



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 06:48 pm BST

PDB ID : 5L2E  
Title : Crystal structure of rat Glutamate receptor delta-2 extracellular domain  
Authors : Cheng, S.; Ozkan, E.  
Deposited on : 2016-08-01  
Resolution : 4.15 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

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

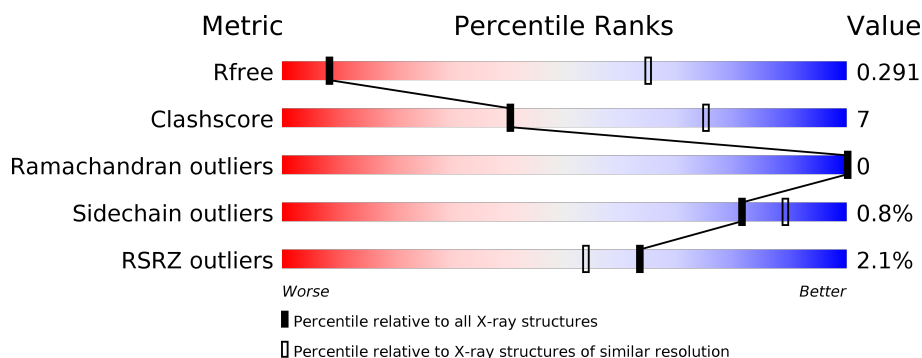
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.15 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))
$R_{free}$	130704	1020 (4.54-3.76)
Clashscore	141614	1028 (4.52-3.80)
Ramachandran outliers	138981	1005 (4.54-3.78)
Sidechain outliers	138945	1024 (4.54-3.76)
RSRZ outliers	127900	1055 (4.62-3.70)

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 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	688	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>19%</div> <div>6%</div> </div> </div>
1	B	688	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>6%</div> </div> </div>
1	C	688	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>6%</div> </div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15408 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 ionotropic, delta-2, Glutamate receptor ionotropic, delta-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	648	Total	C	N	O	S	0	0	0
			5136	3248	889	973	26			
1	B	648	Total	C	N	O	S	0	0	0
			5136	3248	889	973	26			
1	C	648	Total	C	N	O	S	0	0	0
			5136	3248	889	973	26			

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	GLY	-	expression tag	UNP Q63226
A	23	SER	-	expression tag	UNP Q63226
A	343	GLN	GLU	conflict	UNP Q63226
A	662	GLY	-	linker	UNP Q63226
A	663	THR	-	linker	UNP Q63226
A	814	HIS	-	expression tag	UNP Q63226
A	815	HIS	-	expression tag	UNP Q63226
A	816	HIS	-	expression tag	UNP Q63226
A	817	HIS	-	expression tag	UNP Q63226
A	818	HIS	-	expression tag	UNP Q63226
A	819	HIS	-	expression tag	UNP Q63226
B	22	GLY	-	expression tag	UNP Q63226
B	23	SER	-	expression tag	UNP Q63226
B	343	GLN	GLU	conflict	UNP Q63226
B	662	GLY	-	linker	UNP Q63226
B	663	THR	-	linker	UNP Q63226
B	814	HIS	-	expression tag	UNP Q63226
B	815	HIS	-	expression tag	UNP Q63226
B	816	HIS	-	expression tag	UNP Q63226
B	817	HIS	-	expression tag	UNP Q63226
B	818	HIS	-	expression tag	UNP Q63226
B	819	HIS	-	expression tag	UNP Q63226

