



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 09:31 PM BST

PDB ID : 5FWX  
Title : Crystal structure of the AMPA receptor GluA2/A4 N-terminal domain heterodimer  
Authors : Garcia-Nafria, J.; Herguedas, B.; Greger, I.H.  
Deposited on : 2016-02-21  
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](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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

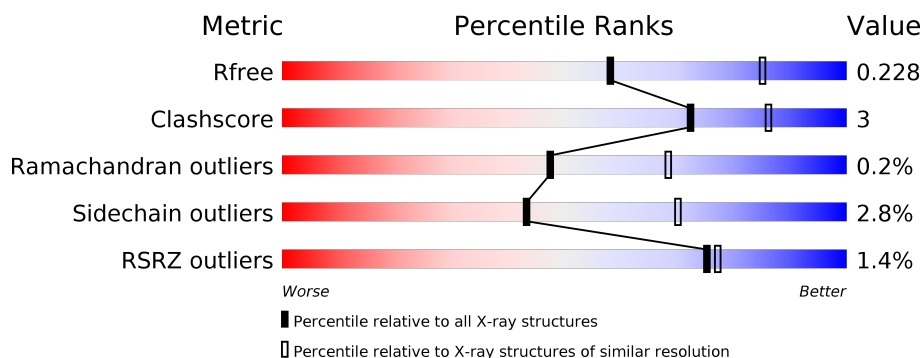
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	385	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>9%</div> <div>9%</div> </div> </div>
1	C	385	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>8%</div> </div> </div>
2	B	389	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>•</div> </div> </div>
2	D	389	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>10%</div> <div>• •</div> </div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11343 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	351	Total	C	N	O	S	0	0	0
			2668	1703	441	515	9			
1	C	356	Total	C	N	O	S	0	1	0
			2671	1704	448	510	9			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ARG	-	expression tag	UNP P19491
A	381	THR	-	expression tag	UNP P19491
A	382	LYS	-	expression tag	UNP P19491
A	383	HIS	-	expression tag	UNP P19491
A	384	HIS	-	expression tag	UNP P19491
A	385	HIS	-	expression tag	UNP P19491
A	386	HIS	-	expression tag	UNP P19491
A	387	HIS	-	expression tag	UNP P19491
A	388	HIS	-	expression tag	UNP P19491
C	380	ARG	-	expression tag	UNP P19491
C	381	THR	-	expression tag	UNP P19491
C	382	LYS	-	expression tag	UNP P19491
C	383	HIS	-	expression tag	UNP P19491
C	384	HIS	-	expression tag	UNP P19491
C	385	HIS	-	expression tag	UNP P19491
C	386	HIS	-	expression tag	UNP P19491
C	387	HIS	-	expression tag	UNP P19491
C	388	HIS	-	expression tag	UNP P19491

- Molecule 2 is a protein called GLUTAMATE RECEPTOR 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	375	Total	C	N	O	S	0	0	0
			2889	1853	485	538	13			

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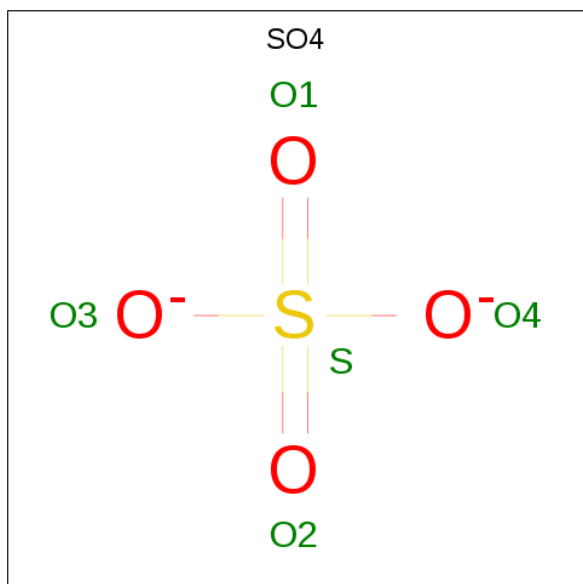
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	375	Total	C	N	O	S	0	0	0
			2928	1873	503	539	13			

There are 18 discrepancies between the modelled and reference sequences:

