



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:00 PM GMT

PDB ID : 3QLU
Title : Crystal structure of the GluK2/GluK5 (GluR6/KA2) ATD dimer assembly
Authors : Kumar, J.; Mayer, M.L.
Deposited on : 2011-02-03
Resolution : 2.91 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

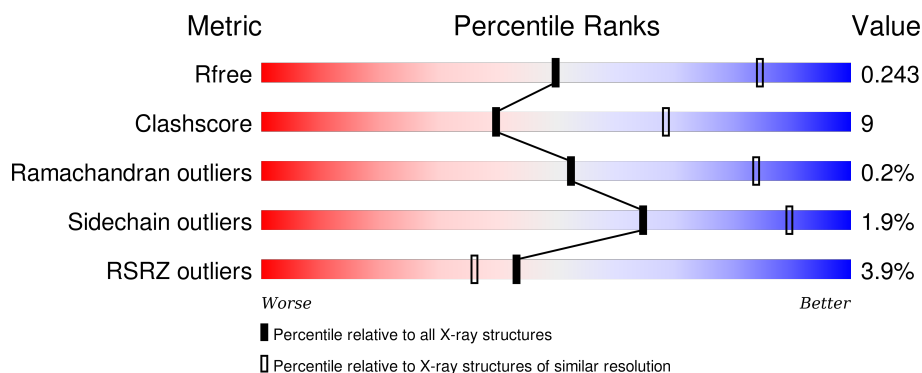
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	393	<div> <div>5%</div> <div>78% 15% • 5%</div> </div>
1	B	393	<div> <div>4%</div> <div>76% 20% • •</div> </div>
2	C	395	<div> <div>3%</div> <div>82% 12% 6%</div> </div>
2	D	395	<div> <div>3%</div> <div>82% 12% 6%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	B	397	-	-	-	X
3	NAG	B	398	-	-	-	X
3	NAG	C	398	X	-	-	X
3	NAG	D	397	X	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 23862 atoms, of which 11853 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 kainate 5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	372	Total	C	H	N	O	S	12	2	0
			5773	1829	2878	499	550	17			
1	B	381	Total	C	H	N	O	S	0	1	0
			5905	1867	2947	509	564	18			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	388	LEU	-	EXPRESSION TAG	UNP Q63273
A	389	GLU	-	EXPRESSION TAG	UNP Q63273
A	390	LEU	-	EXPRESSION TAG	UNP Q63273
A	391	VAL	-	EXPRESSION TAG	UNP Q63273
A	392	PRO	-	EXPRESSION TAG	UNP Q63273
A	393	ARG	-	EXPRESSION TAG	UNP Q63273
B	388	LEU	-	EXPRESSION TAG	UNP Q63273
B	389	GLU	-	EXPRESSION TAG	UNP Q63273
B	390	LEU	-	EXPRESSION TAG	UNP Q63273
B	391	VAL	-	EXPRESSION TAG	UNP Q63273
B	392	PRO	-	EXPRESSION TAG	UNP Q63273
B	393	ARG	-	EXPRESSION TAG	UNP Q63273

- Molecule 2 is a protein called Glutamate receptor, ionotropic kainate 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	372	Total	C	H	N	O	S	0	0	0
			5848	1885	2897	503	547	16			
2	D	373	Total	C	H	N	O	S	0	0	0
			5882	1894	2915	504	552	17			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	213	ASN	ALA	ENGINEERED MUTATION	UNP P42260
C	215	SER	GLY	ENGINEERED MUTATION	UNP P42260
C	390	LEU	-	EXPRESSION TAG	UNP P42260
C	391	GLU	-	EXPRESSION TAG	UNP P42260
C	392	LEU	-	EXPRESSION TAG	UNP P42260
C	393	VAL	-	EXPRESSION TAG	UNP P42260
C	394	PRO	-	EXPRESSION TAG	UNP P42260
C	395	ARG	-	EXPRESSION TAG	UNP P42260
D	213	ASN	ALA	ENGINEERED MUTATION	UNP P42260
D	215	SER	GLY	ENGINEERED MUTATION	UNP P42260
D	390	LEU	-	EXPRESSION TAG	UNP P42260
D	391	GLU	-	EXPRESSION TAG	UNP P42260
D	392	LEU	-	EXPRESSION TAG	UNP P42260
D	393	VAL	-	EXPRESSION TAG	UNP P42260
D	394	PRO	-	EXPRESSION TAG	UNP P42260
D	395	ARG	-	EXPRESSION TAG	UNP P42260