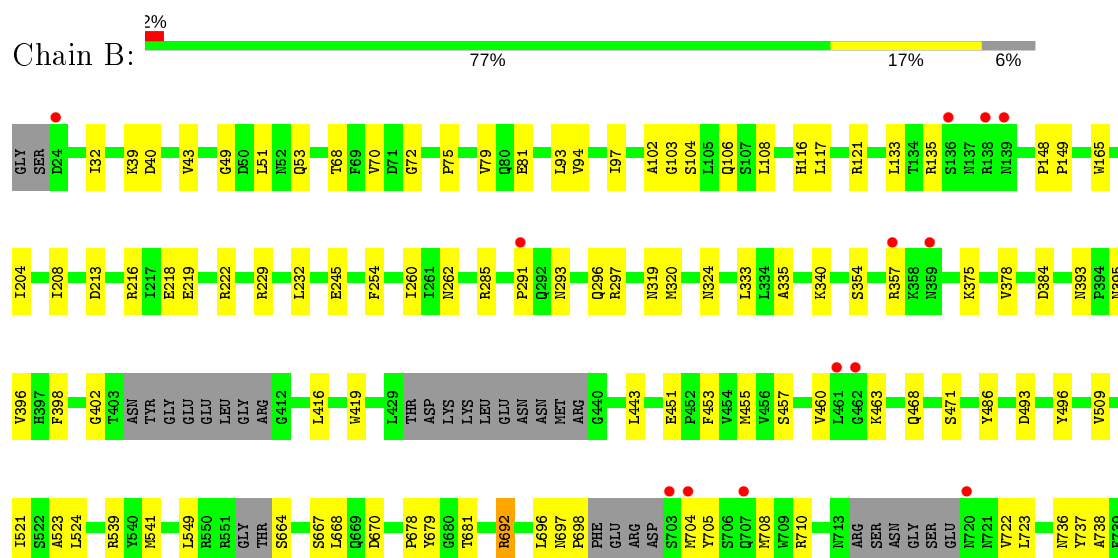
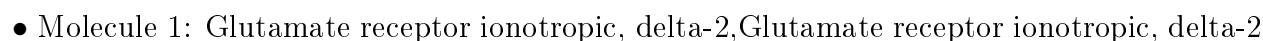
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Chain	Residue	Modelled	Actual	Comment	Reference
C	22	GLY	-	expression tag	UNP Q63226
C	23	SER	-	expression tag	UNP Q63226
C	343	GLN	GLU	conflict	UNP Q63226
C	662	GLY	-	linker	UNP Q63226
C	663	THR	-	linker	UNP Q63226
C	814	HIS	-	expression tag	UNP Q63226
C	815	HIS	-	expression tag	UNP Q63226
C	816	HIS	-	expression tag	UNP Q63226
C	817	HIS	-	expression tag	UNP Q63226
C	818	HIS	-	expression tag	UNP Q63226
C	819	HIS	-	expression tag	UNP Q63226

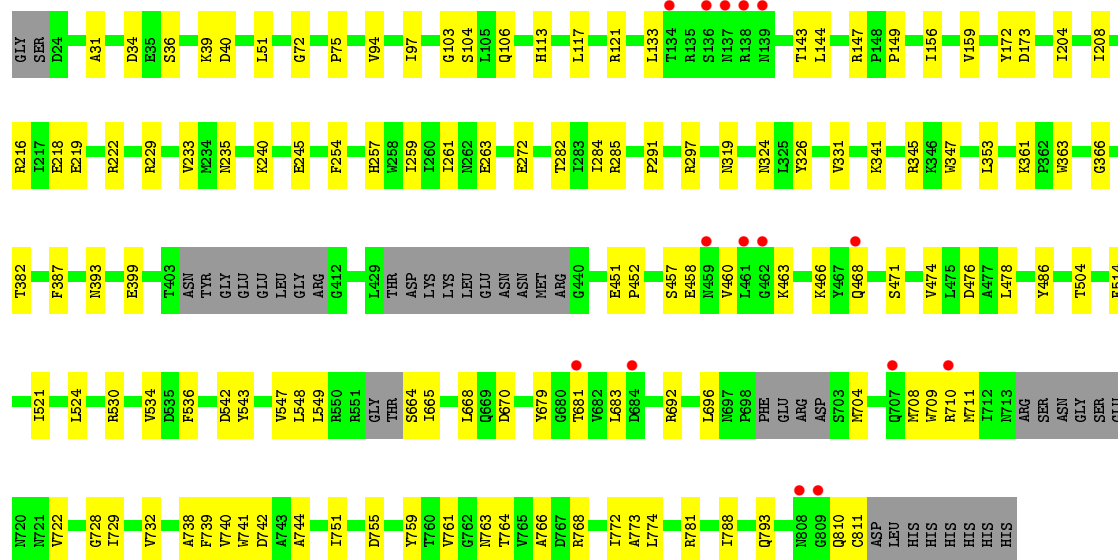
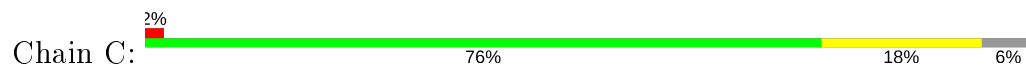