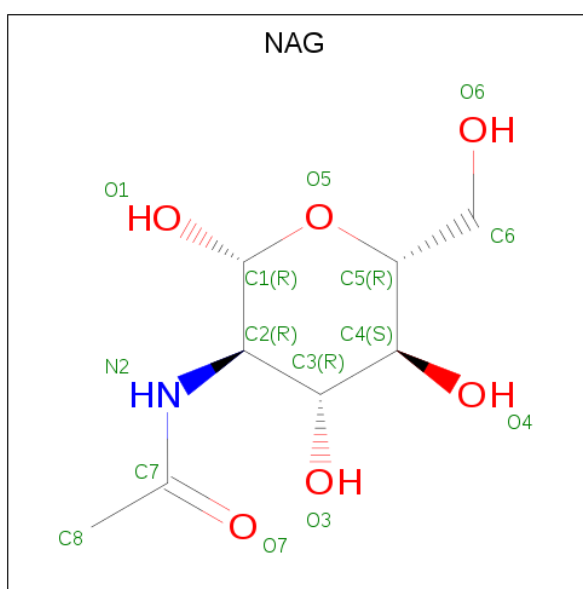
Chain	Residue	Modelled	Actual	Comment	Reference
B	381	ARG	-	expression tag	UNP P19493
B	382	THR	-	expression tag	UNP P19493
B	383	LYS	-	expression tag	UNP P19493
B	384	HIS	-	expression tag	UNP P19493
B	385	HIS	-	expression tag	UNP P19493
B	386	HIS	-	expression tag	UNP P19493
B	387	HIS	-	expression tag	UNP P19493
B	388	HIS	-	expression tag	UNP P19493
B	389	HIS	-	expression tag	UNP P19493
D	381	ARG	-	expression tag	UNP P19493
D	382	THR	-	expression tag	UNP P19493
D	383	LYS	-	expression tag	UNP P19493
D	384	HIS	-	expression tag	UNP P19493
D	385	HIS	-	expression tag	UNP P19493
D	386	HIS	-	expression tag	UNP P19493
D	387	HIS	-	expression tag	UNP P19493
D	388	HIS	-	expression tag	UNP P19493
D	389	HIS	-	expression tag	UNP P19493

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	34	Total O 34 34	0	0
5	B	32	Total O 32 32	0	0

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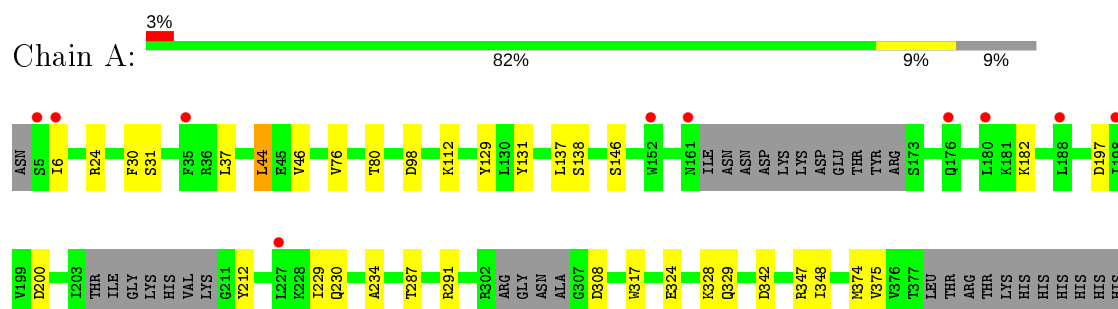
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	32	Total	O	0	0
			32	32		
5	D	27	Total	O	0	0
			27	27		

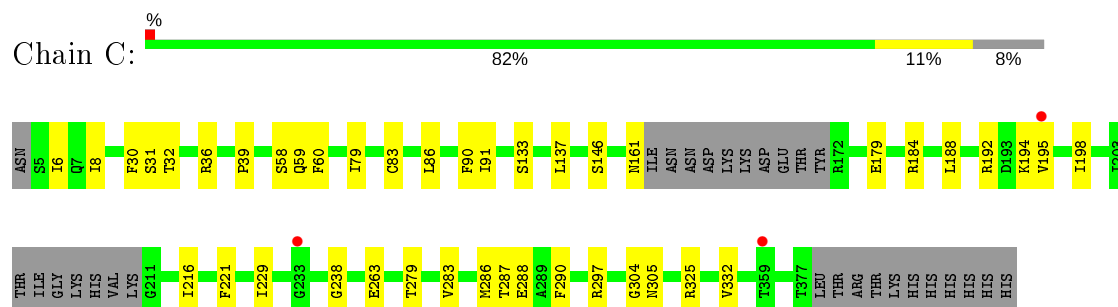
### 3 Residue-property plots [i](#)

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.

