



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:10 AM UTC

PDB ID : 1OMW / pdb_00001omw
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

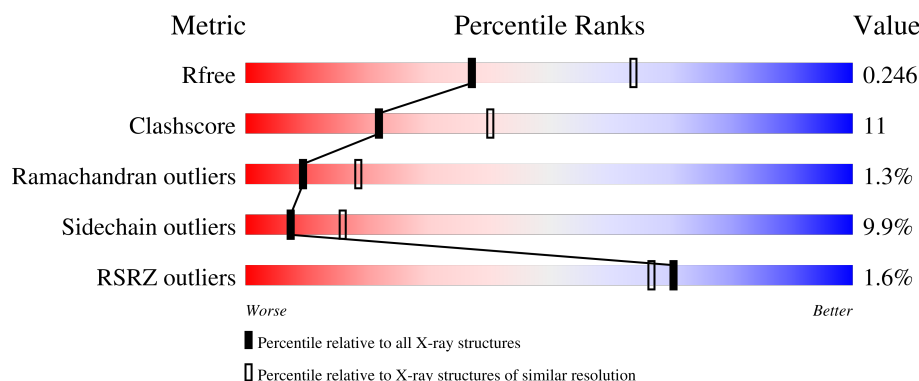
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	0% 63% 23% • 11%
2	B	340	2% 58% 30% 11% •
3	G	74	5% 55% 19% 8% 18%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CMT	G	68	-	X	-	-

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 mutation	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

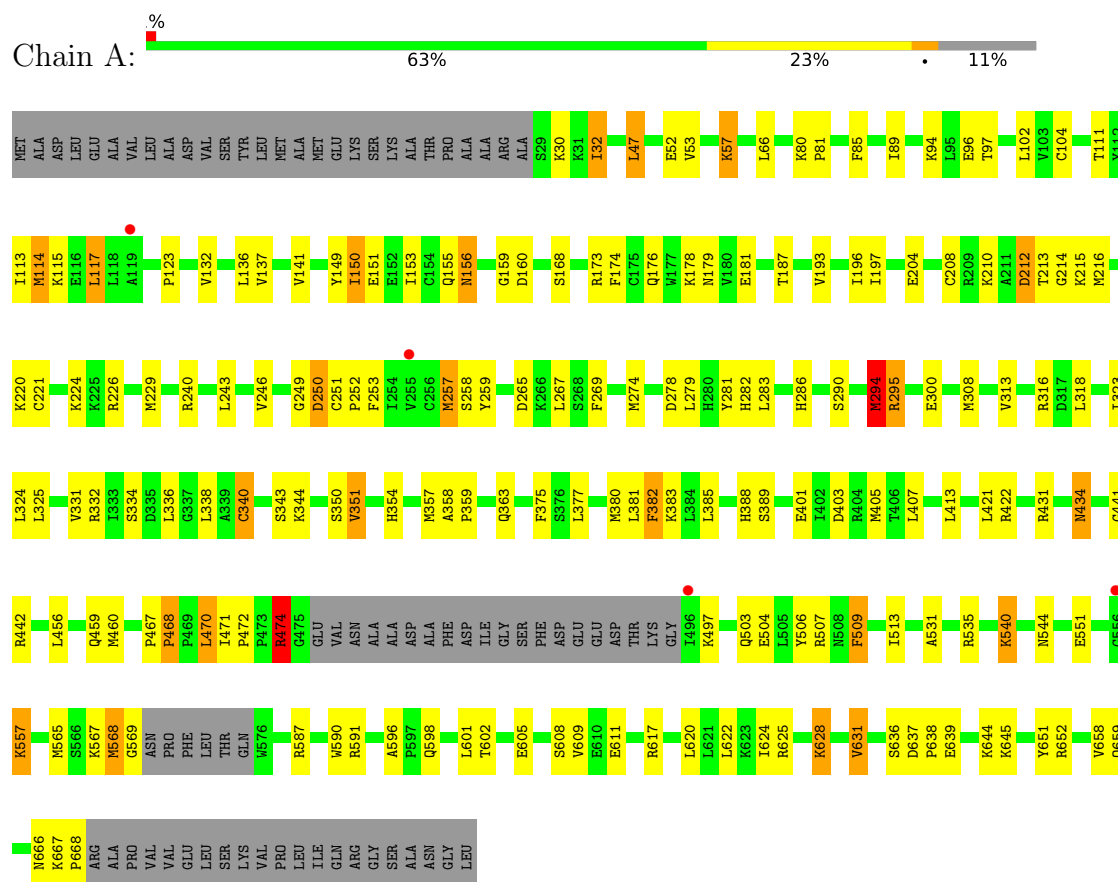
- Molecule 4 is water.

