



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 08:40 am BST

PDB ID : 3H5W
Title : Crystal structure of the GluR2-ATD in space group P212121 without solvent
Authors : Jin, R.; Singh, S.K.; Gu, S.; Furukawa, H.; Sobolevsky, A.; Zhou, J.; Jin, Y.; Gouaux, E.
Deposited on : 2009-04-22
Resolution : 2.69 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

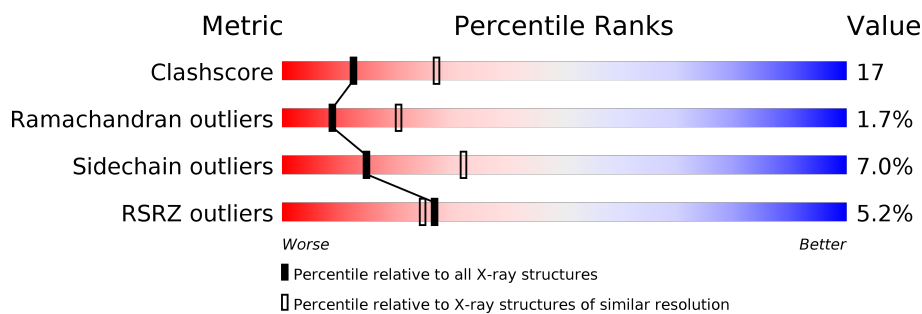
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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 ≥ 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	394	<div> <div>2%</div> <div>63%</div> <div>27%</div> <div>6%</div> </div>
1	B	394	<div> <div>8%</div> <div>66%</div> <div>24%</div> <div>7%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5404 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 Glutamate receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	1	0	0
			2805	1784	472	540	9			
1	B	366	Total	C	N	O	S	0	0	0
			2599	1645	438	508	8			

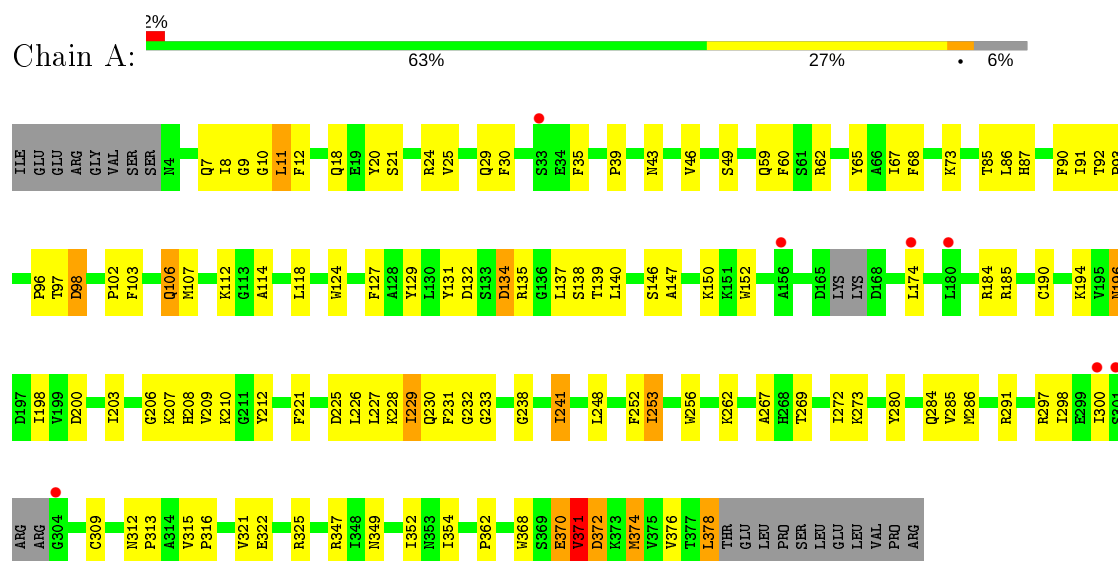
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	ILE	-	EXPRESSION TAG	UNP P19491
A	-3	GLU	-	EXPRESSION TAG	UNP P19491
A	-2	GLU	-	EXPRESSION TAG	UNP P19491
A	-1	ARG	-	EXPRESSION TAG	UNP P19491
A	384	LEU	-	EXPRESSION TAG	UNP P19491
A	385	GLU	-	EXPRESSION TAG	UNP P19491
A	386	LEU	-	EXPRESSION TAG	UNP P19491
A	387	VAL	-	EXPRESSION TAG	UNP P19491
A	388	PRO	-	EXPRESSION TAG	UNP P19491
A	389	ARG	-	EXPRESSION TAG	UNP P19491
B	-4	ILE	-	EXPRESSION TAG	UNP P19491
B	-3	GLU	-	EXPRESSION TAG	UNP P19491
B	-2	GLU	-	EXPRESSION TAG	UNP P19491
B	-1	ARG	-	EXPRESSION TAG	UNP P19491
B	384	LEU	-	EXPRESSION TAG	UNP P19491
B	385	GLU	-	EXPRESSION TAG	UNP P19491
B	386	LEU	-	EXPRESSION TAG	UNP P19491
B	387	VAL	-	EXPRESSION TAG	UNP P19491
B	388	PRO	-	EXPRESSION TAG	UNP P19491
B	389	ARG	-	EXPRESSION TAG	UNP P19491

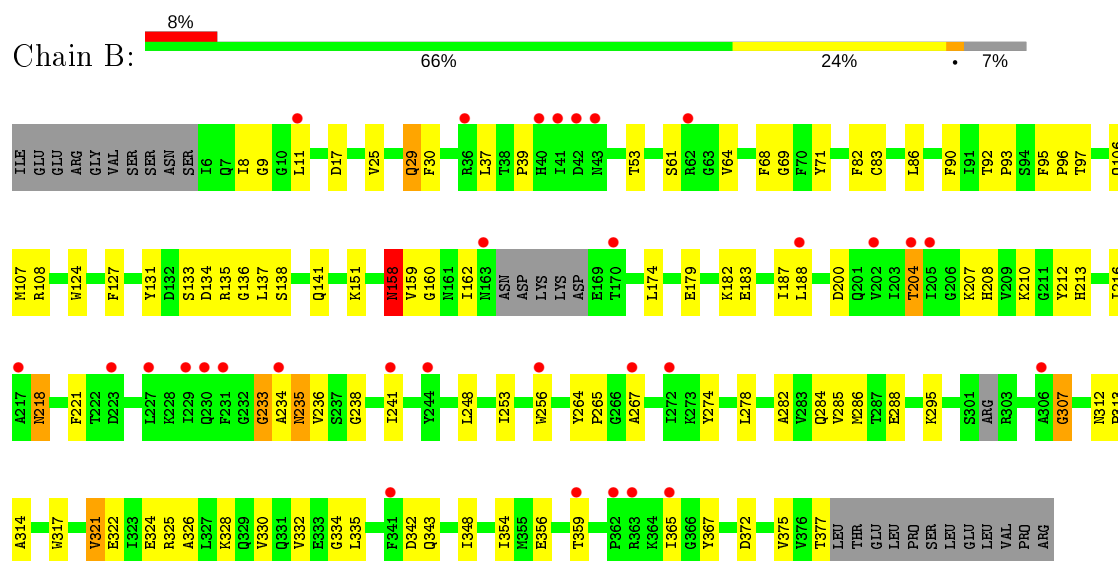
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Glutamate receptor 2



• Molecule 1: Glutamate receptor 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.87Å 96.36Å 108.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.69 48.18 – 2.69	Depositor EDS
