



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:47 AM GMT

PDB ID : 3C4Y  
Title : Crystal Structure of Apo form of G protein coupled receptor kinase 1 at 7.51Å  
Authors : Singh, P.; Tesmer, J.J.G.  
Deposited on : 2008-01-30  
Resolution : 7.51 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](mailto: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.

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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

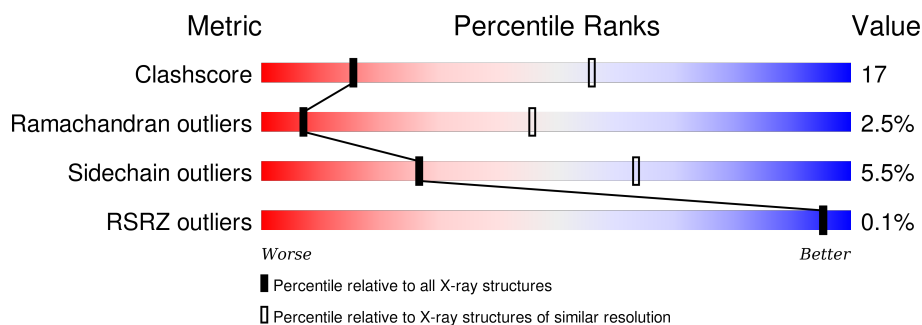
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 7.51 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))
Clashscore	102246	1063 (10.00-3.70)
Ramachandran outliers	100387	1035 (9.50-3.66)
Sidechain outliers	100360	1005 (9.50-3.66)
RSRZ outliers	91569	1013 (9.50-3.66)

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  $\geq 3$ , 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	543	
1	B	543	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7629 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.

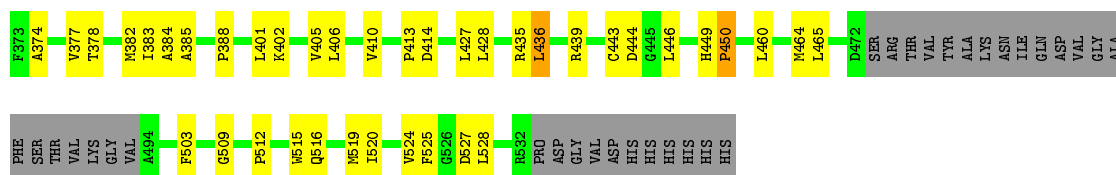
- Molecule 1 is a protein called Rhodopsin kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	478	Total	C	N	O	S	0	0	0
			3854	2474	666	695	19			
1	B	466	Total	C	N	O	S	0	0	0
			3775	2427	649	680	19			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	536	VAL	-	EXPRESSION TAG	UNP P28327
A	537	ASP	-	EXPRESSION TAG	UNP P28327
A	538	HIS	-	EXPRESSION TAG	UNP P28327
A	539	HIS	-	EXPRESSION TAG	UNP P28327
A	540	HIS	-	EXPRESSION TAG	UNP P28327
A	541	HIS	-	EXPRESSION TAG	UNP P28327
A	542	HIS	-	EXPRESSION TAG	UNP P28327
A	543	HIS	-	EXPRESSION TAG	UNP P28327
B	536	VAL	-	EXPRESSION TAG	UNP P28327
B	537	ASP	-	EXPRESSION TAG	UNP P28327
B	538	HIS	-	EXPRESSION TAG	UNP P28327
B	539	HIS	-	EXPRESSION TAG	UNP P28327
B	540	HIS	-	EXPRESSION TAG	UNP P28327
B	541	HIS	-	EXPRESSION TAG	UNP P28327
B	542	HIS	-	EXPRESSION TAG	UNP P28327
B	543	HIS	-	EXPRESSION TAG	UNP P28327





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.31Å 123.31Å 192.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 7.51 19.94 – 7.51	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-7.51) 100.0 (19.94-7.51)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.03 (at 7.78Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.182 , (Not available) 0.183 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	540.3	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.14 , 153.3	EDS
Estimated twinning fraction	0.043 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 2230 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7629	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	224.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.85% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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](#)

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	0.39	0/3944	0.53	0/5316
1	B	0.38	0/3862	0.53	0/5205
All	All	0.39	0/7806	0.53	0/10521

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	LEU	Peptide
1	A	116	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	3854	0	3820	133	0
1	B	3775	0	3748	130	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7629	0	7568	262	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 17.

