



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:07 am GMT

PDB ID : 5FWY
Title : Crystal structure of the AMPA receptor GluA2/A3 N-terminal domain heterodimer
Authors : Herguedas, B.; Garcia-Nafria, J.; Greger, I.H.
Deposited on : 2016-02-21
Resolution : 2.12 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

<http://wwpdb.org/validation/2016/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
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

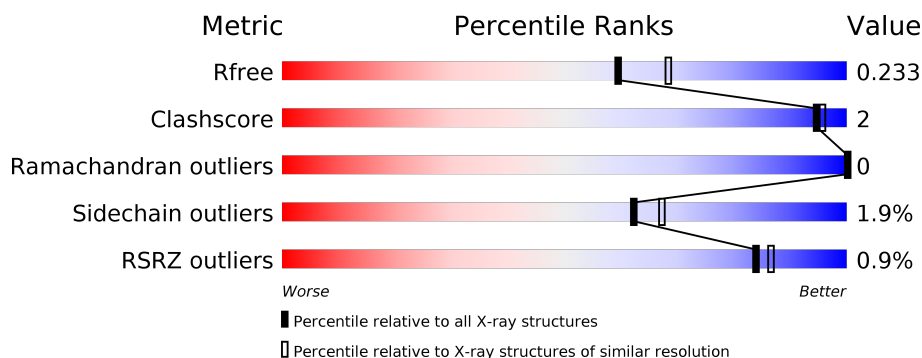
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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}	100719	4988 (2.14-2.10)
Clashscore	112137	5557 (2.14-2.10)
Ramachandran outliers	110173	5504 (2.14-2.10)
Sidechain outliers	110143	5505 (2.14-2.10)
RSRZ outliers	101464	5021 (2.14-2.10)

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. 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>%</div> <div> <div></div> <div>88%</div> <div>8%</div> <div>•</div> </div> </div>
1	C	385	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>5%</div> <div>•</div> </div> </div>
2	B	390	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>6%</div> <div>• •</div> </div> </div>
2	D	390	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>8%</div> <div>• •</div> </div> </div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	C	1378	-	-	-	X
3	NAG	C	1379	-	-	-	X
4	SO4	B	1387	-	-	-	X
4	SO4	B	1389	-	-	-	X
4	SO4	B	1390	-	-	-	X
4	SO4	D	1385	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12549 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	0	1	0
			2956	1885	501	561	9			
1	C	367	Total	C	N	O	S	0	1	0
			2927	1870	495	553	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 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	379	Total	C	N	O	S	0	0	0
			3069	1952	536	565	16			

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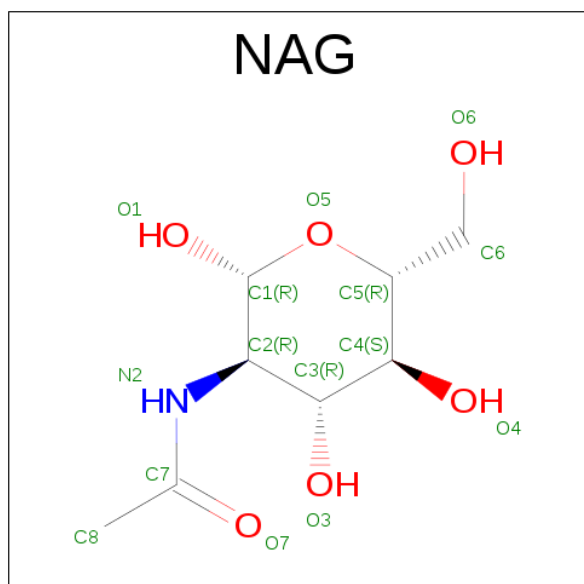
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	377	Total	C	N	O	S	0	1	0
			3059	1949	533	560	17			

There are 18 discrepancies between the modelled and reference sequences:

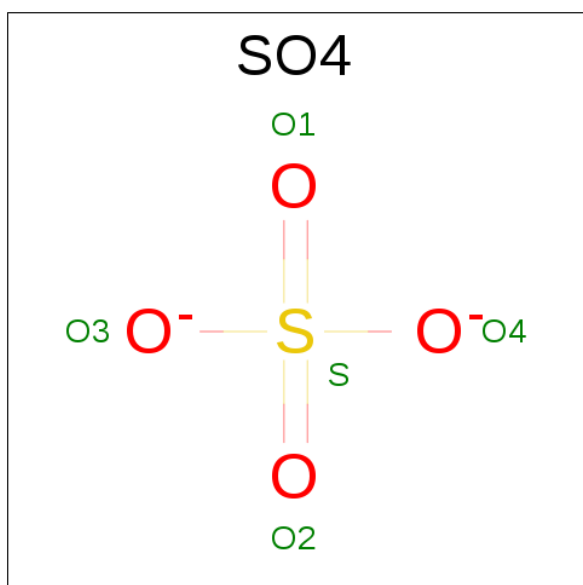
Chain	Residue	Modelled	Actual	Comment	Reference
B	382	GLY	-	EXPRESSION TAG	UNP P19492
B	383	THR	-	EXPRESSION TAG	UNP P19492
B	384	LYS	-	EXPRESSION TAG	UNP P19492
B	385	HIS	-	EXPRESSION TAG	UNP P19492
B	386	HIS	-	EXPRESSION TAG	UNP P19492
B	387	HIS	-	EXPRESSION TAG	UNP P19492
B	388	HIS	-	EXPRESSION TAG	UNP P19492
B	389	HIS	-	EXPRESSION TAG	UNP P19492
B	390	HIS	-	EXPRESSION TAG	UNP P19492
D	382	GLY	-	EXPRESSION TAG	UNP P19492
D	383	THR	-	EXPRESSION TAG	UNP P19492
D	384	LYS	-	EXPRESSION TAG	UNP P19492
D	385	HIS	-	EXPRESSION TAG	UNP P19492
D	386	HIS	-	EXPRESSION TAG	UNP P19492
D	387	HIS	-	EXPRESSION TAG	UNP P19492
D	388	HIS	-	EXPRESSION TAG	UNP P19492
D	389	HIS	-	EXPRESSION TAG	UNP P19492
D	390	HIS	-	EXPRESSION TAG	UNP P19492

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



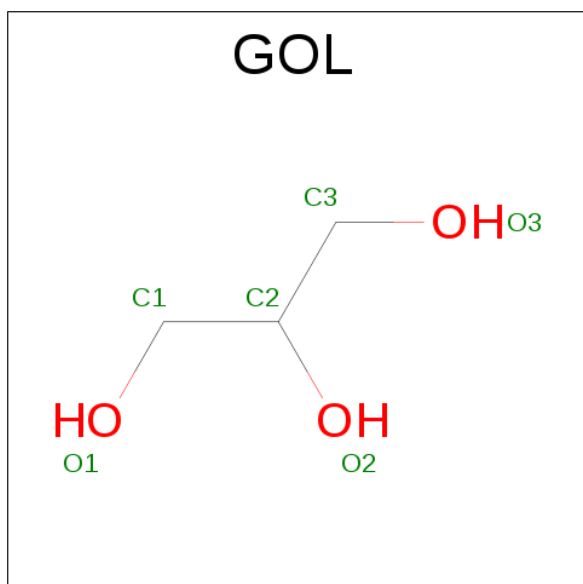
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O S	0	0
			5	4 1		
4	B	1	Total	O S	0	0
			5	4 1		

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	88	Total	O	0	0
			88	88		
6	B	102	Total	O	0	0
			102	102		