- Molecule 1: Glutamate receptor ionotropic, delta-2, Glutamate receptor ionotropic, delta-2





- Molecule 1: Glutamate receptor ionotropic, delta-2, Glutamate receptor ionotropic, delta-2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	179.17Å 179.17Å 214.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.58 – 4.15 46.58 – 4.15	Depositor EDS
% Data completeness (in resolution range)	98.5 (46.58-4.15) 98.5 (46.58-4.15)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.26 (at 4.14Å)	Xtriage
Refinement program	PHENIX (dev_2481: ???)	Depositor
R, $R_{free}$	0.211 , 0.260 0.241 , 0.291	Depositor DCC
$R_{free}$ test set	1973 reflections (6.55%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.0	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 18.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.378 for -h,-k,l	Xtriage
Reported twinning fraction	0.490 for -h,-k,l	Depositor
Outliers	0 of 30109 reflections	Xtriage
$F_o, F_c$ correlation	0.78	EDS
Total number of atoms	15408	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.17% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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	0.28	0/5235	0.46	0/7090
1	B	0.26	0/5235	0.45	0/7090
1	C	0.26	0/5235	0.45	0/7090
All	All	0.27	0/15705	0.45	0/21270

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

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	5136	0	5057	81	0
1	B	5136	0	5057	68	1
1	C	5136	0	5057	73	1
All	All	15408	0	15171	220	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (220) 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:C:458:GLU:HB2	1:C:466:LYS:HB2	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ASP:O	1:A:395:ASN:ND2	2.21	0.74
1:C:103:GLY:HA2	1:C:133:LEU:HD21	1.69	0.74
1:B:40:ASP:OD1	1:B:324:ASN:ND2	2.22	0.72
1:C:39:LYS:NZ	1:C:319:ASN:O	2.22	0.72
1:A:664:SER:N	1:A:759:TYR:HH	1.87	0.71
1:B:471:SER:HB3	1:B:521:ILE:HG22	1.71	0.71
1:B:103:GLY:HA2	1:B:133:LEU:HD21	1.73	0.71
1:C:476:ASP:OD1	1:C:486:TYR:OH	2.08	0.71
1:A:539:ARG:NH1	1:A:542:ASP:OD1	2.23	0.70
1:B:679:TYR:HB3	1:B:738:ALA:HB3	1.74	0.70
1:A:729:ILE:HD12	1:A:749:VAL:HG11	1.73	0.69
1:C:471:SER:HB3	1:C:521:ILE:HG22	1.72	0.69
1:C:353:LEU:HD11	1:C:363:TRP:HB2	1.77	0.67