% Data completeness (in resolution range)	98.6 (19.96-2.69) 93.3 (48.18-2.69)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.215 , 0.291 0.220 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	71.3	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 79.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5404	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% 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 [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	0.44	0/2860	0.58	0/3878
1	B	0.38	0/2651	0.54	0/3612
All	All	0.41	0/5511	0.56	0/7490

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2805	0	2639	93	0
1	B	2599	0	2254	79	0
All	All	5404	0	4893	172	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 (172) 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:A:230:GLN:HE21	1:A:232:GLY:H	1.01	0.95
1:A:97:THR:HG23	1:A:106:GLN:HE22	1.31	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ILE:CD1	1:A:352:ILE:HG12	2.02	0.89
1:A:35:PHE:HE2	1:A:291:ARG:HG2	1.38	0.89
1:B:282:ALA:O	1:B:286:MET:HG3	1.73	0.88
1:A:35:PHE:CE2	1:A:291:ARG:HG2	2.14	0.82
1:A:97:THR:HG23	1:A:106:GLN:NE2	1.93	0.82
1:A:371:VAL:O	1:A:371:VAL:HG23	1.81	0.80
1:A:210:LYS:HG2	1:A:233:GLY:HA3	1.66	0.77
1:A:230:GLN:NE2	1:A:232:GLY:H	1.80	0.77
1:B:37:LEU:O	1:B:39:PRO:HD3	1.84	0.77
1:A:85:THR:HG22	1:A:86:LEU:HD23	1.65	0.76
1:A:349:ASN:H	1:A:370:GLU:HG2	1.49	0.76
1:B:317:TRP:O	1:B:321:VAL:HG23	1.86	0.76
1:B:83:CYS:SG	1:B:90:PHE:HB2	2.26	0.75
1:A:378:LEU:HD13	1:A:378:LEU:H	1.52	0.74
1:B:210:LYS:HA	1:B:233:GLY:HA2	1.68	0.74
1:A:18:GLN:HE22	1:A:273:LYS:H	1.35	0.74
1:A:241:ILE:HD11	1:A:352:ILE:HG12	1.71	0.73
1:B:9:GLY:H	1:B:64:VAL:HG11	1.53	0.72
1:A:97:THR:H	1:A:106:GLN:NE2	1.87	0.72
1:B:356:GLU:HG3	1:B:365:ILE:HG12	1.71	0.72
1:B:221:PHE:CD1	1:B:238:GLY:HA3	2.25	0.71
1:A:262:LYS:HE2	1:A:262:LYS:HA	1.72	0.71
1:A:96:PRO:HA	1:A:106:GLN:HE21	1.56	0.70
1:B:307:GLY:H	1:B:312:ASN:HD22	1.40	0.70
1:A:73:LYS:HD3	1:A:134:ASP:HA	1.73	0.70
1:A:230:GLN:HE21	1:A:232:GLY:N	1.85	0.67
1:A:229:ILE:HG12	1:A:231:PHE:CE2	2.29	0.67
