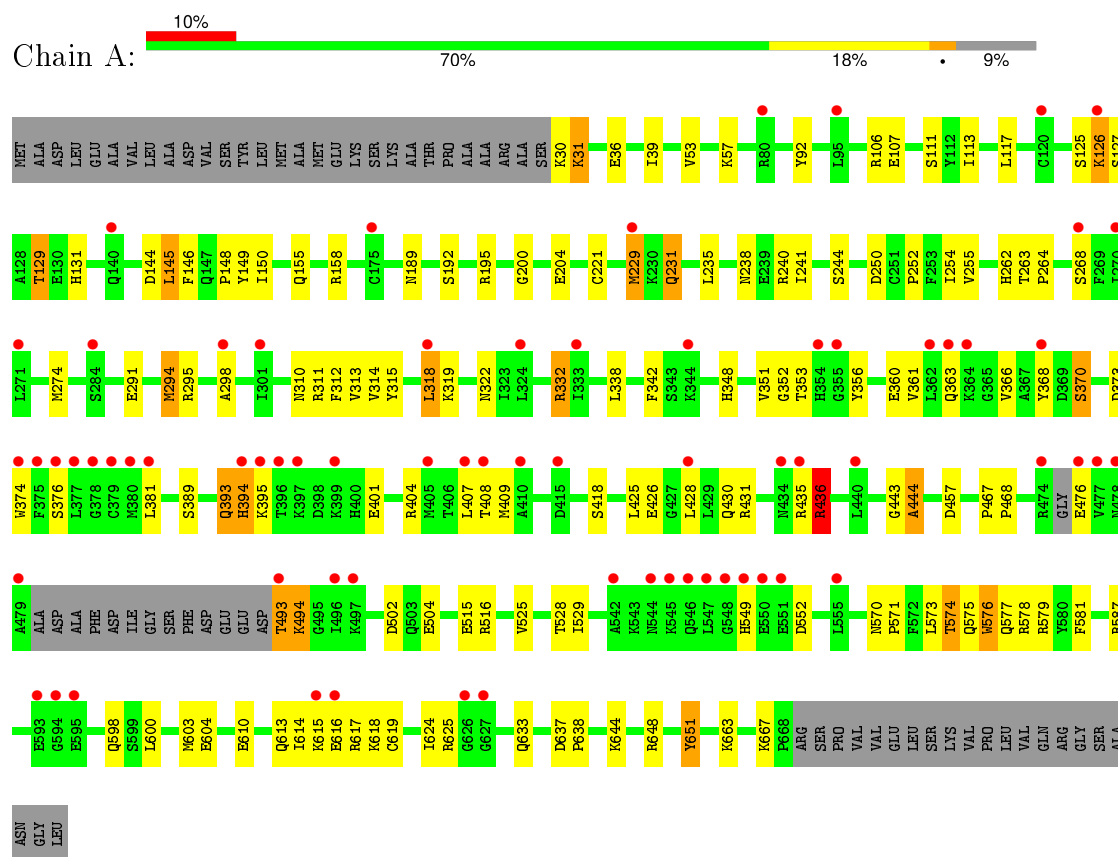
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	35	Total	O	0	0
			35	35		
5	B	32	Total	O	0	0
			32	32		
5	G	2	Total	O	0	0
			2	2		

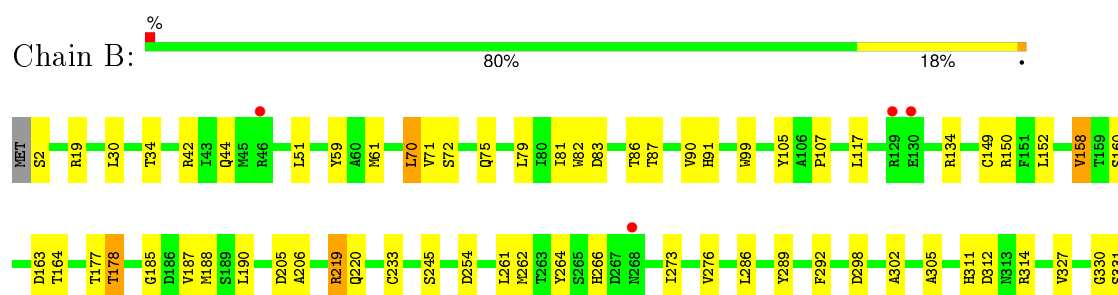
3 Residue-property plots

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: Beta-adrenergic receptor kinase 1