1:A:504:THR:HB	1:A:514:PHE:HZ	1.59	0.67
1:C:208:ILE:HD12	1:C:245:GLU:HG3	1.75	0.67
1:B:681:THR:HB	1:B:740:VAL:HB	1.76	0.66
1:B:72:GLY:HA2	1:B:97:ILE:HD11	1.77	0.66
1:A:681:THR:HB	1:A:740:VAL:HB	1.77	0.65
1:A:681:THR:O	1:A:722:VAL:HG13	1.97	0.65
1:A:117:LEU:HD13	1:A:144:LEU:HB2	1.78	0.64
1:A:39:LYS:NZ	1:A:319:ASN:O	2.30	0.64
1:A:225:ASP:OD1	1:A:228:ARG:NH1	2.31	0.63
1:A:103:GLY:HA2	1:A:133:LEU:HD21	1.80	0.63
1:A:208:ILE:HD12	1:A:245:GLU:HG3	1.81	0.63
1:C:36:SER:O	1:C:121:ARG:NH2	2.32	0.62
1:C:549:LEU:HD21	1:C:761:VAL:HG22	1.81	0.62
1:A:36:SER:O	1:A:121:ARG:NH2	2.33	0.62
1:C:94:VAL:HG22	1:C:117:LEU:HB2	1.82	0.62
1:C:692:ARG:HE	1:C:696:LEU:HD11	1.63	0.62
1:C:665:ILE:HG23	1:C:670:ASP:HB2	1.81	0.61
1:B:208:ILE:HD12	1:B:245:GLU:HG3	1.83	0.61
1:A:341:LYS:HG2	1:A:347:TRP:HA	1.82	0.61
1:A:291:PRO:O	1:A:297:ARG:NE	2.34	0.60
1:C:664:SER:N	1:C:759:TYR:HH	1.99	0.60
1:B:681:THR:O	1:B:722:VAL:HG13	2.02	0.60
1:A:218:GLU:HG2	1:A:222:ARG:HH22	1.67	0.59
1:C:681:THR:O	1:C:722:VAL:HG13	2.02	0.59
1:B:68:THR:HG21	1:B:81:GLU:HB3	1.84	0.59
1:A:692:ARG:NH2	1:A:696:LEU:HD11	2.19	0.58
1:A:204:ILE:HG22	1:A:245:GLU:HG2	1.84	0.58
1:A:243:ILE:HD11	1:A:260:ILE:HD11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ASP:OD2	1:B:121:ARG:NH1	2.34	0.57
1:C:681:THR:HB	1:C:740:VAL:HB	1.86	0.57
1:B:384:ASP:O	1:B:395:ASN:ND2	2.30	0.57
1:C:291:PRO:O	1:C:297:ARG:NE	2.36	0.57
1:A:181:ILE:HD11	1:A:197:LEU:HD21	1.87	0.57
1:B:165:TRP:CE2	1:B:229:ARG:HD3	2.40	0.56
1:C:173:ASP:OD2	1:C:235:ASN:ND2	2.32	0.56
1:C:679:TYR:H	1:C:711:MET:HE2	1.69	0.56
1:A:451:GLU:HG2	1:A:455:MET:HG2	1.86	0.56
1:A:682:VAL:HA	1:A:723:LEU:O	2.05	0.56
1:B:291:PRO:O	1:B:297:ARG:NE	2.38	0.56
1:A:664:SER:N	1:A:759:TYR:OH	2.39	0.56
1:C:460:VAL:HB	1:C:463:LYS:HD2	1.87	0.55
1:C:156:ILE:HD13	1:C:261:ILE:HG21	1.88	0.55
1:C:285:ARG:NE	1:C:399:GLU:OE2	2.33	0.55
1:B:705:TYR:HA	1:B:708:MET:HB2	1.89	0.55
1:A:353:LEU:HD11	1:A:363:TRP:HB2	1.89	0.54
1:B:354:SER:HB3	1:B:357:ARG:HG3	1.88	0.54
1:C:106:GLN:HG2	1:C:143:THR:HG21	1.89	0.54
1:A:72:GLY:HA2	1:A:97:ILE:HD11	1.89	0.53
1:B:254:PHE:O	1:B:793:GLN:HG2	2.07	0.53
1:C:457:SER:HB3	1:C:468:GLN:HG2	1.89	0.53
1:C:72:GLY:HA2	1:C:97:ILE:HD11	1.89	0.53
1:B:667:SER:OG	1:B:670:ASP:OD1	2.22	0.53