1:A:65:TYR:CE1	1:A:300:ILE:HB	2.30	0.67
1:B:8:ILE:HA	1:B:64:VAL:HG13	1.77	0.67
1:B:8:ILE:O	1:B:8:ILE:HG13	1.96	0.65
1:B:218:ASN:HD22	1:B:218:ASN:C	2.00	0.64
1:B:234:ALA:O	1:B:236:VAL:HG23	1.98	0.63
1:B:354:ILE:O	1:B:365:ILE:HG13	1.99	0.63
1:A:207:LYS:HB3	1:A:208:HIS:HA	1.81	0.60
1:B:317:TRP:CZ3	1:B:321:VAL:HG21	2.37	0.60
1:B:288:GLU:HG3	1:B:332:VAL:HG11	1.84	0.59
1:A:112:LYS:HE2	1:A:138:SER:OG	2.03	0.59
1:B:367:TYR:CZ	1:B:375:VAL:HG21	2.40	0.57
1:B:8:ILE:O	1:B:39:PRO:HA	2.05	0.56
1:A:241:ILE:HD12	1:A:352:ILE:HG12	1.87	0.56
1:A:371:VAL:CG2	1:A:371:VAL:O	2.53	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:MET:HE1	1:B:285:VAL:HG11	1.88	0.56
1:A:107:MET:HE1	1:A:285:VAL:HG11	1.88	0.55
1:A:349:ASN:N	1:A:370:GLU:HG2	2.21	0.55
1:B:218:ASN:ND2	1:B:218:ASN:C	2.59	0.55
1:B:9:GLY:H	1:B:64:VAL:CG1	2.19	0.55
1:A:11:LEU:HD22	1:A:67:ILE:HG21	1.89	0.55
1:A:368:TRP:CZ2	1:A:372:ASP:HA	2.41	0.55
1:A:8:ILE:O	1:A:39:PRO:HA	2.06	0.55
1:A:184:ARG:HA	1:A:212:TYR:CD2	2.43	0.53
1:A:9:GLY:HA3	1:A:59:GLN:OE1	2.09	0.53
1:A:229:ILE:HG12	1:A:231:PHE:CZ	2.44	0.53
1:A:12:PHE:O	1:A:43:ASN:HA	2.09	0.53
1:A:226:LEU:O	1:A:229:ILE:HG23	2.09	0.53
1:A:112:LYS:CE	1:A:138:SER:HB3	2.39	0.52
1:B:131:TYR:CG	1:B:158:ASN:HA	2.43	0.52
1:B:307:GLY:HA3	1:B:312:ASN:ND2	2.25	0.52
1:B:317:TRP:CE3	1:B:321:VAL:HG21	2.44	0.52
1:A:206:GLY:C	1:A:207:LYS:HG2	2.30	0.52
1:A:86:LEU:O	1:A:87:HIS:HB2	2.09	0.52
1:A:7:GLN:O	1:A:65:TYR:HD2	1.92	0.52
1:A:118:LEU:HA	1:A:374:MET:HE1	1.92	0.52
1:B:210:LYS:HA	1:B:233:GLY:CA	2.39	0.52
1:A:132:ASP:HB2	1:A:190:CYS:HA	1.91	0.52
1:A:97:THR:H	1:A:106:GLN:HE21	1.57	0.52
1:A:221:PHE:CD1	1:A:238:GLY:HA3	2.46	0.51
1:B:96:PRO:HD3	1:B:108:ARG:HD2	1.92	0.51
1:B:86:LEU:HA	1:B:314:ALA:CB	2.41	0.51
1:A:196:ASN:C	1:A:196:ASN:HD22	2.14	0.51
1:B:107:MET:HE1	1:B:285:VAL:CB	2.41	0.51
1:A:252:PHE:HD2	1:A:253:ILE:HD12	1.76	0.51
1:A:21:SER:O	1:A:25:VAL:HG23	2.11	0.50
1:A:112:LYS:HE2	1:A:138:SER:CB	2.42	0.50
1:A:124:TRP:HA	1:A:185:ARG:NH1	2.26	0.50
1:A:147:ALA:HA	1:A:152:TRP:HB2	1.94	0.50
1:B:29:GLN:O	1:B:29:GLN:OE1	2.29	0.50
1:B:321:VAL:O	1:B:325:ARG:HB2	2.12	0.50
