Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:22 PM GMT

PDB ID	:	1OMW
Title	:	Crystal Structure of the complex between G Protein-Coupled Receptor Kinase 2 and Heterotrimeric G Protein beta 1 and gamma 2 subunits
Authors	:	Lodowski, D.T.; Pitcher, J.A.; Capel, W.D.; Lefkowitz, R.J.; Tesmer, J.J.G.
Deposited on	:	2003-02-26
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

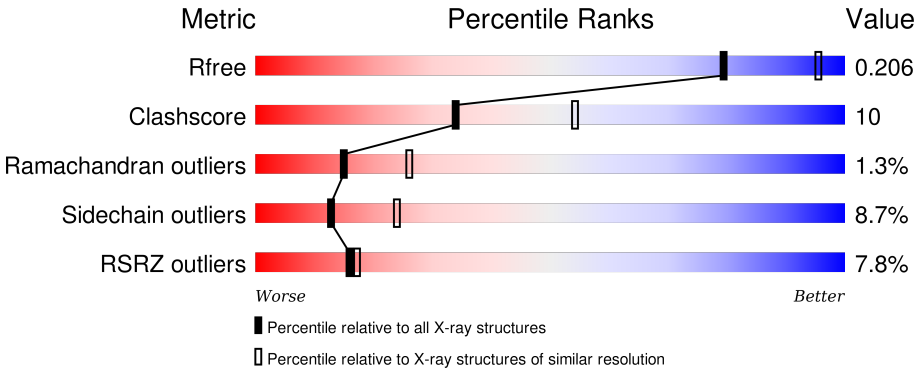
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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	689	9% 65% 21% • 11%
2	B	340	5% 61% 33% 5% •
3	G	74	5% 53% 24% 5% 18%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8151 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 G-protein coupled receptor kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	614	Total	C	N	O	S	0	0	0
			5037	3216	876	909	36			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	670	ALA	SER	ENGINEERED	UNP P21146

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	339	Total	C	N	O	S	0	0	0
			2607	1607	468	511	21			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	61	Total	C	N	O	S	0	0	0
			481	305	83	89	4			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-5	HIS	-	EXPRESSION TAG	UNP P63212
G	-4	HIS	-	EXPRESSION TAG	UNP P63212
G	-3	HIS	-	EXPRESSION TAG	UNP P63212
G	-2	HIS	-	EXPRESSION TAG	UNP P63212
G	-1	HIS	-	EXPRESSION TAG	UNP P63212
G	0	HIS	-	EXPRESSION TAG	UNP P63212
G	68	CMT	CYS	MODIFIED RESIDUE	UNP P63212

- Molecule 4 is water.

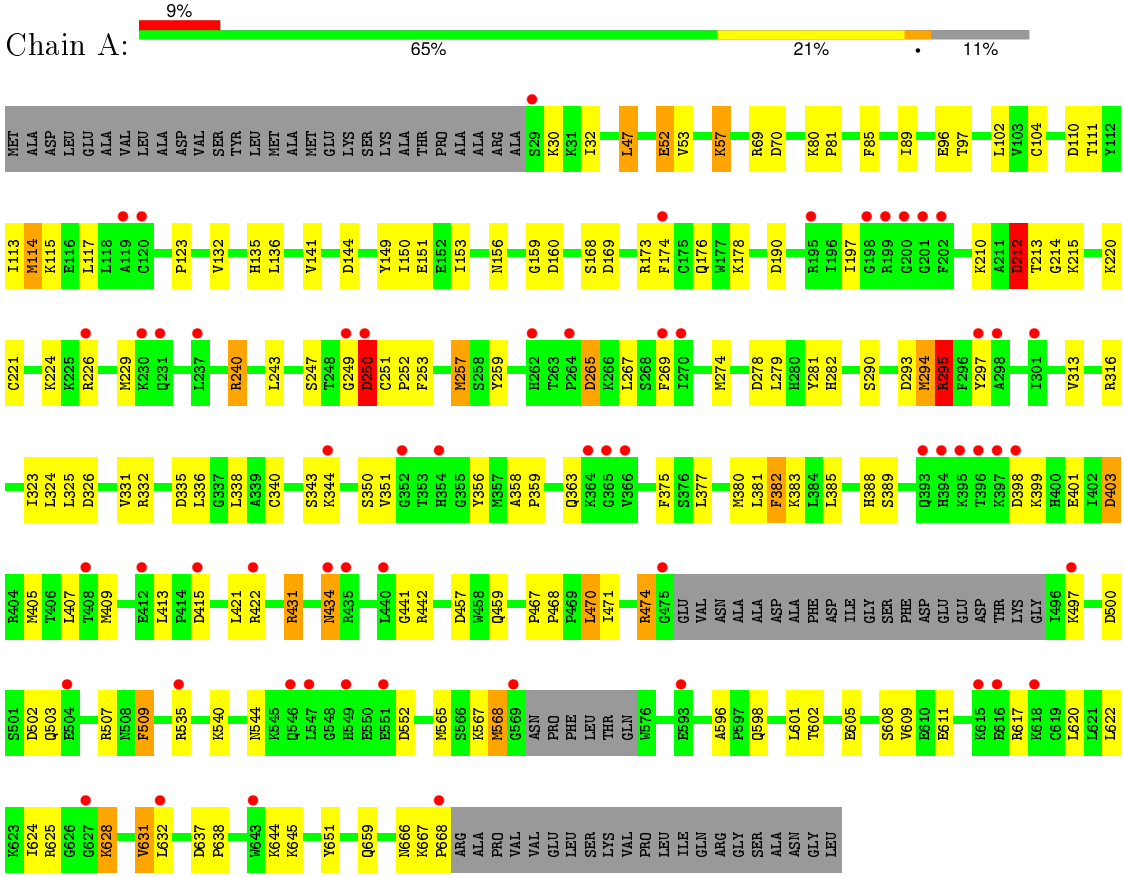
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	14	Total O 14 14	0	0
4	B	10	Total O 10 10	0	0
4	G	2	Total O 2 2	0	0