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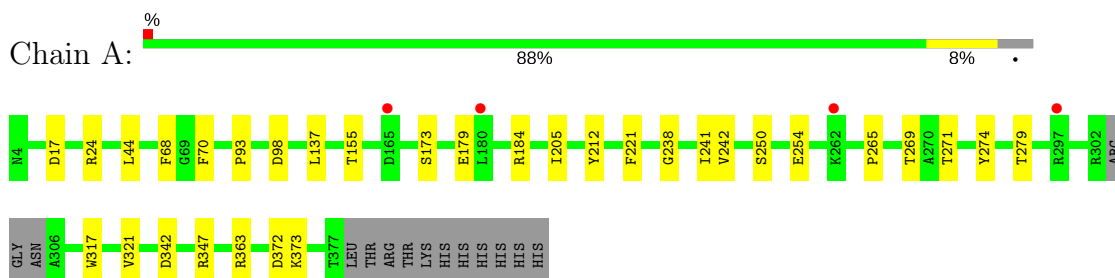
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	87	Total	O	0	0
			87	87		
6	D	75	Total	O	0	0
			75	75		

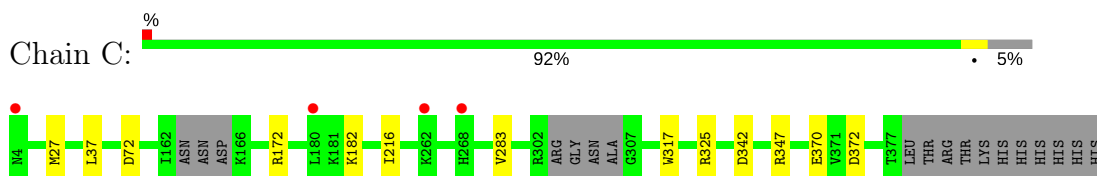
3 Residue-property plots

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.