1:A:87:HIS:CG	1:A:316:PRO:HB3	2.47	0.49
1:B:179:GLU:OE2	1:B:179:GLU:HA	2.12	0.49
1:B:183:GLU:HG3	1:B:183:GLU:O	2.11	0.49
1:A:370:GLU:C	1:A:372:ASP:H	2.16	0.49
1:A:90:PHE:CE2	1:A:92:THR:HB	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ASP:CG	1:A:138:SER:HB2	2.34	0.48
1:B:97:THR:H	1:B:106:GLN:NE2	2.12	0.48
1:B:86:LEU:HA	1:B:314:ALA:HB2	1.96	0.48
1:A:368:TRP:CZ3	1:A:370:GLU:HA	2.48	0.48
1:B:210:LYS:C	1:B:212:TYR:H	2.16	0.48
1:B:342:ASP:HB3	1:B:348:ILE:HD13	1.95	0.48
1:B:274:TYR:O	1:B:278:LEU:HG	2.13	0.48
1:B:107:MET:HE1	1:B:285:VAL:CG1	2.44	0.47
1:B:179:GLU:OE2	1:B:182:LYS:HA	2.13	0.47
1:A:8:ILE:HD12	1:A:286:MET:CE	2.44	0.47
1:B:158:ASN:C	1:B:160:GLY:H	2.18	0.47
1:A:267:ALA:O	1:A:269:THR:HG23	2.14	0.47
1:A:312:ASN:HA	1:A:313:PRO:C	2.33	0.47
1:B:354:ILE:CG2	1:B:365:ILE:HD11	2.44	0.47
1:A:114:ALA:HA	1:A:368:TRP:CD1	2.49	0.47
1:B:200:ASP:O	1:B:204:THR:HG22	2.14	0.47
1:B:107:MET:HE1	1:B:285:VAL:HB	1.97	0.47
1:B:90:PHE:CE2	1:B:92:THR:HB	2.50	0.47
1:A:30:PHE:CZ	1:A:284:GLN:HB2	2.50	0.46
1:B:68:PHE:CD2	1:B:68:PHE:C	2.88	0.46
1:A:129:TYR:CE1	1:A:131:TYR:HB3	2.50	0.46
1:A:229:ILE:HG13	1:A:230:GLN:N	2.28	0.46
1:A:10:GLY:HA2	1:A:68:PHE:O	2.15	0.46
1:A:209:VAL:HG23	1:A:210:LYS:N	2.30	0.46
1:A:98:ASP:OD2	1:A:138:SER:HB2	2.15	0.46
1:A:67:ILE:O	1:A:90:PHE:HA	2.16	0.46
1:A:8:ILE:HD12	1:A:286:MET:HE1	1.98	0.46
1:A:207:LYS:CB	1:A:208:HIS:HA	2.44	0.45
1:B:354:ILE:HD12	1:B:354:ILE:N	2.31	0.45
1:A:225:ASP:O	1:A:228:LYS:HB2	2.16	0.45
1:A:253:ILE:HA	1:A:256:TRP:HB3	1.98	0.45
1:B:90:PHE:HE2	1:B:92:THR:HB	1.81	0.45
1:A:20:TYR:CE2	1:A:24:ARG:HD2	2.52	0.45
1:B:158:ASN:O	1:B:160:GLY:N	2.42	0.45
1:A:298:ILE:HD13	1:A:322:GLU:HG2	1.97	0.45
1:B:241:ILE:HG13	1:B:241:ILE:O	2.17	0.45
1:A:91:ILE:HG23	1:A:107:MET:HE2	1.99	0.44
1:B:187:ILE:C	1:B:188:LEU:HD12	2.38	0.44
1:B:208:HIS:O	1:B:212:TYR:CE2	2.70	0.44
1:B:317:TRP:O	1:B:321:VAL:CG2	2.63	0.44
1:A:106:GLN:O	1:A:347:ARG:HG2	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:PHE:HA	1:B:96:PRO:HD3	1.85	0.44
1:A:127:PHE:HB2	1:A:185:ARG:O	2.18	0.44
1:A:227:LEU:CD1	1:A:362:PRO:HG3	2.47	0.44
1:B:216:ILE:HD12	1:B:216:ILE:N	2.33	0.44