1:B:216:ARG:HG3	1:B:219:GLU:H	1.74	0.53
1:B:218:GLU:HG2	1:B:222:ARG:HH22	1.74	0.52
1:A:285:ARG:NE	1:A:399:GLU:OE2	2.30	0.52
1:B:664:SER:N	1:B:759:TYR:HH	2.08	0.52
1:A:402:GLY:HA3	1:A:416:LEU:HD11	1.91	0.52
1:B:204:ILE:HG22	1:B:245:GLU:HG2	1.92	0.52
1:C:144:LEU:HB3	1:C:387:PHE:CE1	2.46	0.51
1:B:39:LYS:NZ	1:B:319:ASN:O	2.43	0.51
1:C:751:ILE:HG23	1:C:810:GLN:HB3	1.92	0.51
1:B:457:SER:HB3	1:B:468:GLN:HG2	1.92	0.51
1:C:548:LEU:HD22	1:C:729:ILE:HD13	1.94	0.50
1:B:402:GLY:HA3	1:B:416:LEU:HD11	1.92	0.50
1:A:527:THR:O	1:A:531:GLU:HG3	2.11	0.50
1:A:692:ARG:HG3	1:A:709:TRP:CZ2	2.47	0.50
1:C:34:ASP:HB2	1:C:97:ILE:HG13	1.93	0.50
1:C:40:ASP:OD2	1:C:121:ARG:NH1	2.39	0.50
1:C:341:LYS:HG2	1:C:347:TRP:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:LEU:HD21	1:A:530:ARG:HD3	1.93	0.49
1:C:259:ILE:HG12	1:C:282:THR:HB	1.94	0.49
1:A:476:ASP:OD1	1:A:486:TYR:OH	2.27	0.49
1:B:51:LEU:HD13	1:B:335:ALA:HB2	1.94	0.49
1:C:218:GLU:HG2	1:C:222:ARG:HH22	1.76	0.49
1:A:267:ASP:OD1	1:A:285:ARG:NH2	2.45	0.48
1:B:451:GLU:HG2	1:B:455:MET:HG2	1.94	0.48
1:A:260:ILE:HG13	1:A:281:LEU:HD11	1.94	0.48
1:B:149:PRO:HD3	1:B:393:ASN:O	2.13	0.48
1:C:31:ALA:HA	1:C:94:VAL:O	2.13	0.48
1:B:493:ASP:N	1:B:493:ASP:OD1	2.39	0.48
1:B:293:ASN:HB2	1:B:296:GLN:HG2	1.95	0.48
1:A:262:ASN:HB3	1:A:265:ILE:HD11	1.96	0.48
1:A:263:GLU:HG2	1:A:398:PHE:HE1	1.79	0.48
1:A:730:GLN:HE21	1:A:734:TYR:HD2	1.61	0.48
1:B:692:ARG:NH1	1:B:696:LEU:HD22	2.28	0.48
1:B:697:ASN:OD1	1:B:698:PRO:HD2	2.12	0.48
1:B:471:SER:HB3	1:B:521:ILE:CG2	2.43	0.47
1:A:173:ASP:OD2	1:A:235:ASN:ND2	2.42	0.47
1:A:543:TYR:H	1:A:769:GLY:HA2	1.79	0.47
1:B:333:LEU:HA	1:B:378:VAL:HG11	1.97	0.47
1:C:240:LYS:HD3	1:C:272:GLU:HG2	1.95	0.47
1:C:149:PRO:HD3	1:C:393:ASN:O	2.15	0.47
1:C:40:ASP:OD1	1:C:324:ASN:ND2	2.47	0.47
1:C:683:LEU:HD13	1:C:722:VAL:HG11	1.97	0.47
1:A:471:SER:HB3	1:A:521:ILE:HG22	1.97	0.46
1:B:453:PHE:CD1	1:B:523:ALA:HB2	2.50	0.46
1:B:692:ARG:HH11	1:B:696:LEU:HD22	1.80	0.46
1:A:697:ASN:OD1	1:A:698:PRO:HD2	2.15	0.46
1:B:460:VAL:HB	1:B:463:LYS:HD2	1.97	0.46
1:B:539:ARG:HA	1:B:770:TYR:O	2.15	0.46
1:A:493:ASP:N	1:A:493:ASP:OD1	2.37	0.46
1:A:457:SER:HB3	1:A:468:GLN:HG2	1.97	0.46
1:C:254:PHE:CE2	1:C:793:GLN:HG3	2.51	0.46
1:A:742:ASP:OD2	1:A:770:TYR:OH	2.30	0.46