- 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	H	N	O	0	0
			27	8	13	1	5		
3	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
3	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
3	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
3	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
3	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
3	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
3	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
3	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
3	C	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
3	C	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
3	C	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
3	D	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
3	D	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
3	D	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

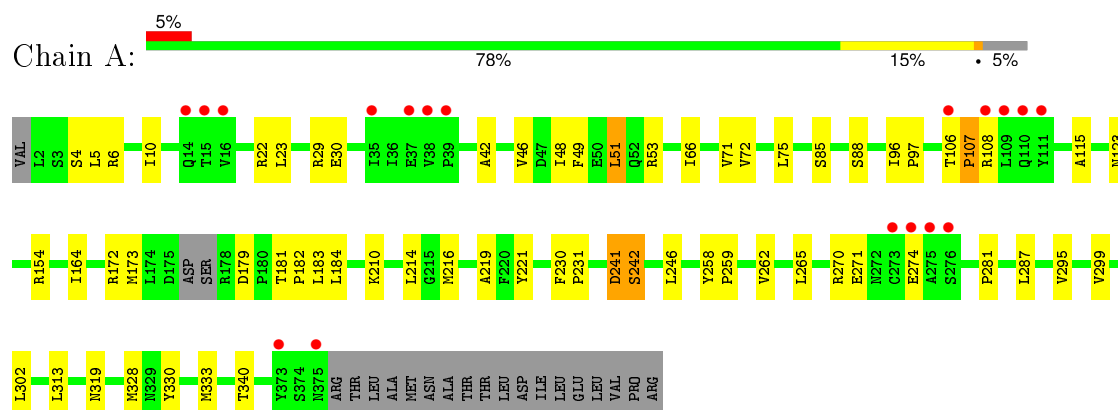
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O	0	0
			1	1		
6	C	2	Total	O	0	0
			2	2		
6	D	3	Total	O	0	0
			3	3		

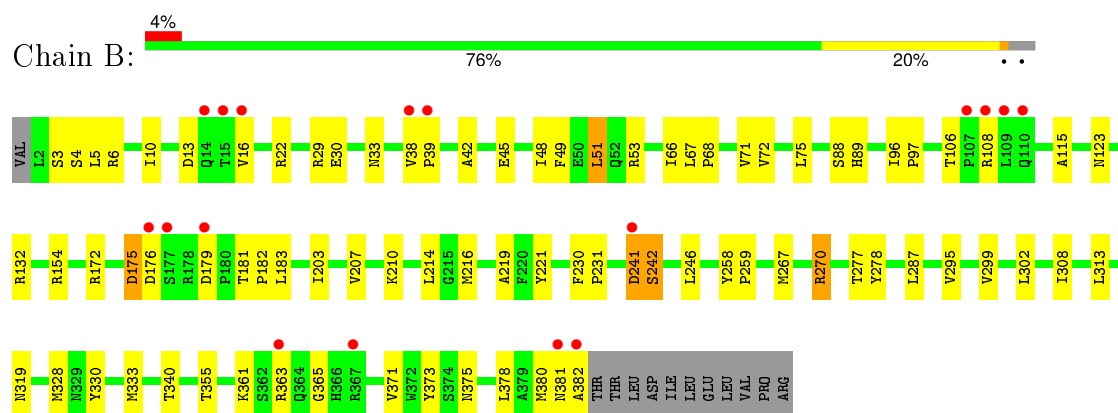
3 Residue-property plots

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

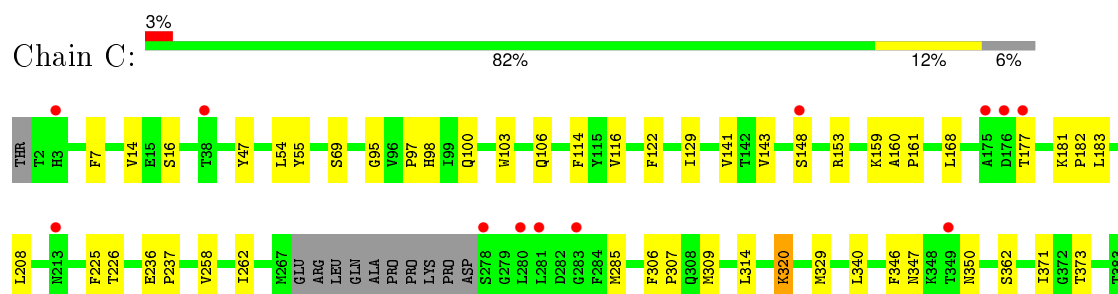
- Molecule 1: Glutamate receptor, ionotropic kainate 5