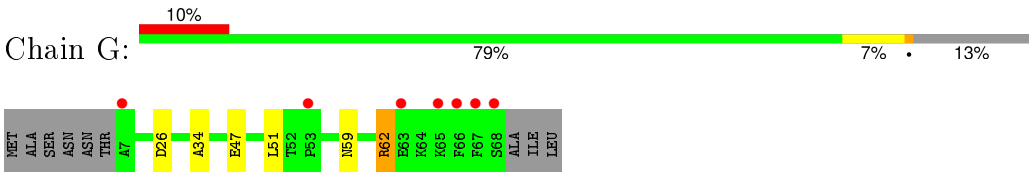


- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1





- Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	61.44Å 241.40Å 212.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.55 – 2.56 24.55 – 2.56	Depositor EDS
% Data completeness (in resolution range)	97.5 (24.55-2.56) 97.7 (24.55-2.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 2.57Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.190 , 0.259 0.190 , 0.255	Depositor DCC
R_{free} test set	2565 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	77.3	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 61.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 50375 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8322	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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: KZQ

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	0.81	2/5238 (0.0%)	0.96	4/7038 (0.1%)
2	B	0.85	0/2666	1.03	6/3613 (0.2%)
3	G	0.82	0/492	0.90	0/661
All	All	0.82	2/8396 (0.0%)	0.98	10/11312 (0.1%)

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	A	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	576	TRP	CB-CG	-5.79	1.39	1.50
1	A	348	HIS	C-O	5.21	1.33	1.23

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	295	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	A	436	ARG	NE-CZ-NH1	6.15	123.38	120.30
2	B	314	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	516	ARG	NE-CZ-NH1	-5.97	117.31	120.30
2	B	219	ARG	NE-CZ-NH1	5.76	123.18	120.30
2	B	312	ASP	CB-CG-OD1	5.75	123.48	118.30
2	B	163	ASP	CB-CG-OD1	5.71	123.44	118.30
1	A	332	ARG	NE-CZ-NH2	-5.58	117.51	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	19	ARG	NE-CZ-NH1	5.49	123.04	120.30
2	B	188	MET	CB-CA-C	-5.36	99.68	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	494	LYS	Peptide
1	A	616	GLU	Peptide

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	5123	0	5114	78	0
2	B	2619	0	2518	40	0
3	G	484	0	496	2	0
4	A	27	0	16	3	0
5	A	35	0	0	3	0
5	B	32	0	0	2	0
5	G	2	0	0	0	0
All	All	8322	0	8144	120	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 7.