1:B:104:SER:HA	1:C:75:PRO:HG2	1.98	0.46
1:A:679:TYR:H	1:A:711:MET:HE2	1.80	0.46
1:B:49:GLY:O	1:B:53:GLN:HG2	2.15	0.46
1:C:204:ILE:HG22	1:C:245:GLU:HG2	1.97	0.46
1:C:457:SER:HB3	1:C:468:GLN:CG	2.46	0.46
1:A:317:ALA:HA	1:A:320:MET:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:ARG:HG3	1:C:219:GLU:H	1.79	0.46
1:C:474:VAL:O	1:C:478:LEU:HG	2.16	0.46
1:B:75:PRO:HG2	1:C:104:SER:HA	1.98	0.45
1:A:165:TRP:CE2	1:A:229:ARG:HD3	2.52	0.45
1:C:692:ARG:NE	1:C:696:LEU:HD11	2.30	0.45
1:B:340:LYS:HE2	1:B:375:LYS:NZ	2.31	0.45
1:B:796:ASP:HA	1:B:799:ILE:HD12	1.98	0.45
1:A:254:PHE:CE2	1:A:793:GLN:HG3	2.52	0.45
1:A:504:THR:HB	1:A:514:PHE:CZ	2.47	0.45
1:A:679:TYR:HB3	1:A:738:ALA:HB3	1.99	0.45
1:A:474:VAL:O	1:A:478:LEU:HG	2.16	0.45
1:B:802:HIS:NE2	1:B:808:ASN:OD1	2.43	0.44
1:C:543:TYR:HD2	1:C:768:ARG:HG3	1.81	0.44
1:A:741:TRP:CG	1:A:742:ASP:N	2.86	0.44
1:C:113:HIS:O	1:C:366:GLY:HA3	2.16	0.44
1:B:398:PHE:O	1:B:419:TRP:N	2.40	0.44
1:A:386:GLU:HG2	1:A:395:ASN:HD21	1.82	0.44
1:B:218:GLU:HG2	1:B:222:ARG:NH2	2.32	0.44
1:A:326:TYR:CD1	1:A:382:THR:HG21	2.53	0.44
1:B:32:ILE:HD13	1:B:68:THR:HB	2.00	0.44
1:B:254:PHE:CE2	1:B:793:GLN:HG3	2.52	0.44
1:B:93:LEU:O	1:B:116:HIS:HA	2.18	0.44
1:C:679:TYR:HB3	1:C:738:ALA:HB3	2.00	0.44
1:B:541:MET:HB3	1:B:770:TYR:HD2	1.81	0.44
1:C:665:ILE:HG22	1:C:761:VAL:HG21	1.99	0.44
1:A:133:LEU:HD23	1:A:135:ARG:HB2	1.99	0.44
1:A:293:ASN:HB2	1:A:296:GLN:HG2	2.00	0.43
1:A:672:SER:HB3	1:A:708:MET:HG3	2.01	0.43
1:B:723:LEU:HD21	1:B:737:TYR:CE2	2.53	0.43
1:C:451:GLU:HA	1:C:452:PRO:HA	1.82	0.43
1:C:810:GLN:O	1:C:811:CYS:HB2	2.17	0.43
1:C:326:TYR:CD1	1:C:382:THR:HG21	2.53	0.43
1:C:728:GLY:O	1:C:732:VAL:HG23	2.18	0.43
1:A:682:VAL:O	1:A:688:TYR:HB2	2.18	0.43
1:B:668:LEU:HD23	1:B:668:LEU:HA	1.76	0.43
1:C:504:THR:HB	1:C:514:PHE:HZ	1.82	0.43
1:A:106:GLN:HG2	1:A:143:THR:HG21	2.01	0.43
1:A:232:LEU:HD11	1:A:258:TRP:CE3	2.53	0.43
1:A:102:ALA:O	1:A:106:GLN:HG3	2.17	0.43
1:A:505:TRP:NE1	1:A:533:VAL:HG11	2.34	0.42
1:C:353:LEU:HD22	1:C:361:LYS:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:678:PRO:HD2	1:B:736:ASN:ND2	2.34	0.42
1:C:774:LEU:HD13	1:C:781:ARG:HB2	2.01	0.42
1:A:173:ASP:N	1:A:173:ASP:OD1	2.51	0.42
1:A:170:ILE:HD11	1:A:184:PHE:HE2	1.83	0.42