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

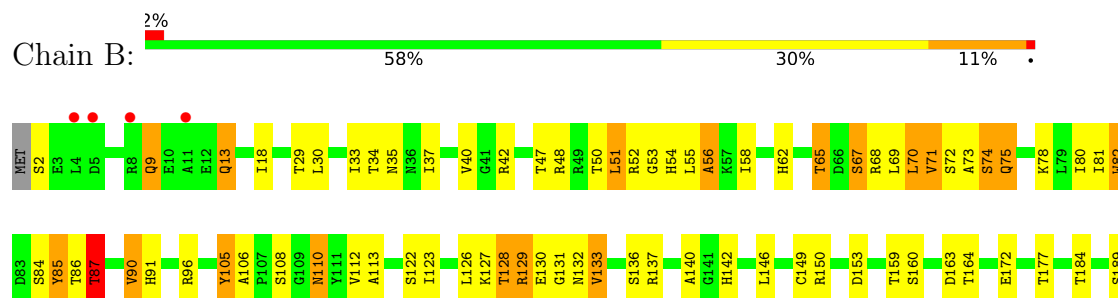
3 Residue-property plots

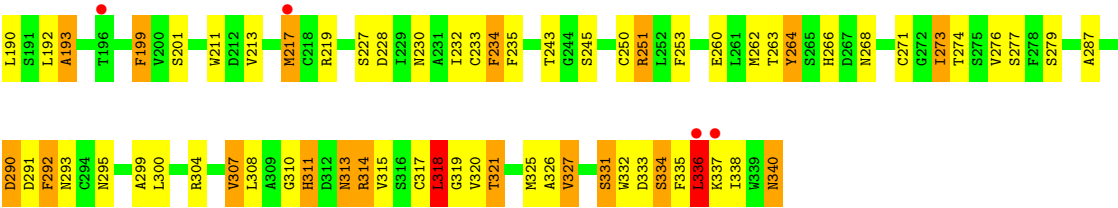
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



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





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



4 Data and refinement statistics

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 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	73.6 (20.00-2.50) 73.6 (20.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.202 , 0.252 0.241 , 0.246	Depositor DCC
R_{free} test set	1942 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	72.8	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	1.23	12/5150 (0.2%)	1.25	18/6918 (0.3%)
2	B	1.66	31/2654 (1.2%)	1.45	20/3597 (0.6%)
3	G	1.61	5/481 (1.0%)	1.48	4/646 (0.6%)
All	All	1.40	48/8285 (0.6%)	1.33	42/11161 (0.4%)