All (262) 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)
1:B:209:THR:HG22	1:B:524:VAL:HG21	1.43	1.00
1:A:209:THR:HG22	1:A:524:VAL:HG21	1.46	0.95
1:B:275:HIS:HA	1:B:279:VAL:HG23	1.51	0.90
1:B:134:ALA:HB2	1:B:146:LEU:HD13	1.52	0.90
1:A:275:HIS:HA	1:A:279:VAL:HG23	1.53	0.88
1:A:134:ALA:HB2	1:A:146:LEU:HD13	1.54	0.87
1:A:250:LEU:HD12	1:A:263:VAL:O	1.76	0.85
1:B:250:LEU:HD12	1:B:263:VAL:O	1.77	0.84
1:B:314:ASP:HB2	1:B:335:LEU:HD13	1.61	0.83
1:B:361:LEU:HD12	1:B:405:VAL:HG11	1.61	0.82
1:A:314:ASP:HB2	1:A:335:LEU:HD13	1.61	0.81
1:B:356:MET:HE1	1:B:361:LEU:HD21	1.60	0.81
1:A:361:LEU:HD12	1:A:405:VAL:HG11	1.64	0.80
1:A:410:VAL:HG21	1:A:428:LEU:HD13	1.63	0.78
1:B:410:VAL:HG21	1:B:428:LEU:HD13	1.68	0.76
1:A:116:GLU:HB3	1:A:117:PRO:HD2	1.70	0.73
1:A:250:LEU:HD21	1:A:262:LEU:HD22	1.74	0.69
1:A:250:LEU:HD11	1:A:262:LEU:HD22	1.75	0.68
1:B:358:PRO:HB3	1:B:406:LEU:HD23	1.75	0.68
1:B:250:LEU:HD21	1:B:262:LEU:HD22	1.75	0.68
1:A:410:VAL:HG21	1:A:428:LEU:CD1	2.24	0.68
1:B:250:LEU:HD11	1:B:262:LEU:HD22	1.76	0.67
1:A:356:MET:HE1	1:A:361:LEU:HD21	1.76	0.67
1:B:238:ILE:HG21	1:B:310:ILE:CD1	2.24	0.67
1:A:353:PRO:HA	1:A:356:MET:HE2	1.77	0.67
1:A:358:PRO:HB3	1:A:406:LEU:HD23	1.75	0.67
1:A:150:VAL:HG22	1:A:154:LEU:CD1	2.25	0.67
1:B:356:MET:CE	1:B:361:LEU:HD21	2.25	0.66
1:A:168:PHE:CZ	1:A:172:LEU:HD11	2.31	0.65
1:A:192:VAL:HG13	1:A:201:VAL:O	1.97	0.65
1:A:356:MET:CE	1:A:361:LEU:HD21	2.27	0.64
1:B:353:PRO:HA	1:B:356:MET:HE2	1.80	0.64
1:B:401:LEU:O	1:B:405:VAL:HG23	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:VAL:HG21	1:B:428:LEU:CD1	2.28	0.63
1:A:305:LEU:HD13	1:A:306:HIS:NE2	2.13	0.63
1:B:168:PHE:CZ	1:B:172:LEU:HD11	2.33	0.63
1:A:377:VAL:HG13	1:A:388:PRO:CD	2.29	0.63
1:A:401:LEU:O	1:A:405:VAL:HG23	1.99	0.62
1:B:305:LEU:HD13	1:B:306:HIS:NE2	2.14	0.62
1:B:150:VAL:HG22	1:B:154:LEU:CD1	2.28	0.62
1:B:212:LEU:HD12	1:B:266:ILE:HD12	1.83	0.61
1:B:192:VAL:HG13	1:B:201:VAL:O	2.00	0.61
1:B:213:TYR:CG	1:B:263:VAL:HG13	2.35	0.61
1:B:302:LEU:HD23	1:B:305:LEU:HD12	1.82	0.61
1:A:302:LEU:HD23	1:A:305:LEU:HD12	1.83	0.60
1:A:238:ILE:HG21	1:A:310:ILE:CD1	2.31	0.60
1:B:251:ALA:HB3	1:B:263:VAL:HG12	1.83	0.60
1:B:305:LEU:HD13	1:B:306:HIS:CD2	2.36	0.60
1:B:305:LEU:HD22	1:B:310:ILE:O	2.02	0.60
1:A:357:ALA:CB	1:A:370:VAL:HG12	2.32	0.60
1:B:377:VAL:HG13	1:B:388:PRO:CD	2.32	0.59
1:A:251:ALA:HB3	1:A:263:VAL:HG12	1.83	0.59