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.

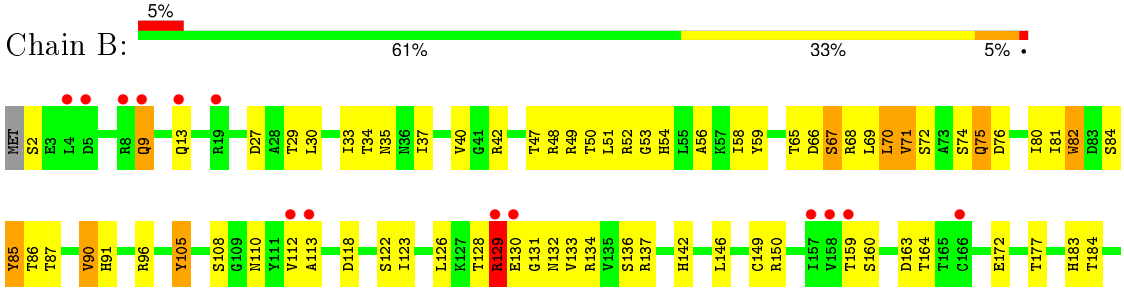
- Molecule 1: G-protein coupled receptor kinase 2

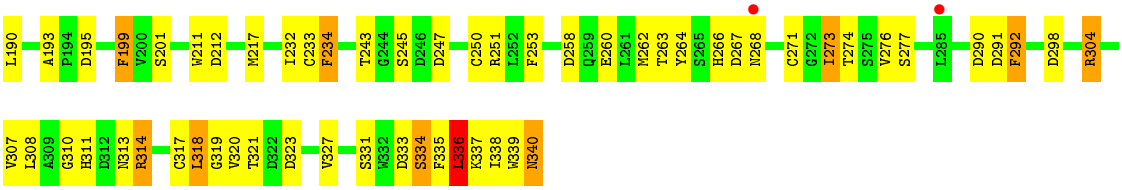
Chain A:



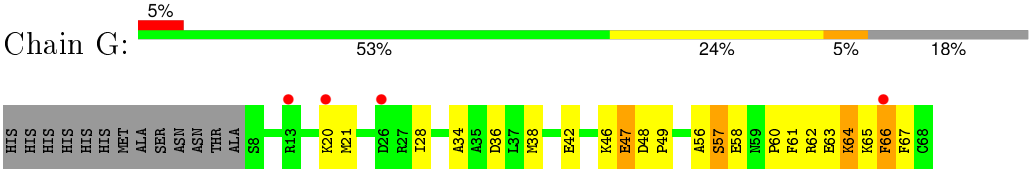
- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) beta subunit 1

Chain B:





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



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	188.20Å 72.50Å 122.79Å 90.00° 115.20° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.94 – 2.50	Depositor EDS
% Data completeness (in resolution range)	73.6 (20.00-2.50) 73.8 (19.94-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.93 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.202 , 0.252 0.199 , 0.206	Depositor DCC
R_{free} test set	1942 reflections (5.08%)	DCC
Wilson B-factor (Å^2)	72.8	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 63.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 38249 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8151	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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: CMT

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	0.98	2/5150 (0.0%)	1.04	21/6918 (0.3%)
2	B	1.31	11/2654 (0.4%)	1.23	19/3597 (0.5%)
3	G	1.45	6/481 (1.2%)	1.22	4/646 (0.6%)
All	All	1.13	19/8285 (0.2%)	1.12	44/11161 (0.4%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	64	LYS	CE-NZ	8.71	1.70	1.49
2	B	85	TYR	CE1-CZ	8.45	1.49	1.38
2	B	335	PHE	CE1-CZ	7.71	1.52	1.37
3	G	66	PHE	CD2-CE2	7.04	1.53	1.39
2	B	335	PHE	CD1-CE1	-7.01	1.25	1.39
2	B	82	TRP	CE3-CZ3	6.22	1.49	1.38
3	G	66	PHE	CD1-CE1	6.21	1.51	1.39
2	B	59	TYR	CD2-CE2	6.16	1.48	1.39
2	B	335	PHE	CD2-CE2	5.96	1.51	1.39
2	B	84	SER	CB-OG	5.77	1.49	1.42
2	B	85	TYR	CG-CD1	5.67	1.46	1.39
1	A	297	TYR	CE1-CZ	-5.58	1.31	1.38
2	B	85	TYR	CD1-CE1	5.53	1.47	1.39
3	G	66	PHE	CE1-CZ	5.36	1.47	1.37
2	B	340	ASN	CB-CG	-5.32	1.38	1.51
3	G	42	GLU	CD-OE1	5.25	1.31	1.25
3	G	67	PHE	CB-CG	-5.18	1.42	1.51
1	A	52	GLU	CD-OE1	5.07	1.31	1.25
2	B	339	TRP	CE3-CZ3	5.05	1.47	1.38

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	110	ASP	CB-CG-OD2	9.02	126.42	118.30
2	B	66	ASP	CB-CG-OD2	8.52	125.97	118.30
2	B	195	ASP	CB-CG-OD2	8.34	125.81	118.30
1	A	212	ASP	CB-CG-OD2	8.31	125.78	118.30
1	A	326	ASP	CB-CG-OD2	7.78	125.30	118.30
1	A	502	ASP	CB-CG-OD2	7.10	124.69	118.30
2	B	76	ASP	CB-CG-OD2	6.95	124.56	118.30
1	A	169	ASP	CB-CG-OD2	6.85	124.47	118.30
2	B	212	ASP	CB-CG-OD2	6.79	124.41	118.30
2	B	118	ASP	CB-CG-OD2	6.76	124.38	118.30
2	B	68	ARG	NE-CZ-NH2	-6.67	116.97	120.30
2	B	27	ASP	CB-CG-OD2	6.62	124.26	118.30
1	A	70	ASP	CB-CG-OD2	6.58	124.22	118.30
1	A	293	ASP	CB-CG-OD1	6.41	124.07	118.30
1	A	190	ASP	CB-CG-OD2	6.39	124.05	118.30
1	A	335	ASP	CB-CG-OD2	6.21	123.89	118.30
2	B	298	ASP	CB-CG-OD2	6.07	123.76	118.30
1	A	144	ASP	CB-CG-OD2	5.94	123.65	118.30
1	A	265	ASP	CB-CG-OD2	5.90	123.61	118.30
2	B	323	ASP	CB-CG-OD2	5.88	123.60	118.30
1	A	415	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	457	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	70	ASP	CB-CG-OD1	-5.69	113.18	118.30
3	G	62	ARG	NE-CZ-NH2	-5.60	117.50	120.30
3	G	36	ASP	CB-CG-OD2	5.59	123.33	118.30
2	B	267	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	295	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	A	409	MET	CG-SD-CE	5.55	109.08	100.20
1	A	500	ASP	CB-CG-OD2	5.54	123.28	118.30
2	B	304	ARG	NE-CZ-NH1	5.49	123.05	120.30
2	B	71	VAL	CB-CA-C	-5.49	100.97	111.40
2	B	247	ASP	CB-CG-OD1	5.44	123.20	118.30
3	G	38	MET	CG-SD-CE	5.43	108.88	100.20
2	B	195	ASP	OD1-CG-OD2	-5.40	113.04	123.30
3	G	48	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	69	ARG	NE-CZ-NH2	-5.22	117.69	120.30
2	B	258	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	250	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	552	ASP	CB-CG-OD1	5.13	122.91	118.30
2	B	129	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	403	ASP	CB-CG-OD2	5.10	122.89	118.30
2	B	336	LEU	CB-CA-C	-5.09	100.53	110.20
2	B	49	ARG	NE-CZ-NH1	-5.01	117.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	68	ARG	NE-CZ-NH1	5.00	122.80	120.30