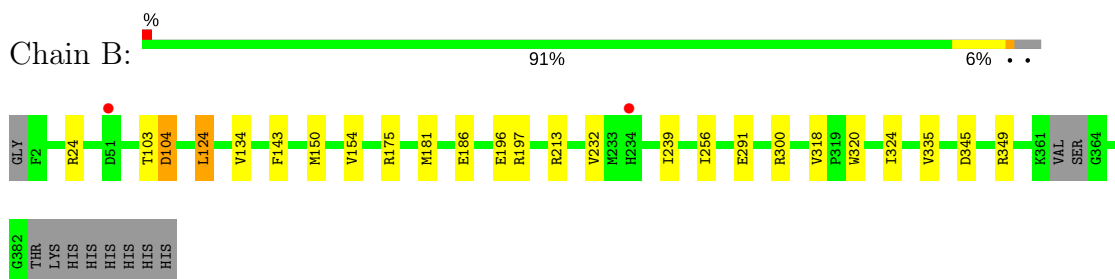
• Molecule 1: GLUTAMATE RECEPTOR 2



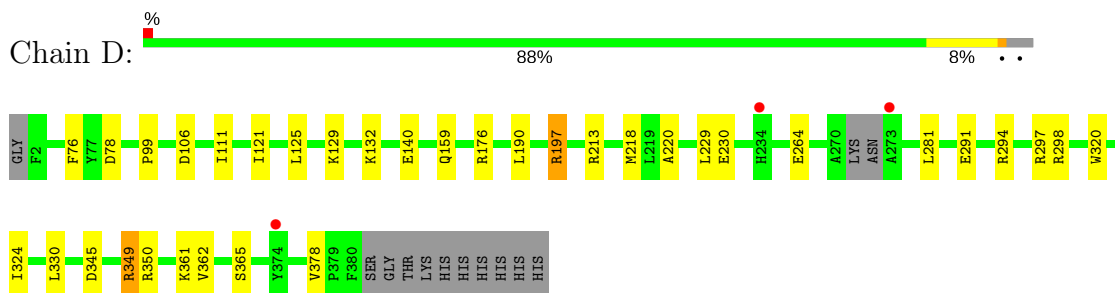
• Molecule 1: GLUTAMATE RECEPTOR 2



• Molecule 2: GLUTAMATE RECEPTOR 3



• Molecule 2: GLUTAMATE RECEPTOR 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	66.27Å 78.52Å 107.85Å 83.36° 87.40° 64.94°	Depositor
Resolution (Å)	41.76 – 2.12 41.75 – 2.12	Depositor EDS
% Data completeness (in resolution range)	90.3 (41.76-2.12) 87.2 (41.75-2.12)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.192 , 0.231 0.198 , 0.233	Depositor DCC
R_{free} test set	4984 reflections (5.23%)	DCC
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.077 for h,h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12549	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	0.81	0/3021	0.89	6/4088 (0.1%)
1	C	0.84	0/2991	0.90	7/4045 (0.2%)
2	B	0.83	1/3140 (0.0%)	0.92	10/4250 (0.2%)
2	D	0.80	1/3133 (0.0%)	0.93	13/4241 (0.3%)
All	All	0.82	2/12285 (0.0%)	0.91	36/16624 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	291	GLU	CD-OE2	5.46	1.31	1.25
2	B	291	GLU	CD-OE2	5.42	1.31	1.25

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	24	ARG	NE-CZ-NH2	-9.20	115.70	120.30
2	D	197	ARG	NE-CZ-NH2	-8.03	116.29	120.30
2	B	24	ARG	NE-CZ-NH1	7.43	124.02	120.30
2	D	345	ASP	CB-CG-OD1	7.04	124.63	118.30
1	C	325	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	C	342	ASP	CB-CG-OD1	6.86	124.48	118.30
1	C	72	ASP	CB-CG-OD2	-6.61	112.35	118.30
2	D	294	ARG	NE-CZ-NH1	6.60	123.60	120.30
2	B	197	ARG	NE-CZ-NH1	6.47	123.54	120.30
2	D	349	ARG	NE-CZ-NH2	-6.38	117.11	120.30
2	B	124	LEU	CA-CB-CG	-6.25	100.92	115.30
1	A	347	ARG	NE-CZ-NH1	6.20	123.40	120.30
2	D	78	ASP	CB-CG-OD1	6.20	123.88	118.30
2	B	175	ARG	NE-CZ-NH2	-6.18	117.21	120.30
2	B	175	ARG	NE-CZ-NH1	6.14	123.37	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	347	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	A	342	ASP	CB-CG-OD1	5.90	123.61	118.30
2	D	78	ASP	CB-CG-OD2	-5.88	113.00	118.30
2	B	104	ASP	CB-CG-OD2	5.87	123.58	118.30
2	B	345	ASP	CB-CG-OD1	5.85	123.57	118.30
2	D	297	ARG	NE-CZ-NH1	5.84	123.22	120.30
2	D	213	ARG	NE-CZ-NH2	-5.82	117.39	120.30
2	B	300	ARG	NE-CZ-NH1	5.73	123.16	120.30
2	B	150	MET	CG-SD-CE	5.64	109.23	100.20
2	D	345	ASP	CB-CG-OD2	-5.59	113.26	118.30
2	D	197	ARG	NE-CZ-NH1	5.54	123.07	120.30
2	D	298	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	24	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	363	ARG	NE-CZ-NH2	-5.50	117.55	120.30
2	D	176	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	C	347	ARG	NE-CZ-NH2	-5.41	117.60	120.30
2	D	350	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	363	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	C	172	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	98	ASP	CB-CG-OD1	5.20	122.98	118.30
1	C	325	ARG	NE-CZ-NH1	5.18	122.89	120.30

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	2956	0	2897	15	0
1	C	2927	0	2875	3	0
2	B	3069	0	2964	11	0
2	D	3059	0	2965	10	0
3	A	28	0	26	0	0
3	B	42	0	39	0	0
3	C	28	0	26	0	0
3	D	42	0	39	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	5	0	0	0	0
4	B	20	0	0	0	0
4	C	5	0	0	0	0
4	D	10	0	0	0	0
5	B	6	0	8	0	0
6	A	88	0	0	0	0
6	B	102	0	0	2	0
6	C	87	0	0	0	0
6	D	75	0	0	0	0
All	All	12549	0	11839	36	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 2.