1:B:166:LEU:HA	1:B:169:LEU:HD12	1.82	0.59
1:A:213:TYR:CG	1:A:263:VAL:HG13	2.38	0.59
1:A:76:LEU:HB2	1:A:86:LEU:HD22	1.83	0.58
1:A:305:LEU:HD13	1:A:306:HIS:CD2	2.37	0.58
1:B:275:HIS:HA	1:B:279:VAL:CG2	2.30	0.58
1:A:166:LEU:HA	1:A:169:LEU:HD12	1.85	0.58
1:B:92:ILE:HG21	1:B:147:LEU:HD13	1.86	0.58
1:B:357:ALA:HB2	1:B:370:VAL:HA	1.85	0.58
1:A:305:LEU:HD22	1:A:310:ILE:O	2.03	0.58
1:A:116:GLU:HB3	1:A:117:PRO:CD	2.34	0.58
1:B:279:VAL:HG12	1:B:280:ASP:N	2.19	0.57
1:A:295:THR:O	1:A:299:VAL:HG23	2.05	0.57
1:A:357:ALA:HB2	1:A:370:VAL:HA	1.86	0.57
1:B:76:LEU:HB2	1:B:86:LEU:HD22	1.87	0.57
1:B:115:LEU:CD2	1:B:131:VAL:HG13	2.35	0.57
1:A:130:THR:HG22	1:A:146:LEU:HD12	1.87	0.56
1:B:134:ALA:CB	1:B:146:LEU:HD13	2.30	0.56
1:B:295:THR:O	1:B:299:VAL:HG23	2.05	0.56
1:B:130:THR:HG22	1:B:146:LEU:HD12	1.86	0.56
1:A:250:LEU:HD11	1:A:252:TYR:O	2.05	0.56
1:B:212:LEU:HD12	1:B:266:ILE:CD1	2.36	0.56
1:A:157:ALA:HB3	1:A:158:PRO:HD3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:LEU:HD21	1:A:446:LEU:HA	1.88	0.56
1:A:361:LEU:HD22	1:A:402:LYS:HD2	1.88	0.56
1:A:357:ALA:HB3	1:A:370:VAL:HG12	1.88	0.55
1:B:250:LEU:HD11	1:B:252:TYR:O	2.07	0.55
1:A:115:LEU:CD2	1:A:131:VAL:HG13	2.37	0.55
1:B:317:PRO:HD3	1:B:378:THR:HG23	1.88	0.54
1:B:322:LEU:HG	1:B:328:VAL:HG12	1.88	0.54
1:B:157:ALA:HB3	1:B:158:PRO:HD3	1.89	0.54
1:A:134:ALA:HB1	1:A:143:PHE:CD2	2.42	0.54
1:A:238:ILE:HD12	1:A:310:ILE:HD11	1.89	0.54
1:B:134:ALA:HB1	1:B:143:PHE:CD2	2.43	0.53
1:B:357:ALA:CB	1:B:370:VAL:HG12	2.38	0.53
1:B:361:LEU:HD22	1:B:402:LYS:HD2	1.90	0.53
1:B:215:CYS:SG	1:B:263:VAL:HG23	2.48	0.52
1:A:92:ILE:HG21	1:A:147:LEU:HD13	1.91	0.52
1:A:147:LEU:O	1:A:150:VAL:HG12	2.09	0.52
1:B:71:LEU:HD12	1:B:171:PHE:HD1	1.75	0.52
1:A:275:HIS:HA	1:A:279:VAL:CG2	2.33	0.52
1:A:377:VAL:HG13	1:A:388:PRO:CG	2.40	0.52
1:A:322:LEU:HG	1:A:328:VAL:HG12	1.91	0.52
1:A:174:TRP:CH2	1:A:525:PHE:HA	2.45	0.52
1:B:174:TRP:CH2	1:B:525:PHE:HA	2.45	0.51
1:A:297:GLN:OE1	1:A:328:VAL:HG22	2.11	0.51
1:B:519:MET:SD	1:B:519:MET:N	2.83	0.51
1:B:251:ALA:HB3	1:B:263:VAL:CG1	2.41	0.51
1:A:150:VAL:HG22	1:A:154:LEU:HD11	1.90	0.51
1:B:67:ILE:HD12	1:B:516:GLN:HG2	1.93	0.51
1:A:251:ALA:HB3	1:A:263:VAL:CG1	2.40	0.51
1:A:238:ILE:HG21	1:A:310:ILE:HD13	1.92	0.50
1:B:247:ILE:HD11	1:B:304:HIS:HB3	1.92	0.50
1:B:91:ASP:HB3	1:B:110:LEU:HD21	1.94	0.50
1:B:436:LEU:HD21	1:B:446:LEU:HA	1.92	0.50