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	5037	0	5042	90	0
2	B	2607	0	2510	66	0
3	G	481	0	493	9	0
4	A	14	0	0	2	0
4	B	10	0	0	0	0
4	G	2	0	0	0	0
All	All	8151	0	8045	164	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 10.

All (164) 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)
3:G:64:LYS:NZ	3:G:64:LYS:CE	1.70	1.53
2:B:217:MET:CE	2:B:217:MET:SD	2.04	1.46
2:B:86:THR:O	2:B:87:THR:HB	1.64	0.96
2:B:163:ASP:O	2:B:164:THR:OG1	1.94	0.86
1:A:363:GLN:O	4:A:698:HOH:O	1.93	0.84
2:B:71:VAL:HG23	2:B:105:TYR:CD2	2.12	0.84
1:A:434:ASN:HD22	1:A:434:ASN:H	1.28	0.79
1:A:294:MET:HE3	1:A:381:LEU:HD13	1.71	0.73
1:A:240:ARG:HG2	1:A:269:PHE:HE1	1.55	0.72
2:B:67:SER:HB3	2:B:321:THR:HB	1.73	0.70
1:A:212:ASP:OD2	4:A:694:HOH:O	2.12	0.68
2:B:333:ASP:O	2:B:334:SER:HB3	1.94	0.67
3:G:47:GLU:O	3:G:49:PRO:HD3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:LEU:HG	2:B:70:LEU:O	1.95	0.66
1:A:413:LEU:HD12	1:A:422:ARG:HG3	1.79	0.65
2:B:313:ASN:O	2:B:314:ARG:C	2.36	0.64
1:A:141:VAL:HG23	1:A:141:VAL:O	1.98	0.64
1:A:132:VAL:HG12	1:A:136:LEU:HD12	1.81	0.63
1:A:609:VAL:HG22	1:A:622:LEU:HD21	1.80	0.63
3:G:56:ALA:HB1	3:G:63:GLU:HB2	1.80	0.63
1:A:609:VAL:HG22	1:A:622:LEU:CD2	2.29	0.62
1:A:474:ARG:N	1:A:474:ARG:HD2	2.15	0.61
1:A:111:THR:O	1:A:115:LYS:HB3	2.01	0.61
2:B:33:ILE:HD12	3:G:34:ALA:HB3	1.83	0.60
2:B:262:MET:HG3	2:B:263:THR:N	2.15	0.60
1:A:274:MET:SD	1:A:332:ARG:HD2	2.42	0.60
1:A:667:LYS:HB3	1:A:668:PRO:HD2	1.83	0.60
3:G:20:LYS:HB3	3:G:21:MET:HE3	1.85	0.59
1:A:173:ARG:HA	1:A:176:GLN:OE1	2.03	0.59
2:B:160:SER:HB3	2:B:190:LEU:HD23	1.84	0.59
2:B:233:CYS:HB2	2:B:276:VAL:HG23	1.84	0.58
1:A:568:MET:HB2	1:A:631:VAL:HG23	1.83	0.58
2:B:318:LEU:C	2:B:318:LEU:CD1	2.72	0.58
1:A:470:LEU:C	1:A:470:LEU:HD12	2.24	0.58
2:B:54:HIS:CE1	2:B:80:ILE:HD12	2.39	0.58
2:B:30:LEU:O	2:B:34:THR:HG23	2.04	0.57
1:A:80:LYS:HB2	1:A:81:PRO:HD3	1.85	0.57
2:B:193:ALA:HB2	2:B:234:PHE:CE2	2.40	0.57
2:B:317:CYS:O	2:B:318:LEU:HB3	2.04	0.57
2:B:128:THR:O	2:B:129:ARG:C	2.43	0.57
1:A:313:VAL:HA	1:A:340:CYS:O	2.04	0.57
1:A:150:ILE:HG22	1:A:151:GLU:N	2.20	0.56
1:A:377:LEU:O	1:A:381:LEU:HG	2.05	0.56
2:B:54:HIS:NE2	2:B:80:ILE:HD12	2.20	0.56
1:A:358:ALA:HB2	1:A:375:PHE:HB3	1.87	0.56
2:B:71:VAL:CG2	2:B:105:TYR:CD2	2.89	0.55
1:A:596:ALA:O	1:A:598:GLN:HG2	2.06	0.55
1:A:474:ARG:HA	1:A:474:ARG:NH1	2.22	0.55
1:A:294:MET:CE	1:A:381:LEU:HD13	2.35	0.54
1:A:249:GLY:O	1:A:251:CYS:N	2.40	0.54
1:A:474:ARG:HA	1:A:474:ARG:HH11	1.72	0.54
1:A:249:GLY:O	1:A:250:ASP:C	2.44	0.54