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	217	MET	SD-CE	9.88	2.04	1.79
2	B	51	LEU	CA-C	-9.38	1.41	1.52
2	B	307	VAL	C-O	-7.81	1.16	1.24
2	B	325	MET	CA-C	-7.55	1.42	1.52
2	B	287	ALA	CA-C	-7.54	1.44	1.52
3	G	56	ALA	CA-C	7.25	1.62	1.52
3	G	64	LYS	CE-NZ	7.16	1.70	1.49
2	B	251	ARG	CA-C	-6.97	1.44	1.52
1	A	216	MET	SD-CE	6.86	1.96	1.79
1	A	565	MET	SD-CE	-6.59	1.63	1.79
2	B	293	ASN	CA-C	-6.44	1.45	1.52
2	B	335	PHE	N-CA	6.36	1.53	1.46
2	B	73	ALA	CA-C	-6.28	1.45	1.52
2	B	299	ALA	CA-CB	-6.23	1.43	1.53
2	B	321	THR	CA-C	-6.11	1.44	1.52
1	A	187	THR	CA-CB	6.01	1.62	1.53
2	B	140	ALA	CA-CB	-6.00	1.44	1.53
2	B	153	ASP	C-O	-5.84	1.19	1.24
2	B	264	TYR	C-O	-5.79	1.17	1.24
2	B	313	ASN	C-O	5.78	1.30	1.23
2	B	290	ASP	N-CA	-5.77	1.38	1.46
1	A	460	MET	SD-CE	5.74	1.93	1.79
3	G	38	MET	SD-CE	5.72	1.93	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	56	ALA	CA-CB	-5.70	1.47	1.54
2	B	71	VAL	CA-CB	-5.67	1.47	1.54
2	B	62	HIS	CA-C	5.66	1.58	1.52
3	G	64	LYS	C-O	5.62	1.30	1.23
2	B	311	HIS	C-O	-5.53	1.17	1.23
2	B	189	SER	CA-C	-5.51	1.45	1.52
2	B	295	ASN	C-O	-5.50	1.17	1.23
1	A	591	ARG	CA-C	5.47	1.59	1.52
2	B	85	TYR	CA-CB	-5.44	1.44	1.53
1	A	155	GLN	C-O	-5.44	1.17	1.24
1	A	351	VAL	CA-C	5.41	1.59	1.52
2	B	201	SER	CA-C	-5.39	1.46	1.52
2	B	318	LEU	C-O	-5.37	1.17	1.24
1	A	32	ILE	CA-CB	5.31	1.61	1.54
1	A	474	ARG	N-CA	5.30	1.52	1.46
2	B	340	ASN	CB-CG	-5.30	1.38	1.52
1	A	196	ILE	CA-CB	5.25	1.59	1.54
2	B	55	LEU	CA-C	-5.20	1.45	1.52
2	B	315	VAL	CA-CB	-5.20	1.48	1.53
3	G	58	GLU	CA-C	5.15	1.59	1.52
1	A	531	ALA	CA-CB	-5.14	1.44	1.53
2	B	56	ALA	C-O	5.14	1.27	1.24
1	A	66	LEU	CA-C	5.12	1.59	1.52
2	B	128	THR	CA-CB	5.09	1.61	1.53
2	B	327	VAL	C-O	5.07	1.29	1.24

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	106	ALA	N-CA-C	-8.30	99.63	109.93
2	B	230	ASN	N-CA-C	7.92	121.01	111.82
1	A	472	PRO	N-CA-C	7.91	118.06	110.47
2	B	71	VAL	CB-CA-C	-7.47	100.97	111.21
1	A	208	CYS	N-CA-C	7.29	118.16	107.88
2	B	331	SER	N-CA-C	6.94	119.62	109.07
2	B	87	THR	N-CA-CB	-6.94	107.16	114.10
1	A	300	GLU	N-CA-C	-6.89	102.35	111.24
2	B	110	ASN	N-CA-C	6.71	119.45	111.33
1	A	283	LEU	N-CA-C	-6.47	104.08	112.23
1	A	340	CYS	N-CA-C	6.32	119.55	108.75
2	B	74	SER	N-CA-C	6.32	118.67	109.07
1	A	179	ASN	N-CA-C	-6.27	104.36	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	551	GLU	N-CA-C	-6.11	98.86	108.63
2	B	65	THR	N-CA-C	6.09	123.77	110.80
1	A	156	ASN	N-CA-C	6.08	118.87	111.82
1	A	294	MET	N-CA-C	-6.07	104.78	111.82
1	A	652	ARG	N-CA-C	-5.92	104.91	111.36
2	B	192	LEU	N-CA-C	-5.85	102.80	110.53
3	G	62	ARG	CA-C-N	-5.71	112.60	122.14
3	G	62	ARG	C-N-CA	-5.71	112.60	122.14
2	B	290	ASP	N-CA-C	-5.57	106.32	113.01
3	G	60	PRO	CA-C-N	-5.55	113.02	122.56
3	G	60	PRO	C-N-CA	-5.55	113.02	122.56
2	B	193	ALA	N-CA-C	-5.49	103.73	110.31
2	B	213	VAL	CB-CA-C	-5.46	104.71	111.70
1	A	587	ARG	N-CA-C	5.38	116.62	108.07
2	B	235	PHE	N-CA-C	-5.32	102.47	110.24
2	B	82	TRP	N-CA-C	5.31	117.94	110.14
2	B	279	SER	N-CA-C	-5.29	103.05	110.35
2	B	73	ALA	CA-C-O	-5.29	115.26	121.44
1	A	258	SER	N-CA-C	-5.27	106.91	113.55
2	B	336	LEU	CB-CA-C	-5.25	100.53	109.51
1	A	590	TRP	N-CA-C	5.21	116.91	109.14
1	A	468	PRO	N-CA-C	5.18	117.02	110.70
2	B	300	LEU	N-CA-C	5.17	119.65	113.23
1	A	557	LYS	CA-C-N	-5.17	115.47	123.17
1	A	557	LYS	C-N-CA	-5.17	115.47	123.17
1	A	94	LYS	N-CA-C	5.15	119.32	113.19
2	B	326	ALA	N-CA-C	5.06	115.84	108.14
2	B	133	VAL	CB-CA-C	-5.05	104.96	111.53
1	A	334	SER	N-CA-C	5.01	116.75	108.48