All (120) 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:42:ARG:NH2	5:B:417:HOH:O	1.89	1.06
2:B:42:ARG:CZ	5:B:417:HOH:O	2.15	0.89
1:A:493:THR:O	1:A:494:LYS:CE	2.28	0.82
1:A:493:THR:O	1:A:494:LYS:HE3	1.82	0.79
1:A:131:HIS:CD2	1:A:148:PRO:HG2	2.24	0.73
1:A:587:ARG:HD2	1:A:600:LEU:HD22	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:TYR:CE2	2:B:75:GLN:HB2	2.29	0.67
1:A:235:LEU:HD11	1:A:338:LEU:HD23	1.77	0.65
1:A:515:GLU:HB2	5:A:804:HOH:O	1.98	0.64
2:B:177:THR:HG22	2:B:178:THR:OG1	1.99	0.63
1:A:291:GLU:OE2	1:A:418:SER:OG	2.18	0.62
1:A:430:GLN:HG3	1:A:435:ARG:O	1.99	0.62
1:A:126:LYS:HG3	1:A:127:SER:N	2.14	0.61
1:A:314:VAL:HG12	1:A:370:SER:HA	1.83	0.60
1:A:235:LEU:CD1	1:A:338:LEU:HD23	2.33	0.59
1:A:274:MET:H	4:A:701:KZQ:HNAB	1.49	0.59
2:B:254:ASP:HB2	2:B:261:LEU:HD11	1.85	0.59
1:A:263:THR:HB	1:A:264:PRO:CD	2.34	0.57
1:A:144:ASP:O	1:A:145:LEU:C	2.43	0.56
2:B:160:SER:HB3	2:B:190:LEU:HD23	1.88	0.56
1:A:493:THR:O	1:A:494:LYS:CD	2.54	0.56
2:B:71:VAL:HG23	2:B:81:ILE:HG12	1.88	0.55
1:A:356:TYR:O	1:A:376:SER:OG	2.21	0.55
2:B:70:LEU:HG	2:B:70:LEU:O	2.05	0.55
2:B:177:THR:HG22	2:B:178:THR:N	2.20	0.55
1:A:617:ARG:HG2	1:A:633:GLN:NE2	2.21	0.55
2:B:30:LEU:O	2:B:34:THR:HG23	2.06	0.54
1:A:195:ARG:HD3	1:A:476:GLU:OE1	2.08	0.54
1:A:238:ASN:HA	1:A:241:ILE:HD12	1.89	0.54
2:B:262:MET:SD	2:B:302:ALA:HB2	2.48	0.54
1:A:525:VAL:O	1:A:529:ILE:HG12	2.09	0.53
2:B:276:VAL:HA	2:B:286:LEU:O	2.08	0.53
1:A:573:LEU:O	1:A:574:THR:C	2.47	0.53
1:A:603:MET:HB3	1:A:651:TYR:HA	1.91	0.52
4:A:701:KZQ:HAG	4:A:701:KZQ:OAL	2.10	0.52
2:B:42:ARG:HD3	2:B:44:GLN:HG2	1.91	0.51
2:B:164:THR:HA	2:B:187:VAL:HG23	1.92	0.51
1:A:637:ASP:HB2	1:A:638:PRO:HD3	1.93	0.51
1:A:374:TRP:CE3	1:A:374:TRP:HA	2.46	0.51
1:A:667:LYS:HE3	5:A:835:HOH:O	2.12	0.49
1:A:318:LEU:HB3	1:A:376:SER:HB3	1.94	0.49
1:A:53:VAL:HG12	1:A:53:VAL:O	2.12	0.49
1:A:107:GLU:O	1:A:111:SER:HB3	2.12	0.49
1:A:604:GLU:HG3	5:A:830:HOH:O	2.12	0.49
1:A:579:ARG:HB2	1:A:581:PHE:CE1	2.47	0.48
1:A:644:LYS:HE3	1:A:648:ARG:CZ	2.44	0.48
2:B:51:LEU:HB3	2:B:82:TRP:CZ3	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:MET:HE3	2:B:70:LEU:HD13	1.96	0.48
1:A:576:TRP:CZ3	1:A:633:GLN:HB2	2.48	0.48
2:B:99:TRP:HB3	2:B:117:LEU:HG	1.96	0.48
3:G:59:ASN:ND2	3:G:62:ARG:HG2	2.29	0.47
1:A:92:TYR:CD1	1:A:92:TYR:C	2.87	0.47
2:B:292:PHE:N	2:B:292:PHE:CD1	2.82	0.47
1:A:401:GLU:HG2	1:A:404:ARG:HE	1.78	0.47
2:B:59:TYR:HE2	2:B:75:GLN:HB2	1.74	0.47
2:B:83:ASP:C	2:B:83:ASP:OD1	2.53	0.47
1:A:360:GLU:HG3	1:A:368:TYR:HB3	1.97	0.47
1:A:312:PHE:HA	1:A:342:PHE:CE1	2.50	0.47
2:B:311:HIS:CE1	2:B:331:SER:HB2	2.50	0.46
1:A:393:GLN:HG3	1:A:394:HIS:H	1.81	0.46
1:A:294:MET:HE3	1:A:298:ALA:HB2	1.98	0.46
1:A:319:LYS:HE2	1:A:353:THR:OG1	2.15	0.45