1:A:279:VAL:HG12	1:A:280:ASP:N	2.25	0.50
1:A:250:LEU:CD2	1:A:262:LEU:HD22	2.41	0.50
1:A:71:LEU:HD12	1:A:171:PHE:HD1	1.76	0.50
1:B:150:VAL:HG22	1:B:154:LEU:HD11	1.94	0.50
1:A:297:GLN:CG	1:A:460:LEU:HD11	2.42	0.50
1:B:377:VAL:HG13	1:B:388:PRO:CG	2.42	0.50
1:A:215:CYS:SG	1:A:263:VAL:HG23	2.52	0.49
1:A:317:PRO:HD3	1:A:378:THR:HG23	1.94	0.49
1:A:333:LEU:N	1:A:333:LEU:HD22	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ALA:CB	1:A:146:LEU:HD13	2.32	0.49
1:B:357:ALA:HB3	1:B:370:VAL:HG12	1.93	0.49
1:A:443:CYS:HB3	1:A:446:LEU:HB3	1.94	0.49
1:B:246:PHE:HB2	1:B:301:GLY:HA2	1.94	0.49
1:A:246:PHE:CE2	1:A:300:SER:HB2	2.48	0.49
1:B:355:PHE:O	1:B:374:ALA:HB2	2.13	0.49
1:B:317:PRO:CD	1:B:378:THR:HG23	2.42	0.49
1:B:213:TYR:CD2	1:B:263:VAL:HG13	2.47	0.49
1:B:67:ILE:HG13	1:B:520:ILE:HD11	1.95	0.49
1:B:148:ARG:HA	1:B:151:LEU:HD12	1.95	0.49
1:B:361:LEU:HD12	1:B:405:VAL:CG1	2.38	0.48
1:A:218:LEU:O	1:A:259:ASP:HA	2.13	0.48
1:A:250:LEU:HD13	1:A:262:LEU:HB3	1.94	0.48
1:B:218:LEU:O	1:B:259:ASP:HA	2.14	0.48
1:A:91:ASP:HB3	1:A:110:LEU:HD21	1.94	0.48
1:A:355:PHE:O	1:A:374:ALA:HB2	2.13	0.48
1:A:36:LEU:HD12	1:A:39:LEU:HD12	1.96	0.48
1:B:250:LEU:HD13	1:B:262:LEU:HB3	1.96	0.48
1:A:176:TRP:CZ3	1:A:177:LEU:HD13	2.49	0.48
1:B:85:ALA:HB1	1:B:154:LEU:HD21	1.96	0.48
1:B:166:LEU:O	1:B:169:LEU:N	2.47	0.47
1:A:168:PHE:CE1	1:A:172:LEU:HD21	2.50	0.47
1:B:168:PHE:CE1	1:B:172:LEU:HD21	2.49	0.47
1:A:67:ILE:HD12	1:A:516:GLN:HG2	1.96	0.47
1:A:150:VAL:HG22	1:A:154:LEU:HG	1.97	0.47
1:B:260:LEU:HD11	1:B:503:PHE:CD2	2.49	0.47
1:B:272:ILE:HG22	1:B:276:ILE:HG13	1.95	0.47
1:B:512:PRO:O	1:B:515:TRP:HB3	2.15	0.47
1:B:333:LEU:N	1:B:333:LEU:HD22	2.30	0.47
1:B:159:PHE:CE2	1:B:163:LEU:HD21	2.49	0.47
1:B:159:PHE:CZ	1:B:163:LEU:HD21	2.49	0.47
1:B:71:LEU:HD12	1:B:171:PHE:CD1	2.50	0.47
1:A:213:TYR:CD2	1:A:263:VAL:HG13	2.50	0.47
1:A:67:ILE:HG13	1:A:520:ILE:HD11	1.97	0.47
1:B:297:GLN:CG	1:B:460:LEU:HD11	2.45	0.47
1:A:159:PHE:CZ	1:A:163:LEU:HD21	2.50	0.47
1:A:297:GLN:HG3	1:A:460:LEU:HD11	1.97	0.46
1:A:519:MET:N	1:A:519:MET:SD	2.88	0.46
1:A:272:ILE:HG22	1:A:276:ILE:HG13	1.96	0.46
1:A:314:ASP:CB	1:A:335:LEU:HD13	2.40	0.46
1:A:250:LEU:CD1	1:A:262:LEU:HD22	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:GLN:OE1	1:B:328:VAL:HG22	2.15	0.46
1:A:91:ASP:CB	1:A:110:LEU:HD21	2.45	0.46
1:B:176:TRP:CZ3	1:B:177:LEU:HD13	2.51	0.46