1:A:243:LEU:HD23	1:A:336:LEU:HD13	1.88	0.54
2:B:85:TYR:CD1	2:B:85:TYR:N	2.75	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:GLN:NE2	2:B:13:GLN:OE1	2.41	0.53
1:A:434:ASN:N	1:A:434:ASN:HD22	2.01	0.52
2:B:232:ILE:HG13	2:B:243:THR:HG22	1.90	0.52
2:B:333:ASP:O	2:B:334:SER:CB	2.55	0.52
1:A:243:LEU:O	1:A:247:SER:OG	2.23	0.52
1:A:96:GLU:HA	1:A:459:GLN:HE22	1.74	0.52
2:B:136:SER:O	2:B:137:ARG:HB2	2.09	0.52
1:A:382:PHE:C	1:A:382:PHE:CD2	2.83	0.52
1:A:343:SER:OG	1:A:344:LYS:HG3	2.10	0.51
2:B:271:CYS:SG	2:B:291:ASP:HB3	2.51	0.51
2:B:112:VAL:HG13	2:B:126:LEU:HD11	1.93	0.51
2:B:108:SER:HB2	2:B:110:ASN:ND2	2.26	0.50
3:G:56:ALA:O	3:G:57:SER:C	2.50	0.50
1:A:240:ARG:HG2	1:A:269:PHE:CE1	2.43	0.49
2:B:91:HIS:CD2	2:B:133:VAL:HG21	2.47	0.49
1:A:282:HIS:HD2	1:A:470:LEU:HG	1.76	0.49
2:B:307:VAL:C	2:B:308:LEU:HD23	2.33	0.49
1:A:252:PRO:HB2	1:A:253:PHE:CE2	2.48	0.49
2:B:51:LEU:HB3	2:B:82:TRP:CZ3	2.48	0.49
1:A:338:LEU:HD12	1:A:338:LEU:N	2.28	0.49
2:B:81:ILE:HG22	2:B:90:VAL:CG2	2.43	0.49
1:A:325:LEU:HD12	1:A:331:VAL:HG12	1.94	0.48
2:B:48:ARG:HE	2:B:340:ASN:HB3	1.78	0.48
1:A:540:LYS:O	1:A:544:ASN:ND2	2.46	0.48
2:B:54:HIS:ND1	2:B:74:SER:HB3	2.29	0.48
1:A:257:MET:SD	1:A:259:TYR:O	2.72	0.47
1:A:377:LEU:O	1:A:377:LEU:HG	2.14	0.47
2:B:318:LEU:HD12	2:B:318:LEU:C	2.35	0.47
2:B:50:THR:C	2:B:51:LEU:HD23	2.35	0.47
1:A:197:ILE:HG22	1:A:197:ILE:O	2.14	0.47
2:B:149:CYS:O	2:B:150:ARG:NH1	2.48	0.46
1:A:624:ILE:HB	1:A:628:LYS:O	2.15	0.46
2:B:128:THR:O	2:B:130:GLU:N	2.49	0.46
1:A:470:LEU:C	1:A:470:LEU:CD1	2.84	0.46
1:A:279:LEU:HD12	1:A:323:ILE:HG21	1.98	0.46
1:A:174:PHE:CZ	1:A:178:LYS:HD3	2.51	0.46
1:A:214:GLY:O	1:A:215:LYS:C	2.54	0.45
2:B:262:MET:HG2	2:B:264:TYR:CZ	2.51	0.45
1:A:565:MET:HE1	1:A:632:LEU:HD13	1.97	0.45
2:B:142:HIS:NE2	2:B:159:THR:OG1	2.27	0.45
1:A:212:ASP:HB3	1:A:213:THR:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:PRO:HB2	1:A:156:ASN:ND2	2.31	0.45
1:A:240:ARG:HG3	1:A:509:PHE:CE1	2.52	0.44
2:B:54:HIS:ND1	2:B:74:SER:CB	2.81	0.44
1:A:80:LYS:N	1:A:81:PRO:CD	2.81	0.44
1:A:159:GLY:O	1:A:160:ASP:C	2.56	0.44
1:A:385:LEU:HD11	1:A:421:LEU:HD11	1.99	0.44
1:A:52:GLU:HG2	1:A:57:LYS:NZ	2.32	0.44
1:A:221:CYS:HA	1:A:267:LEU:O	2.17	0.44
3:G:58:GLU:O	3:G:60:PRO:HD3	2.17	0.44
1:A:281:TYR:O	1:A:281:TYR:CG	2.68	0.44
2:B:47:THR:HG23	2:B:47:THR:O	2.18	0.44
2:B:292:PHE:CD1	2:B:292:PHE:N	2.85	0.44
1:A:316:ARG:NH2	1:A:351:VAL:HG11	2.32	0.44
1:A:224:LYS:HE2	1:A:267:LEU:HD21	1.99	0.44
1:A:197:ILE:O	1:A:197:ILE:CG2	2.65	0.43
1:A:622:LEU:HA	1:A:622:LEU:HD23	1.88	0.43