1:A:294:MET:HE3	1:A:381:LEU:HD13	1.97	0.45
2:B:152:LEU:HD21	2:B:158:VAL:CG2	2.46	0.45
1:A:274:MET:SD	1:A:332:ARG:HD2	2.55	0.45
1:A:30:LYS:HG2	1:A:31:LYS:N	2.31	0.45
1:A:311:ARG:O	1:A:313:VAL:HG23	2.16	0.45
2:B:61:MET:CE	2:B:70:LEU:HD13	2.46	0.45
1:A:408:THR:HA	1:A:431:ARG:HD3	1.98	0.45
2:B:298:ASP:OD1	2:B:298:ASP:C	2.54	0.45
1:A:129:THR:HG23	1:A:149:TYR:OH	2.17	0.45
1:A:613:GLN:NE2	1:A:618:LYS:HG3	2.31	0.45
1:A:614:ILE:O	1:A:615:LYS:C	2.55	0.44
2:B:30:LEU:HD12	3:G:34:ALA:HB1	2.00	0.44
1:A:254:ILE:HG22	1:A:255:VAL:N	2.33	0.44
1:A:443:GLY:O	1:A:444:ALA:C	2.56	0.44
1:A:570:ASN:HB3	1:A:573:LEU:HD12	1.99	0.44
1:A:155:GLN:HG2	1:A:158:ARG:HH21	1.82	0.44
2:B:90:VAL:HG12	2:B:91:HIS:CD2	2.52	0.44
1:A:315:TYR:OH	1:A:322:ASN:HB3	2.18	0.43
1:A:144:ASP:O	1:A:146:PHE:N	2.51	0.43
1:A:315:TYR:N	1:A:373:ASP:OD2	2.42	0.43
1:A:573:LEU:C	1:A:575:GLN:N	2.69	0.43
1:A:263:THR:HB	1:A:264:PRO:HD2	2.00	0.43
1:A:252:PRO:HA	1:A:332:ARG:NH2	2.33	0.43
2:B:233[B]:CYS:SG	2:B:276:VAL:HG23	2.58	0.43
2:B:164:THR:HG22	2:B:185:GLY:C	2.39	0.43
2:B:152:LEU:HD23	2:B:152:LEU:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:LEU:C	1:A:600:LEU:HD12	2.39	0.43
1:A:363:GLN:HB3	1:A:366:VAL:HG21	2.01	0.43
1:A:425:LEU:O	1:A:426:GLU:C	2.56	0.42
2:B:273:ILE:HG13	2:B:289:TYR:CE2	2.54	0.42
1:A:428:LEU:O	1:A:436:ARG:HD3	2.20	0.42
1:A:570:ASN:HA	1:A:571:PRO:HD2	1.81	0.42
2:B:86:THR:O	2:B:87:THR:OG1	2.24	0.42
1:A:598:GLN:HA	1:A:598:GLN:OE1	2.20	0.42
1:A:149:TYR:O	1:A:150:ILE:C	2.56	0.42
1:A:318:LEU:HD12	1:A:319:LYS:N	2.34	0.42
1:A:312:PHE:HA	1:A:342:PHE:CZ	2.54	0.42
1:A:274:MET:HE2	1:A:332:ARG:HB2	2.02	0.42
2:B:262:MET:HG2	2:B:264:TYR:CZ	2.55	0.42
1:A:294:MET:O	1:A:294:MET:HG2	2.20	0.42
2:B:134:ARG:HD3	2:B:134:ARG:HA	1.89	0.42
1:A:581:PHE:N	1:A:581:PHE:CD1	2.88	0.41
1:A:467:PRO:HA	1:A:468:PRO:HD3	1.81	0.41
2:B:42:ARG:HG2	2:B:305:ALA:O	2.19	0.41
1:A:294:MET:CE	1:A:298:ALA:HB2	2.49	0.41
1:A:351:VAL:HG12	1:A:352:GLY:N	2.35	0.41
1:A:200:GLY:O	4:A:701:KZQ:CAX	2.69	0.41
1:A:125:SER:O	1:A:129:THR:OG1	2.39	0.41
2:B:327:VAL:HB	2:B:339:TRP:HB2	2.02	0.41
1:A:361:VAL:HA	1:A:368:TYR:CE2	2.56	0.41
2:B:219:ARG:O	2:B:220:GLN:HG3	2.20	0.41
2:B:330:GLY:CA	2:B:336:LEU:HD23	2.51	0.41
2:B:205:ASP:O	2:B:206:ALA:HB3	2.20	0.41
1:A:310:ASN:HD22	1:A:310:ASN:HA	1.56	0.41
2:B:72:SER:O	2:B:79:LEU:HA	2.21	0.40
2:B:149:CYS:O	2:B:150:ARG:NH1	2.55	0.40
1:A:624:ILE:HG22	1:A:625:ARG:H	1.87	0.40
1:A:36:GLU:O	1:A:39:ILE:HG22	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	619/689 (90%)	548 (88%)	60 (10%)	11 (2%)	11	19
2	B	339/340 (100%)	309 (91%)	30 (9%)	0	100	100
3	G	60/71 (84%)	57 (95%)	2 (3%)	1 (2%)	11	20
All	All	1018/1100 (92%)	914 (90%)	92 (9%)	12 (1%)	16	30