1:B:248:LEU:HD13	1:B:334:GLY:O	2.17	0.44
1:B:17:ASP:HB3	1:B:265:PRO:HB2	2.00	0.43
1:A:29:GLN:HG2	1:A:280:TYR:OH	2.19	0.43
1:B:264:TYR:O	1:B:267:ALA:HB3	2.19	0.43
1:B:295:LYS:HE3	1:B:295:LYS:HB2	1.70	0.43
1:A:146:SER:HB3	1:A:150:LYS:HE3	2.01	0.43
1:A:112:LYS:HD3	1:A:139:THR:HA	2.01	0.43
1:A:194:LYS:O	1:A:198:ILE:HG13	2.19	0.43
1:A:9:GLY:CA	1:A:59:GLN:OE1	2.67	0.42
1:A:62:ARG:HA	1:A:62:ARG:HD3	1.74	0.42
1:B:312:ASN:HB3	1:B:313:PRO:CD	2.48	0.42
1:A:112:LYS:HE3	1:A:138:SER:HB3	2.00	0.42
1:A:196:ASN:O	1:A:200:ASP:HB2	2.18	0.42
1:B:68:PHE:CD2	1:B:69:GLY:N	2.86	0.42
1:B:188:LEU:HD12	1:B:188:LEU:N	2.34	0.42
1:B:96:PRO:HG3	1:B:108:ARG:O	2.20	0.42
1:B:133:SER:HA	1:B:137:LEU:HD21	2.01	0.42
1:B:207:LYS:HA	1:B:208:HIS:HA	1.57	0.42
1:B:210:LYS:CA	1:B:233:GLY:HA2	2.42	0.42
1:A:92:THR:HA	1:A:93:PRO:HD3	1.84	0.42
1:B:375:VAL:O	1:B:375:VAL:HG23	2.20	0.42
1:B:30:PHE:CZ	1:B:284:GLN:HB2	2.55	0.42
1:A:102:PRO:O	1:A:103:PHE:HB2	2.20	0.42
1:B:326:ALA:O	1:B:330:VAL:HG23	2.20	0.42
1:A:96:PRO:HA	1:A:106:GLN:NE2	2.30	0.41
1:B:133:SER:HB3	1:B:137:LEU:HD11	2.01	0.41
1:B:213:HIS:HA	1:B:235:ASN:HB3	2.01	0.41
1:A:96:PRO:HA	1:A:106:GLN:HG2	2.02	0.41
1:A:256:TRP:CZ2	1:A:267:ALA:HA	2.56	0.41
1:A:354:ILE:HD11	1:A:368:TRP:HB2	2.01	0.41
1:A:60:PHE:CD2	1:A:309:CYS:HB3	2.56	0.41
1:B:124:TRP:HB3	1:B:127:PHE:HD2	1.86	0.41
1:B:324:GLU:HG2	1:B:328:LYS:HD2	2.03	0.41
1:B:53:THR:HG23	1:B:82:PHE:CZ	2.56	0.41
1:B:92:THR:HA	1:B:93:PRO:HD3	1.77	0.41
1:B:138:SER:HA	1:B:141:GLN:HG3	2.03	0.40
1:B:25:VAL:HG21	1:B:256:TRP:HZ3	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:LEU:HD13	1:A:140:LEU:HD22	2.02	0.40
1:A:321:VAL:O	1:A:325:ARG:HB2	2.21	0.40
1:B:248:LEU:HD22	1:B:335:LEU:HD23	2.03	0.40
1:A:325:ARG:HH11	1:A:325:ARG:HG3	1.87	0.40
1:B:133:SER:HA	1:B:134:ASP:CB	2.50	0.40
1:B:307:GLY:N	1:B:312:ASN:HD22	2.13	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	365/394 (93%)	335 (92%)	27 (7%)	3 (1%)	19	40
1	B	360/394 (91%)	308 (86%)	43 (12%)	9 (2%)	5	12
All	All	725/788 (92%)	643 (89%)	70 (10%)	12 (2%)	9	20

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	159	VAL
1	B	151	LYS
1	B	235	ASN
1	A	174	LEU