1:A:354:GLY:O	1:A:377:VAL:HG21	2.16	0.46
1:B:443:CYS:HB3	1:B:446:LEU:HB3	1.97	0.46
1:A:159:PHE:CE2	1:A:163:LEU:HD21	2.50	0.46
1:B:62:CYS:SG	1:B:72:PHE:HB2	2.56	0.46
1:B:152:ALA:O	1:B:156:GLN:HG3	2.15	0.46
1:A:260:LEU:HD11	1:A:503:PHE:CD2	2.50	0.46
1:B:147:LEU:O	1:B:150:VAL:HG12	2.16	0.46
1:B:143:PHE:CD2	1:B:146:LEU:HD22	2.51	0.46
1:B:91:ASP:CB	1:B:110:LEU:HD21	2.45	0.46
1:B:204:CYS:SG	1:B:215:CYS:HB2	2.56	0.46
1:A:152:ALA:O	1:A:156:GLN:HG3	2.16	0.46
1:B:150:VAL:HG22	1:B:154:LEU:HG	1.97	0.45
1:B:115:LEU:HD23	1:B:131:VAL:HG13	1.98	0.45
1:A:377:VAL:HG13	1:A:388:PRO:HG3	1.98	0.45
1:A:317:PRO:CD	1:A:378:THR:HG23	2.46	0.45
1:A:238:ILE:CG2	1:A:310:ILE:CD1	2.95	0.45
1:B:250:LEU:CD2	1:B:262:LEU:HD22	2.43	0.45
1:B:314:ASP:CB	1:B:335:LEU:HD13	2.40	0.45
1:A:71:LEU:HD12	1:A:171:PHE:CD1	2.52	0.45
1:A:166:LEU:O	1:A:169:LEU:N	2.48	0.45
1:B:293:PHE:CE1	1:B:465:LEU:HD22	2.51	0.45
1:B:250:LEU:CD1	1:B:262:LEU:HD22	2.44	0.45
1:A:339:LEU:HD21	1:A:346:THR:HG22	1.99	0.45
1:A:213:TYR:HB3	1:A:263:VAL:HG13	1.98	0.45
1:B:354:GLY:O	1:B:377:VAL:HG21	2.17	0.45
1:B:297:GLN:HG3	1:B:460:LEU:HD11	1.99	0.45
1:A:148:ARG:HA	1:A:151:LEU:HD12	1.99	0.45
1:A:265:THR:HG21	1:A:329:ARG:NH2	2.32	0.45
1:A:384:ALA:O	1:A:385:ALA:HB3	2.17	0.45
1:A:361:LEU:HD13	1:A:402:LYS:HA	2.00	0.44
1:A:62:CYS:SG	1:A:72:PHE:HB2	2.56	0.44
1:A:177:LEU:HD12	1:A:180:GLN:HG3	1.98	0.44
1:B:291:ALA:CB	1:B:383:ILE:HD11	2.47	0.44
1:A:306:HIS:HD2	1:A:310:ILE:O	2.00	0.44
1:B:377:VAL:HG13	1:B:388:PRO:HG3	1.99	0.44
1:A:204:CYS:SG	1:A:215:CYS:HB2	2.57	0.44
1:B:302:LEU:HD22	1:B:306:HIS:CE1	2.51	0.44
1:A:512:PRO:O	1:A:515:TRP:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:LEU:HD11	1:B:528:LEU:O	2.18	0.44
1:A:36:LEU:CD1	1:A:208:ALA:HB1	2.48	0.44
1:B:256:THR:OG1	1:B:257:LYS:N	2.50	0.44
1:A:291:ALA:CB	1:A:383:ILE:HD11	2.47	0.44
1:B:361:LEU:HD13	1:B:402:LYS:HA	1.98	0.44
1:B:384:ALA:O	1:B:385:ALA:HB3	2.18	0.44
1:B:168:PHE:O	1:B:171:PHE:HB3	2.17	0.44
1:B:213:TYR:HB3	1:B:263:VAL:HG13	2.00	0.43
1:B:302:LEU:CD2	1:B:305:LEU:HD12	2.48	0.43
1:A:39:LEU:HD21	1:A:186:TRP:CZ3	2.54	0.43
1:A:75:PHE:CE1	1:A:79:HIS:CE1	3.06	0.43
1:A:168:PHE:O	1:A:171:PHE:HB3	2.18	0.43
1:A:143:PHE:CD2	1:A:146:LEU:HD22	2.54	0.43
1:A:85:ALA:HB1	1:A:154:LEU:HD21	2.00	0.43
1:B:127:ASP:N	1:B:127:ASP:OD1	2.49	0.43
1:B:36:LEU:HD12	1:B:39:LEU:HD12	2.00	0.43