- Molecule 1: Glutamate receptor, ionotropic kainate 5

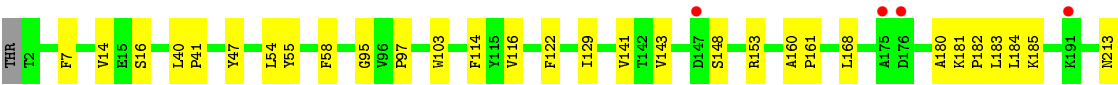
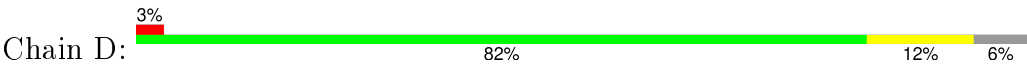


- Molecule 2: Glutamate receptor, ionotropic kainate 2



GLU
SER
GLN
LYS
GLY
LYS
LEU
LEU
LEU
VAL
PRO
ARG

- Molecule 2: Glutamate receptor, ionotropic kainate 2



SER
GLN
LYS
GLY
LYS
LEU
GLU
LEU
VAL
PRO
ARG

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.63Å 139.55Å 195.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.97 – 2.91 29.97 – 2.91	Depositor EDS
% Data completeness (in resolution range)	98.5 (29.97-2.91) 98.5 (29.97-2.91)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 2.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.197 , 0.256 0.183 , 0.243	Depositor DCC
R_{free} test set	1991 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	41.5	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 39760 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	23862	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, CL

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	0.33	0/2955	0.56	3/4006 (0.1%)
1	B	0.32	0/3016	0.55	3/4091 (0.1%)
2	C	0.32	0/3017	0.45	0/4085
2	D	0.32	0/3033	0.45	0/4106
All	All	0.32	0/12021	0.51	6/16288 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	270	ARG	NE-CZ-NH1	-13.08	113.76	120.30
1	A	270	ARG	NE-CZ-NH2	12.60	126.60	120.30
1	B	270	ARG	NE-CZ-NH2	-12.09	114.26	120.30
1	B	270	ARG	NE-CZ-NH1	11.99	126.30	120.30
1	B	270	ARG	CD-NE-CZ	5.68	131.55	123.60
1	A	270	ARG	CD-NE-CZ	5.44	131.22	123.60

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	2895	2878	2886	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2958	2947	2955	65	1
2	C	2951	2897	2907	45	0
2	D	2967	2915	2925	46	0
3	A	70	65	65	5	0
3	B	70	65	65	1	0
3	C	42	39	39	1	0
3	D	42	39	39	1	1
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	B	6	8	8	2	0
6	A	1	0	0	0	0
6	C	2	0	0	0	0
6	D	3	0	0	0	0
All	All	12009	11853	11889	209	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 9.