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	5037	0	5042	93	0
2	B	2607	0	2510	71	0
3	G	481	0	493	10	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	173	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 11.

All (173) 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:CE	3:G:64:LYS:NZ	1.70	1.53
2:B:217:MET:SD	2:B:217:MET:CE	2.04	1.46
1:A:294:MET:HE3	1:A:381:LEU:HD13	1.43	1.01
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: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
2:B:313:ASN:O	2:B:314:ARG:C	2.36	0.69
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
2:B:70:LEU:O	2:B:70:LEU:HG	1.95	0.66
1:A:413:LEU:HD12	1:A:422:ARG:HG3	1.79	0.65
1:A:141:VAL:O	1:A:141:VAL:HG23	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:470:LEU:HD12	1:A:470:LEU:C	2.24	0.62
2:B:318:LEU:C	2:B:318:LEU:CD1	2.72	0.62
1:A:609:VAL:HG22	1:A:622:LEU:CD2	2.29	0.62
2:B:128:THR:O	2:B:129:ARG:C	2.43	0.61
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:249:GLY:O	1:A:250:ASP:C	2.44	0.58
1:A:568:MET:HB2	1:A:631:VAL:HG23	1.83	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
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
1:A:382:PHE:CD2	1:A:382:PHE:C	2.83	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
1:A:226:ARG:HA	1:A:229:MET:HE2	1.88	0.56
2:B:217:MET:HE2	2:B:219:ARG:HG2	1.87	0.56
2:B:71:VAL:CG2	2:B:105:TYR:CD2	2.89	0.55
3:G:56:ALA:O	3:G:57:SER:C	2.50	0.55
1:A:354:HIS:HA	1:A:357:MET:HE2	1.88	0.55
1:A:596:ALA:O	1:A:598:GLN:HG2	2.06	0.55
1:A:474:ARG:NH1	1:A:474:ARG:HA	2.22	0.55
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:243:LEU:HD23	1:A:336:LEU:HD13	1.88	0.54
2:B:307:VAL:C	2:B:308:LEU:HD23	2.33	0.54
2:B:85:TYR:CD1	2:B:85:TYR:N	2.75	0.54
2:B:9:GLN:NE2	2:B:13:GLN:OE1	2.41	0.53
2:B:30:LEU:HD23	2:B:262:MET:HE2	1.89	0.53
1:A:434:ASN:HD22	1:A:434:ASN:N	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: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
2:B:318:LEU:C	2:B:318:LEU:HD12	2.35	0.52
2:B:50:THR:C	2:B:51:LEU:HD23	2.35	0.51
1:A:343:SER:OG	1:A:344:LYS:HG3	2.10	0.51
1:A:114:MET:HE2	1:A:114:MET:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:214:GLY:O	1:A:215:LYS:C	2.54	0.50
2:B:163:ASP:C	2:B:164:THR:HG1	2.03	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
1:A:470:LEU:C	1:A:470:LEU:CD1	2.84	0.49
1:A:159:GLY:O	1:A:160:ASP:C	2.56	0.49
1:A:252:PRO:HB2	1:A:253:PHE:CE2	2.48	0.49
1:A:338:LEU:HD12	1:A:338:LEU:N	2.28	0.49
2:B:51:LEU:HB3	2:B:82:TRP:CZ3	2.48	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:637:ASP:O	1:A:638:PRO:C	2.55	0.47
1:A:257:MET:SD	1:A:259:TYR:O	2.72	0.47
1:A:568:MET:HE3	1:A:569:GLY:H	1.80	0.47