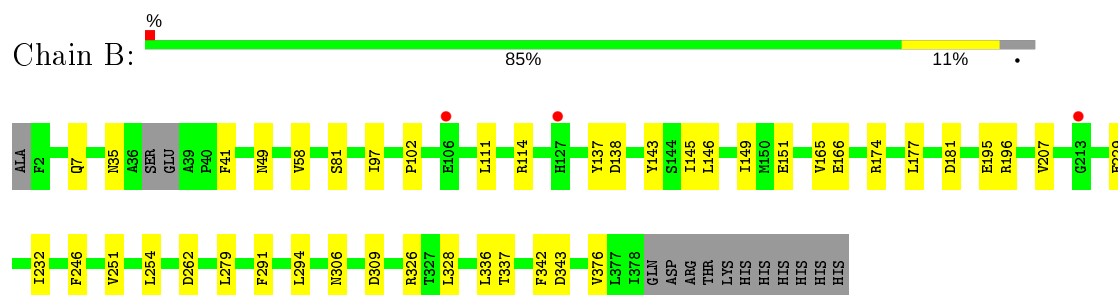
#### • Molecule 1: GLUTAMATE RECEPTOR 2



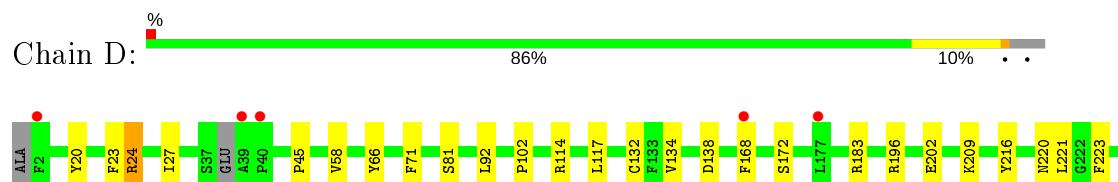
#### • Molecule 1: GLUTAMATE RECEPTOR 2



#### • Molecule 2: GLUTAMATE RECEPTOR 4



#### • Molecule 2: GLUTAMATE RECEPTOR 4







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.07Å 156.63Å 77.12Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	39.16 – 2.50 39.16 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.2 (39.16-2.50) 96.2 (39.16-2.50)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.04 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.172 , 0.238 0.178 , 0.228	Depositor DCC
$R_{free}$ test set	2416 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.6	Xtriage
Anisotropy	0.800	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 29.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.478 for h,-k,-l	Xtriage
Reported twinning fraction	0.497 for H, K, L 0.503 for -h,-k,l	Depositor
Outliers	0 of 48167 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11343	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.25 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1415e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, SO4

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	0.78	0/2722	0.84	4/3698 (0.1%)
1	C	0.71	0/2729	0.82	2/3712 (0.1%)
2	B	0.71	0/2956	0.84	3/4024 (0.1%)
2	D	0.71	0/2996	0.85	4/4070 (0.1%)
All	All	0.72	0/11403	0.84	13/15504 (0.1%)

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	1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	24	ARG	NE-CZ-NH2	-9.49	115.56	120.30
1	A	347	ARG	NE-CZ-NH1	7.71	124.16	120.30
2	D	348	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	C	325	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	C	325	ARG	NE-CZ-NH1	6.56	123.58	120.30
2	B	309	ASP	CB-CG-OD1	6.37	124.03	118.30
2	D	24	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	308	ASP	CB-CG-OD1	5.79	123.51	118.30
2	B	262	ASP	CB-CG-OD2	-5.47	113.38	118.30
2	D	183	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	291	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	24	ARG	CG-CD-NE	5.22	122.76	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	326	ARG	NE-CZ-NH1	5.05	122.82	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	31	SER	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	2668	0	2501	14	0
1	C	2671	0	2470	17	0
2	B	2889	0	2742	20	0
2	D	2928	0	2807	25	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	D	14	0	13	2	0
5	A	34	0	0	0	0
5	B	32	0	0	1	0
5	C	32	0	0	0	0
5	D	27	0	0	0	0
All	All	11343	0	10559	74	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 3.