All (209) 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:5:LEU:HD11	3:A:397:NAG:H81	1.49	0.94
1:A:42:ALA:HB3	3:A:397:NAG:H83	1.64	0.79
2:D:97:PRO:HA	2:D:329:MET:CE	2.15	0.77
2:C:97:PRO:HA	2:C:329:MET:CE	2.20	0.72
1:A:107:PRO:HB2	1:A:108:ARG:CA	2.19	0.71
2:C:320:LYS:H	2:C:320:LYS:HD2	1.54	0.71
2:D:97:PRO:CB	2:D:329:MET:HE2	2.21	0.70
1:A:30:GLU:OE2	1:B:33:ASN:HB2	1.90	0.70
1:A:107:PRO:HB2	1:A:108:ARG:C	2.14	0.68
1:A:115:ALA:CA	1:A:328:MET:HE3	2.25	0.66
1:A:214:LEU:HB2	1:A:216:MET:HE2	1.77	0.66
1:A:30:GLU:OE2	1:B:33:ASN:CB	2.44	0.66
1:A:115:ALA:HA	1:A:328:MET:HE3	1.78	0.66
1:B:214:LEU:HB2	1:B:216:MET:HE2	1.78	0.65
2:D:116:VAL:CG1	2:D:346:PHE:CE1	2.81	0.64
1:B:214:LEU:CB	1:B:216:MET:HE2	2.27	0.64
1:A:271:GLU:CB	1:B:3:SER:CB	2.77	0.62
2:C:141:VAL:HG13	2:C:168:LEU:HD12	1.81	0.62
1:A:107:PRO:HB2	1:A:108:ARG:HA	1.80	0.61
2:C:97:PRO:CB	2:C:329:MET:HE2	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:320:LYS:HD2	2:C:320:LYS:N	2.16	0.61
1:B:381:ASN:O	1:B:382:ALA:HB2	2.00	0.60
2:C:116:VAL:CG1	2:C:346:PHE:CE1	2.84	0.60
2:D:97:PRO:HA	2:D:329:MET:HE1	1.83	0.60
2:D:141:VAL:HG13	2:D:168:LEU:HD12	1.82	0.60
1:A:10:ILE:CG2	1:A:51:LEU:HD12	2.32	0.60
1:A:4:SER:HA	1:A:42:ALA:HB1	1.84	0.58
1:B:179:ASP:O	1:B:182:PRO:HD2	2.03	0.58
2:C:262:ILE:HD13	2:C:285:MET:CE	2.33	0.58
2:C:97:PRO:HG3	2:C:329:MET:HE2	1.86	0.58
1:A:179:ASP:O	1:A:182:PRO:HD2	2.04	0.57
2:D:306:PHE:CE1	2:D:327:ARG:HG2	2.39	0.57
1:B:4:SER:HA	1:B:42:ALA:HB1	1.86	0.57
1:B:51:LEU:CD2	1:B:53:ARG:O	2.53	0.57
2:C:97:PRO:HA	2:C:329:MET:HE1	1.85	0.57
2:D:97:PRO:HB3	2:D:329:MET:HE2	1.85	0.57
1:B:10:ILE:CG2	1:B:51:LEU:HD12	2.34	0.56
2:D:262:ILE:HD13	2:D:285:MET:CE	2.35	0.56
1:B:96:ILE:HD11	1:B:313:LEU:HD12	1.87	0.56
1:A:29[B]:ARG:HD3	1:B:30:GLU:OE2	2.06	0.56
1:A:214:LEU:CD2	1:A:216:MET:HE1	2.35	0.56
2:C:373:THR:HG21	3:C:398:NAG:O6	2.06	0.56
1:B:230:PHE:N	1:B:231:PRO:CD	2.69	0.56
1:A:97:PRO:HA	1:A:328:MET:CE	2.36	0.56
2:D:143:VAL:HG23	2:D:168:LEU:HD11	1.87	0.55
1:B:97:PRO:HA	1:B:328:MET:CE	2.37	0.55
1:A:230:PHE:N	1:A:231:PRO:CD	2.70	0.55
2:D:97:PRO:CA	2:D:329:MET:CE	2.83	0.55
1:B:210:LYS:O	1:B:214:LEU:HD13	2.06	0.55
2:C:143:VAL:HG23	2:C:168:LEU:HD11	1.88	0.55
1:B:181:THR:N	1:B:182:PRO:CD	2.69	0.55
1:A:214:LEU:CB	1:A:216:MET:HE2	2.35	0.54