1:B:549:LEU:HD21	1:B:761:VAL:HG22	2.02	0.42
1:C:668:LEU:HD12	1:C:764:THR:CG2	2.49	0.42
1:C:542:ASP:HB3	1:C:766:ALA:CB	2.49	0.42
1:C:668:LEU:HD23	1:C:668:LEU:HA	1.89	0.42
1:A:354:SER:HB3	1:A:357:ARG:HG3	2.01	0.42
1:C:692:ARG:HG3	1:C:709:TRP:CZ2	2.55	0.42
1:C:704:MET:O	1:C:708:MET:N	2.50	0.42
1:B:232:LEU:HB2	1:B:260:ILE:HG12	2.00	0.42
1:C:147:ARG:NH2	1:C:263:GLU:OE1	2.53	0.42
1:A:325:LEU:HD22	1:A:381:LEU:HB3	2.02	0.42
1:C:547:VAL:HA	1:C:739:PHE:O	2.20	0.42
1:C:772:ILE:HD12	1:C:788:ILE:HD11	2.02	0.42
1:C:668:LEU:HD12	1:C:764:THR:HG23	2.01	0.41
1:C:742:ASP:OD1	1:C:744:ALA:N	2.52	0.41
1:A:254:PHE:CD2	1:A:792:GLN:HB3	2.55	0.41
1:A:672:SER:OG	1:A:704:MET:HB2	2.20	0.41
1:B:148:PRO:CB	1:B:396:VAL:HB	2.49	0.41
1:B:443:LEU:H	1:B:486:TYR:HA	1.86	0.41
1:A:254:PHE:HD2	1:A:792:GLN:HB3	1.85	0.41
1:B:43:VAL:HG21	1:B:320:MET:HE3	2.02	0.41
1:B:704:MET:O	1:B:708:MET:N	2.51	0.41
1:C:741:TRP:CG	1:C:742:ASP:N	2.88	0.41
1:B:496:TYR:O	1:B:509:VAL:HG23	2.20	0.41
1:A:51:LEU:HD13	1:A:335:ALA:HB2	2.03	0.41
1:B:262:ASN:O	1:B:285:ARG:HA	2.21	0.41
1:B:744:ALA:HB1	1:B:805:TRP:CZ2	2.56	0.41
1:B:102:ALA:O	1:B:106:GLN:HG3	2.20	0.41
1:A:442:VAL:HA	1:A:485:ASN:O	2.21	0.41
1:A:676:ASP:OD1	1:A:676:ASP:N	2.54	0.41
1:A:31:ALA:HA	1:A:94:VAL:O	2.20	0.41
1:B:741:TRP:CG	1:B:742:ASP:N	2.89	0.41
1:C:229:ARG:HA	1:C:257:HIS:O	2.21	0.41
1:C:536:PHE:CE1	1:C:773:ALA:HB2	2.56	0.41
1:B:70:VAL:HG12	1:B:81:GLU:HG3	2.03	0.41
1:C:159:VAL:HG21	1:C:284:ILE:CD1	2.50	0.41
1:A:692:ARG:CZ	1:A:696:LEU:HD11	2.50	0.41
1:A:692:ARG:HG3	1:A:709:TRP:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:ARG:HA	1:A:770:TYR:O	2.21	0.41
1:A:156:ILE:HD13	1:A:261:ILE:HG21	2.03	0.41
1:A:263:GLU:HG2	1:A:398:PHE:CE1	2.55	0.40
1:A:262:ASN:O	1:A:285:ARG:HA	2.20	0.40
1:A:93:LEU:O	1:A:116:HIS:HA	2.21	0.40
1:B:133:LEU:HD23	1:B:135:ARG:HB2	2.02	0.40
1:B:94:VAL:HG22	1:B:117:LEU:HB2	2.03	0.40
1:A:692:ARG:HH21	1:A:696:LEU:HD11	1.83	0.40
1:C:172:TYR:HA	1:C:233:VAL:O	2.21	0.40
1:C:530:ARG:O	1:C:534:VAL:HG22	2.20	0.40
1:C:51:LEU:HD12	1:C:331:VAL:HG12	2.03	0.40
1:A:519:ILE:HD13	1:A:784:PHE:HE2	1.86	0.40
1:B:213:ASP:OD1	1:B:213:ASP:N	2.54	0.40
1:B:79:VAL:HG13	1:B:108:LEU:HD22	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:755:ASP:O	1:C:345:ARG:NH1[6_656]	2.09	0.11