All (74) 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)
2:D:27:ILE:HD13	2:D:45:PRO:HG3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:MET:SD	1:A:375:VAL:N	2.69	0.65
2:D:290:THR:HG21	2:D:328:LEU:HG	1.80	0.62
2:D:350:ASN:HD21	4:D:1381:NAG:C1	2.12	0.62
1:A:76:VAL:O	1:A:80:THR:HG23	2.03	0.57
1:A:112:LYS:NZ	1:A:138:SER:OG	2.29	0.56
1:C:6:ILE:HD13	1:C:290:PHE:CD1	2.41	0.56
2:B:254:LEU:HD22	2:B:336:LEU:CD1	2.36	0.55
2:D:71:PHE:CD2	2:D:301:ILE:HD12	2.40	0.55
1:C:91:ILE:HD13	1:C:286:MET:SD	2.46	0.55
1:C:194:LYS:O	1:C:198:ILE:HD12	2.06	0.55
2:B:246:PHE:HA	2:B:251:VAL:HG11	1.90	0.54
1:C:60:PHE:CE2	1:C:86:LEU:HD13	2.43	0.53
2:D:279:LEU:HD23	2:D:337:THR:HG21	1.90	0.53
2:D:220:ASN:C	2:D:220:ASN:OD1	2.43	0.53
2:B:165:VAL:HG23	2:B:196:ARG:HD3	1.90	0.53
2:D:117:LEU:HD13	2:D:221:LEU:HD21	1.91	0.53
2:D:20:TYR:CE2	2:D:24:ARG:HD2	2.44	0.53
2:D:290:THR:OG1	2:D:328:LEU:HD23	2.09	0.53
1:C:31:SER:HB2	1:C:36:ARG:HG3	1.91	0.52
2:B:254:LEU:HD22	2:B:336:LEU:HD13	1.91	0.52
2:D:350:ASN:ND2	4:D:1381:NAG:C1	2.73	0.52
2:B:58:VAL:HG21	2:B:81:SER:HB2	1.91	0.52
1:C:83:CYS:SG	1:C:90:PHE:HB2	2.49	0.52
1:C:79:ILE:HD12	1:C:90:PHE:CE1	2.45	0.52
1:C:133:SER:HA	1:C:137:LEU:HD21	1.92	0.50
2:D:209:LYS:O	2:D:216:TYR:OH	2.18	0.50
1:C:30:PHE:O	1:C:287:THR:HG21	2.12	0.50
2:B:229:GLU:HA	2:B:232:ILE:HD12	1.93	0.50
1:A:229:ILE:N	1:A:230:GLN:HA	2.26	0.49
2:B:111:LEU:HD22	2:B:328:LEU:HD22	1.94	0.49
1:A:212:TYR:O	1:A:234:ALA:HB1	2.13	0.49
1:C:288:GLU:HG3	1:C:332:VAL:HG11	1.95	0.48
2:B:137:TYR:O	2:B:165:VAL:HG22	2.13	0.48
2:D:27:ILE:HD13	2:D:45:PRO:CG	2.43	0.48
2:B:111:LEU:HD21	2:B:342:PHE:CE2	2.48	0.48
2:B:97:ILE:N	2:B:97:ILE:HD12	2.29	0.48
2:D:275:TYR:CE2	2:D:276:THR:HG23	2.49	0.48
1:A:342:ASP:HB3	1:A:348:ILE:HD13	1.97	0.47
1:C:58:SER:HB2	1:C:59:GLN:HE21	1.78	0.47
2:D:223:PHE:CD1	2:D:240:GLY:HA3	2.51	0.46
2:B:279:LEU:HD23	2:B:337:THR:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:THR:O	1:C:283:VAL:HG23	2.17	0.45
2:D:23:PHE:CE2	2:D:27:ILE:HD11	2.52	0.45
2:D:279:LEU:CD2	2:D:337:THR:HG21	2.47	0.45
2:D:247:ASN:N	2:D:247:ASN:HD22	2.14	0.45
2:B:49:ASN:ND2	5:B:2002:HOH:O	2.50	0.44
1:A:30:PHE:O	1:A:287:THR:HG21	2.18	0.44
2:D:66:TYR:CE2	2:D:92:LEU:HD13	2.53	0.44
2:D:66:TYR:CZ	2:D:92:LEU:HD13	2.52	0.44
1:C:8:ILE:O	1:C:39:PRO:HA	2.18	0.43
1:C:188:LEU:HD12	1:C:216:ILE:HD13	1.99	0.43
2:B:145:ILE:HG22	2:B:149:ILE:HD12	2.01	0.43
1:C:304:GLY:HA2	1:C:305:ASN:HA	1.83	0.43
1:A:44:LEU:CD1	1:A:46:VAL:HG12	2.49	0.42
1:A:137:LEU:HD12	2:B:143:TYR:HB3	2.01	0.42
1:A:129:TYR:CE1	1:A:131:TYR:HB3	2.54	0.42
2:B:343:ASP:C	2:B:343:ASP:OD1	2.58	0.42
1:A:197:ASP:O	1:A:200:ASP:HB3	2.19	0.42
2:B:137:TYR:CZ	2:B:146:LEU:HD22	2.55	0.42
2:D:71:PHE:HD2	2:D:301:ILE:HD12	1.81	0.42
1:C:192:ARG:O	1:C:195:VAL:HG22	2.19	0.42
2:D:102:PRO:HD3	2:D:114:ARG:HD2	2.01	0.42
2:D:138:ASP:OD2	2:D:196:ARG:NH1	2.53	0.42
1:C:221:PHE:CD1	1:C:238:GLY:HA3	2.54	0.42
2:D:117:LEU:HD13	2:D:221:LEU:CD2	2.49	0.41
2:B:138:ASP:OD2	2:B:196:ARG:NH1	2.53	0.41
1:A:6:ILE:HB	1:A:37:LEU:HD12	2.01	0.41
2:B:41:PHE:CZ	2:B:291:PHE:HB2	2.56	0.41
2:D:343:ASP:C	2:D:343:ASP:OD1	2.59	0.41
2:D:58:VAL:HG11	2:D:81:SER:HB2	2.03	0.41
1:A:324:GLU:O	1:A:328:LYS:HG3	2.21	0.41
2:B:102:PRO:HD3	2:B:114:ARG:HD2	2.03	0.41
1:A:137:LEU:HD12	2:B:143:TYR:CB	2.52	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	343/385 (89%)	331 (96%)	11 (3%)	1 (0%)	41	61
1	C	351/385 (91%)	332 (95%)	18 (5%)	1 (0%)	41	61
2	B	371/389 (95%)	359 (97%)	11 (3%)	1 (0%)	41	61
2	D	369/389 (95%)	358 (97%)	11 (3%)	0	100	100
All	All	1434/1548 (93%)	1380 (96%)	51 (4%)	3 (0%)	47	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	182	LYS
2	B	35	ASN
1	C	229	ILE