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	250	ASP
1	A	444	ALA
3	G	62	ARG
1	A	145	LEU
1	A	407	LEU
1	A	229	MET
1	A	370	SER
1	A	395	LYS
1	A	231	GLN
1	A	394	HIS
1	A	409	MET
1	A	113	ILE

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	560/609 (92%)	525 (94%)	35 (6%)	22	40
2	B	284/283 (100%)	276 (97%)	8 (3%)	51	76
3	G	51/58 (88%)	48 (94%)	3 (6%)	24	44
All	All	895/950 (94%)	849 (95%)	46 (5%)	29	51

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LYS
1	A	57	LYS
1	A	106	ARG
1	A	117	LEU
1	A	126	LYS
1	A	129	THR
1	A	189	ASN
1	A	192	SER
1	A	204	GLU
1	A	221	CYS
1	A	229	MET
1	A	231	GLN
1	A	240	ARG
1	A	244	SER
1	A	262	HIS
1	A	268	SER
1	A	294	MET
1	A	318	LEU
1	A	389	SER
1	A	393	GLN
1	A	436	ARG
1	A	457	ASP
1	A	493	THR
1	A	502	ASP
1	A	504	GLU
1	A	528	THR
1	A	549	HIS
1	A	552	ASP
1	A	574	THR
1	A	577	GLN
1	A	578	ARG
1	A	610	GLU
1	A	619	CYS
1	A	651	TYR
1	A	663	LYS
2	B	2	SER
2	B	70	LEU
2	B	105	TYR
2	B	107	PRO
2	B	158	VAL
2	B	178	THR
2	B	245	SER

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Mol	Chain	Res	Type
2	B	266	HIS
3	G	26	ASP
3	G	47	GLU
3	G	51	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	HIS
1	A	131	HIS
1	A	189	ASN
1	A	262	HIS
1	A	310	ASN
1	A	633	GLN
2	B	110	ASN
2	B	155	ASN
2	B	239	ASN
2	B	259	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

1 ligand 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	$\# Z > 2$
4	KZQ	A	701	-	28,30,30	1.81	7 (25%)	37,43,43	2.89	15 (40%)

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	KZQ	A	701	-	-	0/12/28/28	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	KZQ	CAR-CAM	-4.12	1.47	1.51
4	A	701	KZQ	CAF-CAD	-3.83	1.34	1.41
4	A	701	KZQ	NAB-NAC	-3.55	1.30	1.37
4	A	701	KZQ	CAN-NAO	-2.90	1.34	1.38
4	A	701	KZQ	CAU-CAR	-2.16	1.49	1.52
4	A	701	KZQ	CAH-NAJ	-2.05	1.37	1.41
4	A	701	KZQ	CAN-CAM	2.83	1.39	1.35