All (36) 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:B:232:VAL:CG1	2:B:239:ILE:HD11	2.32	0.58
1:A:269:THR:HG23	1:A:271:THR:O	2.04	0.58
2:D:106:ASP:OD1	2:D:349:ARG:NH2	2.40	0.55
1:A:17:ASP:HB3	1:A:265:PRO:HB2	1.88	0.54
2:B:134:VAL:HG21	2:B:181:MET:HG3	1.88	0.54
1:A:241:ILE:HD12	1:A:242:VAL:HG23	1.93	0.51
2:B:256:ILE:HD12	6:B:2029:HOH:O	2.11	0.50
1:A:137:LEU:HD12	2:B:143:PHE:CD1	2.46	0.50
1:A:70:PHE:CE2	1:A:93:PRO:HG2	2.47	0.50
2:B:349:ARG:HD2	6:B:2098:HOH:O	2.11	0.50
1:A:221:PHE:CD1	1:A:238:GLY:HA3	2.47	0.49
1:C:27:MET:CE	1:C:283:VAL:HG13	2.42	0.49
2:D:121:ILE:HG23	2:D:218:MET:CE	2.43	0.48
2:B:103:THR:OG1	2:B:104:ASP:N	2.46	0.48
1:A:68:PHE:CZ	1:A:279:THR:HG23	2.49	0.48
2:D:76:PHE:CE2	2:D:99:PRO:HG2	2.50	0.47
1:A:241:ILE:HD11	1:A:274:TYR:HB2	1.97	0.46
1:A:179:GLU:OE2	1:A:212:TYR:OH	2.28	0.45
2:D:99:PRO:HB3	2:D:281:LEU:HB3	1.99	0.45
2:B:181:MET:HE3	2:B:186:GLU:HG3	1.98	0.45
2:B:232:VAL:HG11	2:B:239:ILE:HD11	2.00	0.44
1:A:250:SER:O	1:A:254:GLU:HG3	2.18	0.44
2:D:125:LEU:HD21	2:D:218:MET:HE2	2.00	0.44
2:D:190:LEU:HD13	2:D:218:MET:CE	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:ASP:O	1:A:373:LYS:HD3	2.19	0.43
1:A:184:ARG:HD2	1:A:212:TYR:CE2	2.54	0.43
2:D:111:ILE:HD13	2:D:330:LEU:HD13	2.00	0.43
1:A:44:LEU:HD23	1:A:44:LEU:N	2.34	0.42
1:C:27:MET:HE3	1:C:283:VAL:HG13	2.00	0.42
2:D:132:LYS:HG3	2:D:159:GLN:HB2	2.00	0.42
2:D:140:GLU:OE2	2:D:197:ARG:NH1	2.52	0.42
2:D:121:ILE:HD11	2:D:220:ALA:HB1	2.02	0.42
1:A:137:LEU:HD12	2:B:143:PHE:CG	2.55	0.41
1:C:27:MET:HE2	1:C:37:LEU:HD12	2.02	0.41
1:A:155:THR:HG23	2:B:154:VAL:HG22	2.02	0.41
2:B:324:ILE:HG21	2:B:324:ILE:HD13	1.87	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	368/385 (96%)	358 (97%)	10 (3%)	0	100	100
1	C	362/385 (94%)	353 (98%)	9 (2%)	0	100	100
2	B	375/390 (96%)	367 (98%)	8 (2%)	0	100	100
2	D	374/390 (96%)	369 (99%)	5 (1%)	0	100	100
All	All	1479/1550 (95%)	1447 (98%)	32 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	320/334 (96%)	316 (99%)	4 (1%)	73	79
1	C	317/334 (95%)	312 (98%)	5 (2%)	68	73
2	B	328/341 (96%)	322 (98%)	6 (2%)	64	69
2	D	328/341 (96%)	318 (97%)	10 (3%)	46	48
All	All	1293/1350 (96%)	1268 (98%)	25 (2%)	62	67