2:D:97:PRO:HG3	2:D:329:MET:HE2	1.88	0.54
1:A:5:LEU:CD1	3:A:397:NAG:H81	2.29	0.54
1:A:51:LEU:CD2	1:A:53:ARG:O	2.56	0.54
1:B:381:ASN:O	1:B:382:ALA:CB	2.55	0.54
2:D:236:GLU:HB3	2:D:237:PRO:HD3	1.90	0.54
2:C:97:PRO:CA	2:C:329:MET:CE	2.86	0.54
2:C:262:ILE:HD13	2:C:285:MET:HE2	1.90	0.54
1:A:5:LEU:HD11	3:A:397:NAG:C8	2.32	0.53
2:C:7:PHE:O	2:C:47:TYR:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:ALA:CA	1:B:328:MET:HE3	2.38	0.53
2:D:97:PRO:CG	2:D:329:MET:HE2	2.40	0.52
1:B:219:ALA:HB2	1:B:242:SER:HB3	1.91	0.52
1:A:181:THR:N	1:A:182:PRO:CD	2.73	0.52
1:A:210:LYS:O	1:A:214:LEU:HD13	2.10	0.52
1:A:219:ALA:HB2	1:A:242:SER:HB3	1.92	0.52
2:C:236:GLU:HB3	2:C:237:PRO:HD3	1.91	0.52
1:B:258:TYR:HB3	1:B:259:PRO:HD3	1.92	0.52
1:B:22:ARG:HB3	5:B:400:GOL:H32	1.91	0.51
2:D:97:PRO:CA	2:D:329:MET:HE2	2.41	0.51
2:C:54:LEU:O	2:C:55:TYR:HB2	2.10	0.51
2:C:97:PRO:HB3	2:C:329:MET:CE	2.40	0.51
2:C:183:LEU:HD23	2:C:183:LEU:C	2.31	0.51
1:A:22:ARG:HG3	1:A:48:ILE:CD1	2.41	0.50
2:D:306:PHE:CZ	2:D:327:ARG:HG2	2.47	0.50
1:B:132:ARG:HG3	1:B:378:LEU:HG	1.93	0.50
2:D:54:LEU:O	2:D:55:TYR:HB2	2.12	0.50
2:D:320:LYS:HE3	2:D:320:LYS:N	2.25	0.50
1:A:258:TYR:HB3	1:A:259:PRO:HD3	1.94	0.50
1:A:96:ILE:HD11	1:A:313:LEU:HD12	1.93	0.50
2:D:7:PHE:O	2:D:47:TYR:HA	2.12	0.49
2:C:97:PRO:CG	2:C:329:MET:HE2	2.42	0.49
1:A:97:PRO:CB	1:A:328:MET:HE2	2.42	0.49
2:D:213:ASN:OD1	3:D:397:NAG:C5	2.60	0.49
2:D:262:ILE:HD13	2:D:285:MET:HE2	1.92	0.49
2:D:97:PRO:HB3	2:D:329:MET:CE	2.43	0.49
1:B:287:LEU:HD23	1:B:340:THR:HG21	1.95	0.49
2:D:262:ILE:CD1	2:D:285:MET:HE2	2.42	0.48
2:C:181:LYS:N	2:C:182:PRO:CD	2.76	0.48
1:B:241:ASP:HB2	1:B:363:ARG:NH1	2.29	0.48
2:D:183:LEU:HD23	2:D:183:LEU:C	2.34	0.48
2:C:97:PRO:CB	2:C:329:MET:CE	2.92	0.48
1:B:214:LEU:CD2	1:B:216:MET:HE1	2.44	0.48
2:C:262:ILE:CD1	2:C:285:MET:HE2	2.44	0.48
2:C:262:ILE:CD1	2:C:285:MET:CE	2.92	0.48
1:B:97:PRO:CB	1:B:328:MET:HE2	2.44	0.47
1:B:97:PRO:HA	1:B:328:MET:HE2	1.95	0.47
1:B:22:ARG:HG3	1:B:48:ILE:CD1	2.44	0.47
1:B:175:ASP:O	1:B:176:ASP:HB2	2.13	0.47
1:A:184:LEU:HB3	1:A:216:MET:HE3	1.96	0.47
1:B:214:LEU:HD22	1:B:216:MET:HE1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:SER:CB	1:A:106:THR:HG21	2.44	0.47
2:C:97:PRO:HB3	2:C:329:MET:HE2	1.96	0.47
2:D:116:VAL:HG13	2:D:346:PHE:CD1	2.50	0.47