1:B:369:SER:HB2	1:B:435:ARG:HD2	2.00	0.43
1:A:85:ALA:HB2	1:A:125:PHE:CZ	2.54	0.43
1:B:201:VAL:HG22	1:B:216:LYS:HG3	2.01	0.43
1:A:150:VAL:HG22	1:A:154:LEU:CG	2.49	0.43
1:B:339:LEU:HD21	1:B:346:THR:HG22	2.01	0.43
1:B:268:ASN:O	1:B:269:GLY:C	2.57	0.43
1:B:134:ALA:HB1	1:B:143:PHE:HD2	1.84	0.43
1:A:201:VAL:HG22	1:A:216:LYS:HG3	2.01	0.43
1:A:36:LEU:HD13	1:A:208:ALA:C	2.39	0.43
1:B:85:ALA:HB2	1:B:125:PHE:CZ	2.54	0.43
1:A:41:LEU:HD11	1:A:528:LEU:O	2.18	0.43
1:A:213:TYR:CG	1:A:263:VAL:CG1	3.02	0.42
1:B:361:LEU:HD13	1:B:402:LYS:HG3	2.01	0.42
1:A:361:LEU:HD13	1:A:402:LYS:HG3	2.01	0.42
1:A:302:LEU:HD22	1:A:306:HIS:CE1	2.55	0.42
1:B:177:LEU:HD12	1:B:180:GLN:HG3	2.01	0.42
1:B:213:TYR:CG	1:B:263:VAL:CG1	3.01	0.42
1:B:66:PRO:HB2	1:B:520:ILE:CD1	2.49	0.42
1:A:256:THR:OG1	1:A:257:LYS:N	2.50	0.42
1:B:36:LEU:CD1	1:B:208:ALA:HB1	2.50	0.42
1:A:134:ALA:HB1	1:A:143:PHE:HD2	1.83	0.42
1:A:115:LEU:HD23	1:A:131:VAL:HG13	2.02	0.42
1:B:323:ASP:OD1	1:B:327:ASN:N	2.52	0.42
1:A:131:VAL:HG12	1:A:135:ARG:NH2	2.35	0.42
1:A:369:SER:HB2	1:A:435:ARG:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:LEU:HD23	1:A:466:THR:N	2.35	0.41
1:A:291:ALA:HB1	1:A:382:MET:HE3	2.02	0.41
1:A:66:PRO:HB2	1:A:520:ILE:CD1	2.51	0.41
1:B:75:PHE:CE1	1:B:79:HIS:CE1	3.08	0.41
1:A:268:ASN:O	1:A:269:GLY:C	2.58	0.41
1:B:150:VAL:HG22	1:B:154:LEU:CG	2.50	0.41
1:B:36:LEU:HD13	1:B:208:ALA:C	2.40	0.41
1:B:238:ILE:HG21	1:B:310:ILE:HD13	2.01	0.41
1:A:316:LYS:HB2	1:A:317:PRO:CD	2.51	0.41
1:A:291:ALA:HB3	1:A:383:ILE:HD11	2.03	0.41
1:B:66:PRO:HB2	1:B:520:ILE:HD13	2.02	0.41
1:A:127:ASP:N	1:A:127:ASP:OD1	2.53	0.41
1:B:358:PRO:O	1:B:406:LEU:HD21	2.21	0.41
1:A:215:CYS:SG	1:A:261:CYS:HB3	2.61	0.41
1:A:169:LEU:HD11	1:B:44:LEU:CD1	2.51	0.41
1:A:297:GLN:HE22	1:A:327:ASN:HB3	1.85	0.41
1:B:67:ILE:CG1	1:B:520:ILE:HD11	2.51	0.41
1:B:316:LYS:HB2	1:B:317:PRO:CD	2.51	0.40
1:B:449:HIS:CG	1:B:450:PRO:HD2	2.57	0.40
1:B:66:PRO:HA	1:B:69:LYS:HB3	2.04	0.40
1:A:293:PHE:CE1	1:A:465:LEU:HD22	2.56	0.40
1:B:372:TYR:O	1:B:427:LEU:HD22	2.21	0.40
1:A:250:LEU:HD22	1:A:262:LEU:HD13	2.03	0.40
1:A:87:GLN:HA	1:A:90:LYS:HB2	2.03	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	470/543 (87%)	401 (85%)	56 (12%)	13 (3%)	<b>6</b> 44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	456/543 (84%)	394 (86%)	52 (11%)	10 (2%)	8 49
All	All	926/1086 (85%)	795 (86%)	108 (12%)	23 (2%)	7 46