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	SER
1	A	205	ILE
1	A	317	TRP
1	A	321	VAL
2	B	124	LEU
2	B	196	GLU
2	B	213	ARG
2	B	318	VAL
2	B	320	TRP
2	B	335	VAL
1	C	182	LYS
1	C	216	ILE
1	C	317	TRP
1	C	370	GLU
1	C	372	ASP
2	D	129	LYS
2	D	229	LEU
2	D	230	GLU
2	D	264	GLU
2	D	320	TRP
2	D	324	ILE
2	D	361	LYS
2	D	362	VAL
2	D	365	SER
2	D	378	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	163	ASN
2	B	108	GLN
2	B	257	GLN
2	B	334	GLN
1	C	7	GLN
1	C	353	ASN
2	D	65	GLN
2	D	83	ASN
2	D	253	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](#)

19 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	$\# Z > 2$
3	NAG	A	1378	1	14,14,15	0.53	0	15,19,21	1.48	2 (13%)
3	NAG	A	1379	1	14,14,15	0.53	0	15,19,21	1.40	2 (13%)
4	SO4	A	1380	-	4,4,4	0.50	0	6,6,6	0.36	0
3	NAG	B	1383	2	14,14,15	0.50	0	15,19,21	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	1384	2	14,14,15	0.60	0	15,19,21	1.24	1 (6%)
3	NAG	B	1385	2	14,14,15	0.50	0	15,19,21	2.46	5 (33%)
4	SO4	B	1386	-	4,4,4	0.35	0	6,6,6	0.15	0
4	SO4	B	1387	-	4,4,4	0.43	0	6,6,6	0.30	0
5	GOL	B	1388	-	5,5,5	0.34	0	5,5,5	0.22	0
4	SO4	B	1389	-	4,4,4	0.54	0	6,6,6	0.30	0
4	SO4	B	1390	-	4,4,4	0.46	0	6,6,6	0.20	0
3	NAG	C	1378	1	14,14,15	0.69	1 (7%)	15,19,21	1.10	2 (13%)
3	NAG	C	1379	1	14,14,15	0.47	0	15,19,21	1.70	3 (20%)
4	SO4	C	1380	-	4,4,4	0.47	0	6,6,6	0.18	0
3	NAG	D	1381	2	14,14,15	0.54	0	15,19,21	1.21	2 (13%)
3	NAG	D	1382	2	14,14,15	0.58	0	15,19,21	0.93	0
3	NAG	D	1383	2	14,14,15	0.48	0	15,19,21	1.17	1 (6%)
4	SO4	D	1384	-	4,4,4	0.41	0	6,6,6	0.16	0
4	SO4	D	1385	-	4,4,4	0.45	0	6,6,6	0.18	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
3	NAG	A	1378	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1379	1	-	0/6/23/26	0/1/1/1
4	SO4	A	1380	-	-	0/0/0/0	0/0/0/0
3	NAG	B	1383	2	-	0/6/23/26	0/1/1/1
3	NAG	B	1384	2	-	0/6/23/26	0/1/1/1
3	NAG	B	1385	2	-	0/6/23/26	0/1/1/1
4	SO4	B	1386	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1387	-	-	0/0/0/0	0/0/0/0
5	GOL	B	1388	-	-	0/4/4/4	0/0/0/0
4	SO4	B	1389	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1390	-	-	0/0/0/0	0/0/0/0
3	NAG	C	1378	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1379	1	-	0/6/23/26	0/1/1/1
4	SO4	C	1380	-	-	0/0/0/0	0/0/0/0
3	NAG	D	1381	2	-	0/6/23/26	0/1/1/1
3	NAG	D	1382	2	-	0/6/23/26	0/1/1/1
3	NAG	D	1383	2	-	0/6/23/26	0/1/1/1
4	SO4	D	1384	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1385	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1378	NAG	C1-C2	2.06	1.55	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1385	NAG	O5-C1-C2	-4.88	104.69	111.47