2:B:243:THR:O	2:B:250:CYS:HA	2.19	0.43
1:A:403:ASP:O	1:A:407:LEU:HD12	2.18	0.43
1:A:149:TYR:O	1:A:153:ILE:HD12	2.19	0.43
2:B:29:THR:O	2:B:33:ILE:HG13	2.18	0.43
1:A:324:LEU:O	1:A:331:VAL:HA	2.19	0.43
2:B:308:LEU:HD23	2:B:308:LEU:N	2.33	0.43
1:A:601:LEU:HD11	1:A:624:ILE:CD1	2.48	0.43
3:G:61:PHE:CD2	3:G:61:PHE:N	2.87	0.43
1:A:226:ARG:HA	1:A:229:MET:HE2	2.00	0.43
1:A:85:PHE:CE1	1:A:89:ILE:HD11	2.53	0.43
2:B:70:LEU:HD11	2:B:336:LEU:HD22	2.01	0.43
2:B:313:ASN:O	2:B:314:ARG:O	2.36	0.43
1:A:229:MET:HB3	1:A:229:MET:HE3	1.93	0.43
1:A:637:ASP:O	1:A:638:PRO:C	2.55	0.43
2:B:183:HIS:HE2	2:B:201:SER:HG	1.63	0.43
1:A:295:ARG:O	1:A:295:ARG:HG3	2.20	0.42
1:A:114:MET:HE2	1:A:114:MET:HA	2.01	0.42
1:A:47:LEU:HB3	1:A:53:VAL:CG2	2.49	0.42
2:B:318:LEU:HD13	2:B:319:GLY:N	2.34	0.42
1:A:383:LYS:HA	1:A:388:HIS:O	2.20	0.42
2:B:199:PHE:CZ	2:B:211:TRP:CD1	3.08	0.42
2:B:47:THR:HA	2:B:338:ILE:O	2.20	0.42
1:A:252:PRO:HB2	1:A:253:PHE:CD2	2.55	0.42
1:A:602:THR:O	1:A:605:GLU:HG2	2.20	0.42
1:A:113:ILE:O	1:A:117:LEU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:MET:CE	1:A:332:ARG:HG3	2.49	0.41
2:B:56:ALA:HB1	2:B:75:GLN:OE1	2.20	0.41
1:A:620:LEU:HD21	1:A:644:LYS:HB2	2.02	0.41
2:B:58:ILE:CD1	2:B:336:LEU:HD12	2.50	0.41
3:G:56:ALA:CB	3:G:63:GLU:HB2	2.48	0.41
1:A:568:MET:HB2	1:A:631:VAL:CG2	2.50	0.41
2:B:172:GLU:HA	2:B:172:GLU:OE1	2.21	0.41
1:A:325:LEU:CD1	1:A:331:VAL:HG12	2.51	0.41
2:B:311:HIS:CE1	2:B:337:LYS:HD2	2.55	0.41
1:A:567:LYS:HA	1:A:631:VAL:O	2.21	0.41
2:B:54:HIS:NE2	2:B:72:SER:OG	2.54	0.41
1:A:401:GLU:O	1:A:405:MET:HG2	2.21	0.41
1:A:359:PRO:HG2	1:A:431:ARG:HA	2.03	0.41
1:A:467:PRO:HA	1:A:468:PRO:HD3	1.71	0.41
2:B:130:GLU:O	2:B:132:ASN:ND2	2.54	0.41
2:B:253:PHE:CD2	2:B:260:GLU:HA	2.56	0.41
2:B:318:LEU:HD12	2:B:318:LEU:O	2.21	0.40
1:A:385:LEU:HD13	1:A:421:LEU:HD21	2.03	0.40
1:A:497:LYS:HE3	1:A:497:LYS:HB2	1.91	0.40
2:B:320:VAL:HG22	2:B:327:VAL:HG22	2.03	0.40
2:B:276:VAL:O	2:B:277:SER:HB3	2.21	0.40
1:A:624:ILE:CG2	1:A:625:ARG:N	2.83	0.40
2:B:113:ALA:HA	2:B:122:SER:O	2.21	0.40
1:A:220:LYS:HB3	1:A:269:PHE:HB2	2.03	0.40
1:A:240:ARG:HH21	1:A:509:PHE:HA	1.86	0.40
2:B:69:LEU:HD22	2:B:82:TRP:O	2.21	0.40
2:B:266:HIS:ND1	2:B:268:ASN:HB2	2.36	0.40
2:B:273:ILE:HG22	2:B:274:THR:N	2.36	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	608/689 (88%)	560 (92%)	44 (7%)	4 (1%)	26 46
2	B	337/340 (99%)	299 (89%)	30 (9%)	8 (2%)	7 11
3	G	59/74 (80%)	49 (83%)	9 (15%)	1 (2%)	11 19
All	All	1004/1103 (91%)	908 (90%)	83 (8%)	13 (1%)	15 26