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	701	KZQ	CAU-CAR-CAM	-8.95	100.92	112.80
4	A	701	KZQ	CAS-CAN-CAM	-7.39	120.19	127.63
4	A	701	KZQ	OAL-CAK-CAM	-4.40	113.74	121.09
4	A	701	KZQ	CAN-NAO-CAP	-3.63	120.78	123.72
4	A	701	KZQ	CAG-CAF-CAD	-3.30	117.30	120.88
4	A	701	KZQ	CAH-CAI-CAE	-2.36	116.70	120.39
4	A	701	KZQ	CAE-CAA-NAB	-2.27	105.73	111.38
4	A	701	KZQ	CAK-CAM-CAN	-2.13	118.87	123.22
4	A	701	KZQ	OAT-CAP-NAQ	-2.09	118.00	122.86
4	A	701	KZQ	CAF-CAG-CAH	2.42	124.60	120.59
4	A	701	KZQ	CAI-CAE-CAD	2.47	123.30	119.89
4	A	701	KZQ	OAL-CAK-NAJ	3.03	130.09	123.84
4	A	701	KZQ	CAM-CAR-NAQ	3.68	112.05	109.10
4	A	701	KZQ	CAS-CAN-NAO	4.92	119.27	113.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	701	KZQ	NAO-CAP-NAQ	5.91	122.61	116.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	701	KZQ	3	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	625/689 (90%)	0.44	70 (11%) 7 6	61, 102, 179, 246	0
2	B	339/340 (99%)	-0.03	4 (1%) 81 80	59, 81, 121, 175	0
3	G	62/71 (87%)	0.44	7 (11%) 7 6	73, 105, 172, 202	0
All	All	1026/1100 (93%)	0.28	81 (7%) 15 14	59, 93, 172, 246	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	394	HIS	7.2
3	G	66	PHE	7.0
2	B	129	ARG	6.5
1	A	474	ARG	6.1
1	A	550	GLU	6.0
1	A	476	GLU	5.7
3	G	67	PHE	5.4
1	A	477	VAL	4.9
3	G	65	LYS	4.6
1	A	407	LEU	4.6
1	A	547	LEU	4.5
1	A	549	HIS	4.4
1	A	363	GLN	4.2
1	A	380	MET	4.0
1	A	478	ASN	4.0
1	A	399	LYS	3.9
1	A	555	LEU	3.8
1	A	377	LEU	3.8
1	A	140	GLN	3.8
1	A	415	ASP	3.7
1	A	396	THR	3.5
1	A	548	GLY	3.5
1	A	594	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	397	LYS	3.4
1	A	355	GLY	3.3
1	A	542	ALA	3.3
1	A	545	LYS	3.3
1	A	270	ILE	3.3
3	G	63	GLU	3.1
1	A	544	ASN	3.1
1	A	551	GLU	3.1
3	G	7	ALA	3.1
1	A	374	TRP	3.0
1	A	381	LEU	3.0
1	A	626	GLY	3.0
1	A	379	CYS	2.9
3	G	68	SER	2.9
1	A	229	MET	2.9
1	A	378	GLY	2.9
1	A	120	CYS	2.9
1	A	362	LEU	2.9
1	A	395	LYS	2.8
1	A	627	GLY	2.8
1	A	375	PHE	2.8
2	B	268	ASN	2.8
1	A	354	HIS	2.8
1	A	408	THR	2.7
1	A	410	ALA	2.7
1	A	616	GLU	2.6
2	B	130	GLU	2.6
1	A	496	ILE	2.6
1	A	333	ILE	2.6
1	A	364	LYS	2.6
1	A	497	LYS	2.5
1	A	376	SER	2.5
1	A	126	LYS	2.4
1	A	434	ASN	2.4
1	A	368	TYR	2.4
1	A	301	ILE	2.4
1	A	493	THR	2.3
1	A	344	LYS	2.3
1	A	95	LEU	2.3
1	A	271	LEU	2.3
1	A	318	LEU	2.3
1	A	479	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	435	ARG	2.2
1	A	428	LEU	2.2
3	G	53	PRO	2.2
1	A	298	ALA	2.2
1	A	284	SER	2.2
1	A	175	CYS	2.2
1	A	593	GLU	2.2
1	A	324	LEU	2.1
2	B	46	ARG	2.1
1	A	595	GLU	2.1
1	A	546	GLN	2.1
1	A	80	ARG	2.1
1	A	615	LYS	2.0
1	A	405	MET	2.0
1	A	268	SER	2.0
1	A	440	LEU	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
4	KZQ	A	701	27/27	0.92	0.16	-0.70	74,101,125,145	0

6.5 Other polymers [i](#)

There are no such residues in this entry.