### 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	273/334 (82%)	268 (98%)	5 (2%)	59	81
1	C	263/334 (79%)	256 (97%)	7 (3%)	44	71
2	B	300/341 (88%)	289 (96%)	11 (4%)	34	60
2	D	308/341 (90%)	299 (97%)	9 (3%)	42	69
All	All	1144/1350 (85%)	1112 (97%)	32 (3%)	43	70

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	98	ASP
1	A	146	SER

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Mol	Chain	Res	Type
1	A	317	TRP
1	A	329	GLN
2	B	7	GLN
2	B	151	GLU
2	B	166	GLU
2	B	174	ARG
2	B	177	LEU
2	B	181	ASP
2	B	195	GLU
2	B	207	VAL
2	B	294	LEU
2	B	306	ASN
2	B	376	VAL
1	C	32	THR
1	C	146	SER
1	C	161	ASN
1	C	179	GLU
1	C	184	ARG
1	C	263	GLU
1	C	297	ARG
2	D	132	CYS
2	D	134	VAL
2	D	168	PHE
2	D	172	SER
2	D	202	GLU
2	D	227	SER
2	D	295	ARG
2	D	301	ILE
2	D	345	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	59	GLN
1	A	158	ASN
1	A	296	GLN
2	B	147	GLN
1	C	59	GLN
1	C	101	HIS
1	C	161	ASN
1	C	296	GLN