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	250	ASP
2	B	65	THR
2	B	75	GLN
2	B	131	GLY
1	A	212	ASP
2	B	314	ARG
3	G	57	SER
2	B	310	GLY
2	B	35	ASN
2	B	129	ARG
1	A	441	GLY
2	B	53	GLY
1	A	509	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	553/611 (90%)	509 (92%)	44 (8%)	15 28
2	B	282/283 (100%)	254 (90%)	28 (10%)	10 18
3	G	50/61 (82%)	45 (90%)	5 (10%)	9 18
All	All	885/955 (93%)	808 (91%)	77 (9%)	13 24

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LYS
1	A	32	ILE
1	A	47	LEU
1	A	57	LYS
1	A	97	THR
1	A	102	LEU
1	A	104	CYS
1	A	114	MET
1	A	135	HIS
1	A	168	SER
1	A	210	LYS
1	A	240	ARG
1	A	257	MET
1	A	265	ASP
1	A	278	ASP
1	A	290	SER
1	A	294	MET
1	A	295	ARG
1	A	350	SER
1	A	356	TYR
1	A	380	MET
1	A	382	PHE
1	A	389	SER
1	A	398	ASP
1	A	399	LYS
1	A	431	ARG
1	A	434	ASN
1	A	442	ARG
1	A	470	LEU
1	A	471	ILE
1	A	474	ARG
1	A	503	GLN
1	A	507	ARG
1	A	535	ARG
1	A	568	MET
1	A	608	SER
1	A	611	GLU
1	A	617	ARG
1	A	628	LYS
1	A	631	VAL
1	A	645	LYS
1	A	651	TYR
1	A	659	GLN

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Mol	Chain	Res	Type
1	A	666	ASN
2	B	2	SER
2	B	9	GLN
2	B	37	ILE
2	B	40	VAL
2	B	42	ARG
2	B	52	ARG
2	B	67	SER
2	B	70	LEU
2	B	90	VAL
2	B	96	ARG
2	B	105	TYR
2	B	123	ILE
2	B	134	ARG
2	B	146	LEU
2	B	177	THR
2	B	184	THR
2	B	199	PHE
2	B	234	PHE
2	B	245	SER
2	B	251	ARG
2	B	273	ILE
2	B	290	ASP
2	B	292	PHE
2	B	304	ARG
2	B	318	LEU
2	B	331	SER
2	B	334	SER
2	B	336	LEU
3	G	28	ILE
3	G	46	LYS
3	G	47	GLU
3	G	65	LYS
3	G	66	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	310	ASN
1	A	434	ASN
1	A	459	GLN
1	A	464	GLN