2:D:129:ILE:CD1	2:D:226:THR:HG22	2.44	0.47
2:D:262:ILE:CD1	2:D:285:MET:CE	2.92	0.47
2:D:97:PRO:CB	2:D:329:MET:CE	2.92	0.47
1:A:115:ALA:C	1:A:328:MET:HE3	2.35	0.47
1:A:97:PRO:HA	1:A:328:MET:HE2	1.95	0.47
1:B:49:PHE:CE1	1:B:66:ILE:HG12	2.50	0.47
1:A:287:LEU:HD23	1:A:340:THR:HG21	1.96	0.46
1:A:172:ARG:HB3	1:A:183:LEU:HD22	1.96	0.46
2:D:258:VAL:O	2:D:262:ILE:HG12	2.16	0.46
2:D:143:VAL:CG2	2:D:168:LEU:HD11	2.46	0.46
1:B:267:MET:HG2	1:B:270:ARG:NH2	2.29	0.46
1:A:6:ARG:HG2	1:A:71:VAL:HG12	1.98	0.46
1:B:214:LEU:HB3	1:B:216:MET:HE2	1.97	0.46
1:B:132:ARG:CG	1:B:378:LEU:HG	2.46	0.46
2:C:129:ILE:CD1	2:C:226:THR:HG22	2.45	0.46
1:A:330:TYR:HA	1:A:333:MET:HE2	1.98	0.46
1:A:29[B]:ARG:NH2	1:A:46:VAL:H	2.14	0.45
2:D:181:LYS:N	2:D:182:PRO:CD	2.78	0.45
1:B:375:ASN:O	1:B:375:ASN:OD1	2.34	0.45
1:A:216:MET:HG2	1:A:221:TYR:CZ	2.52	0.45
1:B:295:VAL:O	1:B:299:VAL:HG23	2.16	0.45
2:D:180:ALA:O	2:D:184:LEU:HG	2.16	0.45
1:B:278:TYR:CD2	3:B:396:NAG:H82	2.52	0.45
1:A:214:LEU:HD22	1:A:216:MET:HE1	1.98	0.45
2:C:306:PHE:N	2:C:307:PRO:HD3	2.32	0.45
2:C:160:ALA:HB3	2:C:161:PRO:HD3	1.98	0.45
1:B:175:ASP:O	1:B:176:ASP:CB	2.64	0.45
2:D:185:LYS:HG3	2:D:214:MET:HE1	1.99	0.45
1:A:97:PRO:CA	1:A:328:MET:HE2	2.46	0.45
1:B:216:MET:HG2	1:B:221:TYR:CZ	2.52	0.45
1:B:72:VAL:HG11	1:B:299:VAL:HG21	1.98	0.45
1:A:23:LEU:HD23	1:A:265:LEU:HD12	1.99	0.45
1:B:97:PRO:CA	1:B:328:MET:HE2	2.46	0.44
1:A:72:VAL:HG11	1:A:299:VAL:HG21	1.99	0.44
1:A:164:ILE:HB	2:C:168:LEU:HB3	1.98	0.44
2:C:143:VAL:CG2	2:C:168:LEU:HD11	2.47	0.44
1:B:172:ARG:HB3	1:B:183:LEU:HD22	2.00	0.44
1:A:30:GLU:OE2	1:B:33:ASN:HB3	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:PHE:CE1	1:A:66:ILE:HG12	2.53	0.44
1:B:214:LEU:HB2	1:B:216:MET:CE	2.48	0.44
1:B:13:ASP:HB3	5:B:400:GOL:O1	2.17	0.44
1:A:246:LEU:CD1	1:A:246:LEU:N	2.81	0.44
1:B:123:ASN:HB3	1:B:154:ARG:O	2.18	0.44
1:B:51:LEU:HD23	1:B:53:ARG:O	2.17	0.44
2:D:160:ALA:HB3	2:D:161:PRO:HD3	1.99	0.44
2:C:116:VAL:HG13	2:C:346:PHE:CD1	2.53	0.43
2:C:160:ALA:N	2:C:161:PRO:CD	2.81	0.43
2:C:69:SER:HA	2:C:314:LEU:O	2.18	0.43
2:C:95:GLY:HA2	2:C:114:PHE:CD2	2.53	0.43
2:C:14:VAL:HG12	2:C:16:SER:N	2.33	0.43
2:D:14:VAL:HG12	2:D:16:SER:N	2.32	0.43
1:A:107:PRO:CB	1:A:108:ARG:HA	2.48	0.43
2:C:362:SER:CB	2:C:371:ILE:HD13	2.48	0.43