1	B	158	ASN
1	B	162	ILE
1	B	174	LEU
1	A	371	VAL
1	B	307	GLY
1	B	136	GLY
1	A	203	ILE
1	B	233	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	284/342 (83%)	263 (93%)	21 (7%)	13	29
1	B	233/342 (68%)	218 (94%)	15 (6%)	17	36
All	All	517/684 (76%)	481 (93%)	36 (7%)	15	32

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	46	VAL
1	A	49	SER
1	A	98	ASP
1	A	106	GLN
1	A	134	ASP
1	A	135	ARG
1	A	196	ASN
1	A	229	ILE
1	A	241	ILE
1	A	248	LEU
1	A	253	ILE
1	A	272	ILE
1	A	297	ARG
1	A	315	VAL
1	A	370	GLU
1	A	371	VAL
1	A	372	ASP
1	A	374	MET
1	A	376	VAL
1	A	378	LEU
1	B	11	LEU
1	B	29	GLN
1	B	61	SER
1	B	71	TYR
1	B	135	ARG
1	B	158	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	204	THR
1	B	218	ASN
1	B	253	ILE
1	B	321	VAL
1	B	322	GLU
1	B	343	GLN
1	B	359	THR
1	B	372	ASP
1	B	377	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	101	HIS
1	A	106	GLN
1	A	196	ASN
1	A	230	GLN
1	A	292	ASN
1	A	296	GLN
1	A	319	GLN
1	B	18	GLN
1	B	106	GLN
1	B	141	GLN
1	B	218	ASN
1	B	240	GLN
1	B	292	ASN
1	B	312	ASN
1	B	319	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 [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, 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	371/394 (94%)	0.04	7 (1%) 66 67	43, 76, 149, 195	1 (0%)
1	B	366/394 (92%)	0.44	31 (8%) 10 8	52, 104, 177, 247	0
All	All	737/788 (93%)	0.24	38 (5%) 27 25	43, 88, 170, 247	1 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	205	ILE	6.0
1	B	267	ALA	5.9
1	B	231	PHE	5.1
1	B	306	ALA	4.9
1	A	304	GLY	4.9
1	B	43	ASN	4.6
1	A	301	SER	4.5
1	B	227	LEU	4.2
1	B	230	GLN	3.7
1	B	229	ILE	3.7
1	B	170	THR	3.5
1	B	244	TYR	3.4
1	B	362	PRO	3.3
1	B	42	ASP	3.2
1	B	202	VAL	3.1
1	B	11	LEU	3.0
1	B	241	ILE	2.9
1	A	300	ILE	2.8
1	B	40	HIS	2.8
1	B	272	ILE	2.8
1	B	204	THR	2.7
1	B	36	ARG	2.7
1	A	156	ALA	2.7
1	B	256	TRP	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	62	ARG	2.6
1	A	180	LEU	2.6
1	B	365	ILE	2.5
1	B	359	THR	2.5
1	B	41	ILE	2.4
1	B	341	PHE	2.4
1	B	217	ALA	2.3
1	B	223	ASP	2.3
1	B	188	LEU	2.2
1	B	234	ALA	2.1
1	A	174	LEU	2.1
1	B	363	ARG	2.1
1	B	163	ASN	2.0
1	A	33	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.