1:A:197:ILE:O	1:A:197:ILE:HG22	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: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
2:B:262:MET:HG2	2:B:264:TYR:CZ	2.51	0.45
1:A:308:MET:HE2	1:A:336:LEU:HD21	1.96	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
1:A:123:PRO:HB2	1:A:156:ASN:ND2	2.31	0.45
1:A:377:LEU:O	1:A:377:LEU:HG	2.14	0.45
1:A:636:SER:OG	1:A:639:GLU:OE1	2.33	0.45
1:A:240:ARG:HG3	1:A:509:PHE:CE1	2.52	0.44
1:A:80:LYS:N	1:A:81:PRO:CD	2.81	0.44
2:B:54:HIS:ND1	2:B:74:SER:CB	2.81	0.44
1:A:52:GLU:HG2	1:A:57:LYS:NZ	2.32	0.44
1:A:178:LYS:NZ	1:A:181:GLU:OE1	2.50	0.44
1:A:385:LEU:HD11	1:A:421:LEU:HD11	1.99	0.44
2:B:68:ARG:O	2:B:84:SER:OG	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	2:B:47:THR:HG23	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:HD23	1:A:622:LEU:HA	1.88	0.43
2:B:243:THR:O	2:B:250:CYS:HA	2.19	0.43
1:A:149:TYR:O	1:A:153:ILE:HD12	2.19	0.43
1:A:403:ASP:O	1:A:407:LEU:HD12	2.18	0.43
3:G:21:MET:N	3:G:21:MET:HE2	2.34	0.43
1:A:324:LEU:O	1:A:331:VAL:HA	2.19	0.43
2:B:29:THR:O	2:B:33:ILE:HG13	2.18	0.43
2:B:332:TRP:C	2:B:334:SER:H	2.26	0.43
1:A:85:PHE:CE1	1:A:89:ILE:HD11	2.53	0.43
1:A:504:GLU:C	1:A:506:TYR:H	2.27	0.43
1:A:601:LEU:HD11	1:A:624:ILE:CD1	2.48	0.43
2:B:308:LEU:HD23	2:B:308:LEU:N	2.33	0.43
3:G:61:PHE:N	3:G:61:PHE:CD2	2.87	0.43
2:B:70:LEU:HD11	2:B:336:LEU:HD22	2.01	0.43
2:B:227:SER:O	2:B:228:ASP:C	2.62	0.43
1:A:229:MET:HE2	1:A:229:MET:HB3	1.89	0.42
1:A:295:ARG:O	1:A:295:ARG:HG3	2.20	0.42
1:A:47:LEU:HB3	1:A:53:VAL:CG2	2.49	0.42
1:A:383:LYS:HA	1:A:388:HIS:O	2.20	0.42
2:B:318:LEU:HD13	2:B:319:GLY:N	2.34	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:113:ILE:O	1:A:117:LEU:HB2	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
3:G:9:ILE:C	3:G:11:GLN:N	2.78	0.42
1:A:274:MET:CE	1:A:332:ARG:HG3	2.49	0.41
1:A:620:LEU:HD21	1:A:644:LYS:HB2	2.02	0.41
2:B:56:ALA:HB1	2:B:75:GLN:OE1	2.20	0.41
2:B:313:ASN:O	2:B:314:ARG:O	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:172:GLU:OE1	2:B:172:GLU:HA	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:401:GLU:O	1:A:405:MET:HG2	2.21	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: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
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:318:LEU:HD12	2:B:318:LEU:O	2.21	0.40
2:B:320:VAL:HG22	2:B:327:VAL:HG22	2.03	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
2:B:276:VAL:O	2:B:277:SER:HB3	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%)	18 34
2	B	337/340 (99%)	299 (89%)	30 (9%)	8 (2%)	4 8
3	G	59/74 (80%)	49 (83%)	9 (15%)	1 (2%)	7 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1004/1103 (91%)	908 (90%)	83 (8%)	13 (1%)	9	18