1:B:29:ARG:NH1	1:B:45:GLU:OE2	2.51	0.43
2:C:258:VAL:O	2:C:262:ILE:HG12	2.19	0.43
1:A:230:PHE:HB3	1:A:231:PRO:HD3	2.00	0.43
1:A:173:MET:HG3	2:C:159:LYS:HE2	1.99	0.43
1:A:5:LEU:CD1	3:A:397:NAG:C8	2.95	0.43
1:A:214:LEU:HD23	1:A:216:MET:HE1	2.00	0.43
2:D:236:GLU:N	2:D:237:PRO:CD	2.81	0.43
2:C:236:GLU:N	2:C:237:PRO:CD	2.82	0.43
2:C:183:LEU:HD23	2:C:183:LEU:O	2.18	0.43
1:B:38:VAL:HA	1:B:39:PRO:C	2.38	0.43
2:D:362:SER:CB	2:D:371:ILE:HD13	2.49	0.43
1:A:214:LEU:HB2	1:A:216:MET:CE	2.47	0.43
2:D:160:ALA:N	2:D:161:PRO:CD	2.81	0.43
1:B:302:LEU:HD23	1:B:308:ILE:HD13	2.01	0.43
2:D:129:ILE:HD11	2:D:226:THR:HG22	2.01	0.43
1:A:123:ASN:HB3	1:A:154:ARG:O	2.18	0.43
1:B:355:THR:HG22	1:B:373:TYR:CD2	2.54	0.43
1:B:330:TYR:HA	1:B:333:MET:HE2	2.01	0.42
1:A:5:LEU:H	1:A:5:LEU:HD12	1.84	0.42
1:B:115:ALA:HA	1:B:328:MET:HE3	2.00	0.42
2:C:309:MET:HE2	2:C:309:MET:HB2	1.78	0.42
1:B:246:LEU:N	1:B:246:LEU:CD1	2.82	0.42
1:B:5:LEU:HD12	1:B:5:LEU:H	1.84	0.42
2:D:103:TRP:CZ2	2:D:153:ARG:HB3	2.55	0.42
1:B:6:ARG:HG2	1:B:71:VAL:HG12	2.01	0.42
1:B:230:PHE:CZ	1:B:361:LYS:HG2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:LEU:HD13	1:A:330:TYR:CD2	2.55	0.42
2:D:95:GLY:HA2	2:D:114:PHE:CD2	2.55	0.42
1:B:67:LEU:HB2	1:B:68:PRO:HD3	2.02	0.42
1:A:75:LEU:N	1:A:75:LEU:HD12	2.35	0.42
1:B:10:ILE:HG21	1:B:51:LEU:HD12	2.00	0.41
1:B:67:LEU:N	1:B:68:PRO:CD	2.83	0.41
1:A:262:VAL:HG22	1:A:281:PRO:HG3	2.03	0.41
2:C:347:ASN:HB3	2:C:350:ASN:OD1	2.20	0.41
2:C:285:MET:CE	2:C:340:LEU:HD13	2.50	0.41
1:A:51:LEU:HD23	1:A:53:ARG:O	2.20	0.41
1:B:203:ILE:O	1:B:207:VAL:HG23	2.21	0.41
2:C:103:TRP:CZ2	2:C:153:ARG:HB3	2.56	0.41
1:B:75:LEU:N	1:B:75:LEU:HD12	2.36	0.41
1:A:295:VAL:O	1:A:299:VAL:HG23	2.21	0.41
1:A:241:ASP:C	1:A:241:ASP:OD1	2.59	0.41
2:D:347:ASN:HB3	2:D:350:ASN:OD1	2.21	0.41
2:D:40:LEU:N	2:D:41:PRO:HD3	2.36	0.41
2:D:285:MET:CE	2:D:340:LEU:HD13	2.51	0.40
1:B:89:HIS:HD2	2:D:58:PHE:HB2	1.86	0.40
2:C:98:HIS:CD2	2:C:100:GLN:HE21	2.40	0.40
1:B:230:PHE:HB3	1:B:231:PRO:HD3	2.03	0.40
2:D:183:LEU:O	2:D:183:LEU:HD23	2.22	0.40
2:D:233:LEU:HD12	2:D:280:LEU:CD1	2.51	0.40
1:B:302:LEU:HD23	1:B:308:ILE:CD1	2.51	0.40
2:C:208:LEU:HD21	2:C:225:PHE:HZ	1.87	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:277:THR:O	3:D:397:NAG:O7[1_455]	2.17	0.03