## 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	636/688 (92%)	610 (96%)	26 (4%)	0	100	100
1	B	636/688 (92%)	611 (96%)	25 (4%)	0	100	100
1	C	636/688 (92%)	614 (96%)	22 (4%)	0	100	100
All	All	1908/2064 (92%)	1835 (96%)	73 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	568/604 (94%)	564 (99%)	4 (1%)	84	90
1	B	568/604 (94%)	563 (99%)	5 (1%)	78	88
1	C	568/604 (94%)	564 (99%)	4 (1%)	84	90
All	All	1704/1812 (94%)	1691 (99%)	13 (1%)	81	89

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	482	LEU
1	A	710	ARG
1	A	755	ASP
1	A	763	ASN
1	B	524	LEU
1	B	692	ARG
1	B	710	ARG
1	B	755	ASP
1	B	763	ASN
1	C	524	LEU
1	C	710	ARG
1	C	755	ASP
1	C	763	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	500	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](#)

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, 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	648/688 (94%)	0.12	11 (1%) 70 61	13, 49, 93, 119	0
1	B	648/688 (94%)	0.20	14 (2%) 62 52	21, 54, 102, 129	0
1	C	648/688 (94%)	0.24	15 (2%) 60 51	26, 60, 110, 128	0
All	All	1944/2064 (94%)	0.18	40 (2%) 63 54	13, 55, 103, 129	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	703	SER	6.8
1	C	137	ASN	4.3
1	C	138	ARG	4.1
1	A	136	SER	3.6
1	A	137	ASN	3.5
1	A	707	GLN	3.4
1	B	720	ASN	3.3
1	B	136	SER	3.2
1	C	134	THR	3.2
1	C	139	ASN	3.2
1	A	24	ASP	3.1
1	B	357	ARG	3.0
1	C	809	GLY	3.0
1	B	139	ASN	2.9
1	C	684	ASP	2.9
1	A	135	ARG	2.9
1	C	462	GLY	2.8
1	C	707	GLN	2.8
1	A	666	GLN	2.7
1	A	703	SER	2.6
1	B	24	ASP	2.5
1	C	808	ASN	2.5
1	C	136	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	461	LEU	2.5
1	B	707	GLN	2.4
1	C	459	ASN	2.4
1	B	462	GLY	2.3
1	C	710	ARG	2.3
1	A	134	THR	2.3
1	B	138	ARG	2.3
1	B	807	LYS	2.3
1	B	291	PRO	2.2
1	C	681	THR	2.2
1	C	468	GLN	2.2
1	A	504	THR	2.1
1	B	704	MET	2.1
1	C	461	LEU	2.1
1	A	297	ARG	2.1
1	B	359	ASN	2.0
1	A	720	ASN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.