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	117	PRO
1	A	266	ILE
1	A	127	ASP
1	A	257	LYS
1	A	269	GLY
1	B	127	ASP
1	B	257	LYS
1	B	269	GLY
1	A	190	PHE
1	A	332	ASP
1	B	190	PHE
1	B	332	ASP
1	A	436	LEU
1	B	436	LEU
1	A	58	PHE
1	A	413	PRO
1	B	58	PHE
1	B	413	PRO
1	A	450	PRO
1	A	509	GLY
1	B	450	PRO
1	B	509	GLY
1	A	197	GLY

### 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	401/449 (89%)	378 (94%)	23 (6%)	25 62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	395/449 (88%)	374 (95%)	21 (5%)	28	64
All	All	796/898 (89%)	752 (94%)	44 (6%)	27	63

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ARG
1	A	99	ASP
1	A	117	PRO
1	A	120	GLN
1	A	123	CYS
1	A	156	GLN
1	A	163	LEU
1	A	168	PHE
1	A	191	ARG
1	A	206	MET
1	A	223	LEU
1	A	246	PHE
1	A	255	GLU
1	A	274	TYR
1	A	305	LEU
1	A	330	ILE
1	A	333	LEU
1	A	382	MET
1	A	414	ASP
1	A	439	ARG
1	A	444	ASP
1	A	464	MET
1	A	527	ASP
1	B	70	ARG
1	B	120	GLN
1	B	123	CYS
1	B	156	GLN
1	B	163	LEU
1	B	168	PHE
1	B	191	ARG
1	B	206	MET
1	B	223	LEU
1	B	246	PHE
1	B	255	GLU
1	B	274	TYR
1	B	305	LEU

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Mol	Chain	Res	Type
1	B	330	ILE
1	B	333	LEU
1	B	382	MET
1	B	414	ASP
1	B	439	ARG
1	B	444	ASP
1	B	464	MET
1	B	527	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	GLN
1	A	173	GLN
1	A	268	ASN
1	A	278	ASN
1	A	306	HIS
1	B	120	GLN
1	B	173	GLN
1	B	268	ASN
1	B	278	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](#)

There are no ligands in this entry.

## 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	478/543 (88%)	-0.75	1 (0%) 95 94	223, 224, 225, 238	1 (0%)
1	B	466/543 (85%)	-0.72	0 100 100	223, 224, 225, 238	0
All	All	944/1086 (86%)	-0.74	1 (0%) 95 95	223, 224, 225, 238	1 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	472	ASP	2.2

### 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](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.