3	C	1379	NAG	C1-C2-N2	-3.76	104.06	110.49
3	A	1379	NAG	C1-C2-N2	-3.40	104.69	110.49
3	A	1378	NAG	O5-C1-C2	-2.34	108.22	111.47
3	A	1379	NAG	C3-C4-C5	-2.08	106.55	110.22
3	D	1381	NAG	C6-C5-C4	2.04	117.78	113.00
3	C	1378	NAG	C2-N2-C7	2.13	126.05	122.94
3	D	1381	NAG	C2-N2-C7	2.28	126.27	122.94
3	C	1379	NAG	C4-C3-C2	2.39	114.51	111.02
3	D	1383	NAG	C4-C3-C2	2.46	114.62	111.02
3	C	1378	NAG	C1-O5-C5	2.48	115.59	112.17
3	B	1385	NAG	C1-O5-C5	2.62	115.78	112.17
3	B	1384	NAG	C1-O5-C5	2.95	116.23	112.17
3	A	1378	NAG	C1-O5-C5	2.96	116.25	112.17
3	B	1385	NAG	C1-C2-N2	3.01	115.64	110.49
3	C	1379	NAG	C1-O5-C5	3.80	117.40	112.17
3	B	1385	NAG	C8-C7-N2	3.83	123.03	116.11
3	B	1385	NAG	C2-N2-C7	4.86	130.03	122.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	371/385 (96%)	-0.23	4 (1%) 80 84	25, 36, 65, 89	0
1	C	367/385 (95%)	-0.21	4 (1%) 80 84	23, 35, 63, 82	0
2	B	379/390 (97%)	-0.25	2 (0%) 90 92	24, 35, 57, 78	0
2	D	377/390 (96%)	-0.26	3 (0%) 86 88	26, 40, 61, 74	0
All	All	1494/1550 (96%)	-0.24	13 (0%) 84 86	23, 37, 62, 89	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	180	LEU	3.7
1	A	180	LEU	3.5
2	D	273	ALA	2.9
2	B	234	HIS	2.8
1	A	262	LYS	2.5
2	D	374	TYR	2.4
1	C	4	ASN	2.3
1	A	165	ASP	2.2
1	C	268	HIS	2.2
1	C	262	LYS	2.2
2	B	51	ASP	2.2
2	D	234	HIS	2.1
1	A	297	ARG	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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	SO4	B	1390	5/5	0.86	0.39	13.35	89,92,95,96	0
4	SO4	B	1389	5/5	0.84	0.24	7.71	62,70,78,78	0
4	SO4	D	1385	5/5	0.91	0.23	4.64	85,87,91,93	0
4	SO4	B	1387	5/5	0.91	0.25	3.87	82,82,88,88	0
3	NAG	C	1379	14/15	0.86	0.17	2.55	44,54,60,61	0
3	NAG	C	1378	14/15	0.93	0.14	2.51	40,47,52,56	0
3	NAG	A	1378	14/15	0.93	0.14	1.80	40,46,52,54	0
3	NAG	A	1379	14/15	0.86	0.19	1.18	45,56,58,61	0
3	NAG	D	1381	14/15	0.84	0.17	0.92	48,57,59,59	0
3	NAG	B	1384	14/15	0.91	0.13	0.80	53,61,64,68	0
4	SO4	A	1380	5/5	0.95	0.12	-0.16	62,64,70,71	0
4	SO4	B	1386	5/5	0.97	0.10	-0.36	68,71,74,74	0
3	NAG	D	1382	14/15	0.91	0.09	-0.58	48,53,55,55	0
5	GOL	B	1388	6/6	0.97	0.08	-1.50	36,38,39,40	0
4	SO4	C	1380	5/5	0.97	0.06	-1.73	56,56,63,64	0
4	SO4	D	1384	5/5	0.95	0.11	-	70,75,76,76	0
3	NAG	B	1383	14/15	0.86	0.18	-	47,58,62,64	0
3	NAG	B	1385	14/15	0.84	0.24	-	69,76,78,80	0
3	NAG	D	1383	14/15	0.81	0.23	-	70,76,79,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.