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Mol	Chain	Res	Type
1	C	329	GLN
2	D	15	ASN
2	D	175	GLN
2	D	247	ASN
2	D	379	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 ⓘ

There are no monosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

7 ligands are 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	$\# Z  > 2$
4	NAG	B	1380	2	14,14,15	0.51	0	17,19,21	1.30	2 (11%)
3	SO4	C	1400	-	4,4,4	0.41	0	6,6,6	0.56	0
4	NAG	D	1381	-	14,14,15	0.69	0	17,19,21	1.85	4 (23%)
3	SO4	D	1380	-	4,4,4	0.37	0	6,6,6	0.28	0
3	SO4	B	1379	-	4,4,4	0.51	0	6,6,6	0.62	0
4	NAG	A	1379	1	14,14,15	0.39	0	17,19,21	1.99	6 (35%)
3	SO4	A	1378	-	4,4,4	0.45	0	6,6,6	0.27	0



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
4	NAG	B	1380	2	-	2/6/23/26	0/1/1/1
4	NAG	D	1381	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1379	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1381	NAG	O5-C1-C2	-5.28	102.94	111.29
4	A	1379	NAG	C8-C7-N2	4.20	123.20	116.10
4	A	1379	NAG	C1-O5-C5	4.17	117.84	112.19
4	D	1381	NAG	C3-C4-C5	3.37	116.25	110.24
4	A	1379	NAG	C2-N2-C7	3.20	127.47	122.90
4	B	1380	NAG	C8-C7-N2	3.08	121.31	116.10
4	B	1380	NAG	C2-N2-C7	3.04	127.23	122.90
4	D	1381	NAG	C1-O5-C5	2.81	116.00	112.19
4	A	1379	NAG	O5-C1-C2	-2.21	107.79	111.29
4	A	1379	NAG	C4-C3-C2	-2.20	107.80	111.02
4	A	1379	NAG	O7-C7-C8	-2.09	118.17	122.06
4	D	1381	NAG	O5-C5-C4	2.00	115.70	110.83

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1380	NAG	C8-C7-N2-C2
4	B	1380	NAG	O7-C7-N2-C2
4	A	1379	NAG	C8-C7-N2-C2
4	A	1379	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1381	NAG	2	0

## 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	351/385 (91%)	-0.32	10 (2%) 53 56	29, 57, 102, 153	0
1	C	356/385 (92%)	-0.29	3 (0%) 86 87	35, 60, 121, 160	0
2	B	375/389 (96%)	-0.40	3 (0%) 86 87	33, 59, 88, 121	0
2	D	375/389 (96%)	-0.39	5 (1%) 77 79	34, 59, 89, 105	0
All	All	1457/1548 (94%)	-0.35	21 (1%) 75 77	29, 59, 99, 160	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	180	LEU	6.8
2	B	106	GLU	4.5
1	C	195	VAL	4.2
2	D	39	ALA	2.8
1	A	176	GLN	2.8
1	C	359	THR	2.8
1	C	233	GLY	2.7
2	D	2	PHE	2.5
1	A	227	LEU	2.5
1	A	35	PHE	2.4
2	B	127	HIS	2.4
1	A	161	ASN	2.3
2	D	40	PRO	2.3
2	D	168	PHE	2.3
1	A	5	SER	2.3
1	A	152	TRP	2.2
1	A	188	LEU	2.2
2	B	213	GLY	2.2
1	A	6	ILE	2.1
2	D	177	LEU	2.1
1	A	198	ILE	2.1

## 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 monosaccharides in this entry.

## 6.4 Ligands [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, 95<sup>th</sup> 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
4	NAG	B	1380	14/15	0.78	0.21	78,97,109,111	0
4	NAG	D	1381	14/15	0.89	0.13	53,64,69,71	0
4	NAG	A	1379	14/15	0.91	0.14	49,63,77,81	0
3	SO4	B	1379	5/5	0.98	0.08	49,51,57,59	0
3	SO4	D	1380	5/5	0.98	0.08	55,56,64,69	0
3	SO4	C	1400	5/5	0.99	0.12	36,37,38,44	0
3	SO4	A	1378	5/5	0.99	0.10	38,45,46,48	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.