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 ⓘ

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%)	502 (91%)	51 (9%)	8	19
2	B	282/283 (100%)	250 (89%)	32 (11%)	5	12
3	G	50/61 (82%)	45 (90%)	5 (10%)	7	15
All	All	885/955 (93%)	797 (90%)	88 (10%)	7	16

All (88) 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

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Mol	Chain	Res	Type
1	A	57	LYS
1	A	97	THR
1	A	102	LEU
1	A	104	CYS
1	A	114	MET
1	A	117	LEU
1	A	137	VAL
1	A	150	ILE
1	A	168	SER
1	A	193	VAL
1	A	204	GLU
1	A	210	LYS
1	A	246	VAL
1	A	257	MET
1	A	265	ASP
1	A	278	ASP
1	A	286	HIS
1	A	290	SER
1	A	294	MET
1	A	295	ARG
1	A	318	LEU
1	A	350	SER
1	A	380	MET
1	A	382	PHE
1	A	389	SER
1	A	434	ASN
1	A	442	ARG
1	A	456	LEU
1	A	470	LEU
1	A	471	ILE
1	A	474	ARG
1	A	503	GLN
1	A	507	ARG
1	A	513	ILE
1	A	535	ARG
1	A	540	LYS
1	A	557	LYS
1	A	568	MET
1	A	608	SER
1	A	611	GLU
1	A	617	ARG
1	A	628	LYS

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Mol	Chain	Res	Type
1	A	631	VAL
1	A	645	LYS
1	A	651	TYR
1	A	658	VAL
1	A	659	GLN
1	A	666	ASN
2	B	2	SER
2	B	9	GLN
2	B	13	GLN
2	B	18	ILE
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	78	LYS
2	B	87	THR
2	B	90	VAL
2	B	96	ARG
2	B	105	TYR
2	B	123	ILE
2	B	127	LYS
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	17	GLU
3	G	28	ILE
3	G	46	LYS
3	G	47	GLU

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Mol	Chain	Res	Type
3	G	65	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	HIS
1	A	262	HIS
1	A	307	HIS
1	A	310	ASN
1	A	388	HIS
1	A	393	GLN
1	A	434	ASN
1	A	459	GLN
1	A	464	GLN
1	A	503	GLN
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	132	ASN
2	B	156	GLN
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	7,7,7	1.33	2 (28%)	6,8,8	3.87	4 (66%)

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	-	4/8/8/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	68	CMT	OXT-C	-2.64	1.26	1.33
3	G	68	CMT	CB-CA	-2.12	1.50	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	68	CMT	CA-CB-SG	-7.23	98.95	114.40
3	G	68	CMT	OXT-C-CA	4.18	122.12	111.50
3	G	68	CMT	C1-OXT-C	3.60	124.08	115.92
3	G	68	CMT	C-CA-N	2.01	116.87	110.82

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	68	CMT	O-C-CA-N
3	G	68	CMT	O-C-OXT-C1
3	G	68	CMT	CA-C-OXT-C1
3	G	68	CMT	OXT-C-CA-N

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	614/689 (89%)	-0.14	4 (0%) 84 81	10, 28, 42, 60	0
2	B	339/340 (99%)	0.19	8 (2%) 59 55	13, 28, 50, 59	0
3	G	60/74 (81%)	0.29	4 (6%) 24 21	18, 35, 46, 47	0
All	All	1013/1103 (91%)	-0.00	16 (1%) 70 67	10, 28, 45, 60	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	4	LEU	4.0
2	B	5	ASP	3.4
2	B	196	THR	3.3
2	B	11	ALA	3.2
2	B	8	ARG	3.1
1	A	556	GLY	3.0
3	G	22	GLU	2.9
3	G	65	LYS	2.7
3	G	26	ASP	2.5
2	B	336	LEU	2.5
1	A	255	VAL	2.5
2	B	217	MET	2.4
1	A	496	ILE	2.3
1	A	119	ALA	2.1
3	G	66	PHE	2.0
2	B	337	LYS	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. 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	B-factors($\text{\AA}^2$)	Q<0.9
3	CMT	G	68	8/8	0.61	0.12	44,48,50,58	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.