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Mol	Chain	Res	Type
1	A	544	ASN
1	A	607	GLN
1	A	656	GLN
2	B	6	GLN
2	B	9	GLN
2	B	13	GLN
2	B	91	HIS
2	B	110	ASN
2	B	176	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	CMT	G	68	3	6,7,7	1.32	1 (16%)	6,8,8	3.60	3 (50%)

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	CMT	G	68	3	-	0/8/8/8	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	68	CMT	OXT-C	-2.51	1.26	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	68	CMT	CA-CB-SG	-6.78	98.95	114.48
3	G	68	CMT	C1-OXT-C	3.45	124.08	115.99
3	G	68	CMT	OXT-C-CA	4.08	122.12	111.53

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)

There are no ligands in this entry.

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, 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	614/689 (89%)	0.46	59 (9%)	10	11	10, 28, 42, 60	0
2	B	339/340 (99%)	0.14	16 (4%)	35	40	13, 28, 50, 59	0
3	G	60/74 (81%)	0.18	4 (6%)	21	23	18, 35, 46, 47	0
All	All	1013/1103 (91%)	0.34	79 (7%)	16	17	10, 28, 45, 60	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	4	LEU	8.2
1	A	396	THR	5.8
1	A	199	ARG	5.8
2	B	8	ARG	5.4
1	A	497	LYS	5.2
1	A	201	GLY	4.8
1	A	618	LYS	4.3
1	A	202	PHE	4.3
1	A	29	SER	4.2
1	A	412	GLU	4.1
1	A	364	LYS	4.1
2	B	129	ARG	4.0
1	A	475	GLY	4.0
2	B	5	ASP	3.8
1	A	435	ARG	3.8
1	A	393	GLN	3.7
1	A	264	PRO	3.7
1	A	200	GLY	3.6
1	A	440	LEU	3.6
2	B	130	GLU	3.5
1	A	546	GLN	3.5
1	A	434	ASN	3.4
1	A	415	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	422	ARG	3.2
1	A	395	LYS	3.2
1	A	569	GLY	3.2
1	A	120	CYS	3.1
1	A	354	HIS	3.1
1	A	616	GLU	3.1
1	A	249	GLY	3.1
1	A	408	THR	3.0
1	A	397	LYS	3.0
1	A	366	VAL	2.9
1	A	237	LEU	2.9
1	A	365	GLY	2.9
3	G	20	LYS	2.9
1	A	226	ARG	2.8
1	A	398	ASP	2.8
2	B	268	ASN	2.7
1	A	593	GLU	2.7
1	A	394	HIS	2.7
1	A	549	HIS	2.7
3	G	26	ASP	2.7
1	A	668	PRO	2.6
1	A	298	ALA	2.6
2	B	285	LEU	2.6
1	A	547	LEU	2.5
1	A	195	ARG	2.5
1	A	632	LEU	2.5
1	A	269	PHE	2.4
2	B	9	GLN	2.4
2	B	13	GLN	2.4
1	A	270	ILE	2.4
1	A	535	ARG	2.4
1	A	230	LYS	2.4
1	A	551	GLU	2.4
1	A	615	LYS	2.3
3	G	13	ARG	2.3
1	A	262	HIS	2.3
1	A	198	GLY	2.3
1	A	344	LYS	2.3
1	A	352	GLY	2.3
2	B	113	ALA	2.2
2	B	157	ILE	2.2
1	A	643	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
3	G	66	PHE	2.2
2	B	19	ARG	2.2
2	B	159	THR	2.2
1	A	504	GLU	2.1
2	B	112	VAL	2.1
1	A	250	ASP	2.1
1	A	297	TYR	2.1
1	A	119	ALA	2.1
1	A	627	GLY	2.1
1	A	231	GLN	2.0
2	B	166	CYS	2.0
2	B	158	VAL	2.0
1	A	301	ILE	2.0
1	A	174	PHE	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	CMT	G	68	8/8	0.77	0.21	-	44,48,50,58	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.