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	370/393 (94%)	356 (96%)	13 (4%)	1 (0%)	46	79
1	B	380/393 (97%)	364 (96%)	14 (4%)	2 (0%)	34	71
2	C	368/395 (93%)	357 (97%)	11 (3%)	0	100	100
2	D	369/395 (93%)	354 (96%)	15 (4%)	0	100	100
All	All	1487/1576 (94%)	1431 (96%)	53 (4%)	3 (0%)	52	84

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	108	ARG
1	A	107	PRO
1	B	365	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	322/346 (93%)	316 (98%)	6 (2%)	65	89
1	B	330/346 (95%)	320 (97%)	10 (3%)	48	83
2	C	322/348 (92%)	317 (98%)	5 (2%)	70	91
2	D	325/348 (93%)	321 (99%)	4 (1%)	78	94
All	All	1299/1388 (94%)	1274 (98%)	25 (2%)	65	89

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

Mol	Chain	Res	Type
1	A	51	LEU
1	A	88	SER
1	A	241	ASP
1	A	242	SER
1	A	274	GLU

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Mol	Chain	Res	Type
1	A	319	ASN
1	B	16	VAL
1	B	51	LEU
1	B	88	SER
1	B	106	THR
1	B	175	ASP
1	B	241	ASP
1	B	242	SER
1	B	319	ASN
1	B	371	VAL
1	B	380	MET
2	C	106	GLN
2	C	122	PHE
2	C	148	SER
2	C	177	THR
2	C	320	LYS
2	D	122	PHE
2	D	148	SER
2	D	318	ARG
2	D	320	LYS

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	255	HIS
1	A	319	ASN
1	A	350	GLN
1	B	89	HIS
1	B	255	HIS
1	B	319	ASN
1	B	350	GLN
2	C	67	GLN
2	C	98	HIS
2	C	105	HIS
2	C	110	ASN
2	C	305	GLN
2	D	67	GLN
2	D	98	HIS
2	D	110	ASN
2	D	305	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 for Mogul analysis.

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	394	1	14,14,15	0.47	0	15,19,21	0.87	0
3	NAG	A	395	1	14,14,15	0.50	0	15,19,21	0.83	0
3	NAG	A	396	1	14,14,15	0.40	0	15,19,21	1.62	1 (6%)
3	NAG	A	397	1	14,14,15	0.52	0	15,19,21	1.35	2 (13%)
3	NAG	A	398	1	14,14,15	0.46	0	15,19,21	1.41	1 (6%)
3	NAG	B	394	1	14,14,15	0.45	0	15,19,21	2.10	6 (40%)
3	NAG	B	395	1	14,14,15	0.40	0	15,19,21	1.83	1 (6%)
3	NAG	B	396	1	14,14,15	0.42	0	15,19,21	1.11	2 (13%)
3	NAG	B	397	1	14,14,15	0.45	0	15,19,21	0.95	1 (6%)
3	NAG	B	398	1	14,14,15	0.50	0	15,19,21	0.76	1 (6%)
5	GOL	B	400	-	5,5,5	0.42	0	5,5,5	0.66	0
3	NAG	C	396	2	14,14,15	0.61	0	15,19,21	0.73	0
3	NAG	C	397	2	14,14,15	0.56	0	15,19,21	1.13	1 (6%)
3	NAG	C	398	2	14,14,15	0.49	0	15,19,21	1.99	2 (13%)
3	NAG	D	396	2	14,14,15	0.54	0	15,19,21	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	D	397	2	14,14,15	0.78	0	15,19,21	1.57	3 (20%)
3	NAG	D	398	2	14,14,15	0.53	0	15,19,21	0.94	1 (6%)

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	394	1	-	0/6/23/26	0/1/1/1
3	NAG	A	395	1	-	0/6/23/26	0/1/1/1
3	NAG	A	396	1	-	0/6/23/26	0/1/1/1
3	NAG	A	397	1	-	0/6/23/26	0/1/1/1
3	NAG	A	398	1	-	0/6/23/26	0/1/1/1
3	NAG	B	394	1	-	0/6/23/26	0/1/1/1
3	NAG	B	395	1	-	0/6/23/26	0/1/1/1
3	NAG	B	396	1	-	0/6/23/26	0/1/1/1
3	NAG	B	397	1	-	0/6/23/26	0/1/1/1
3	NAG	B	398	1	-	0/6/23/26	0/1/1/1
5	GOL	B	400	-	-	0/4/4/4	0/0/0/0
3	NAG	C	396	2	-	0/6/23/26	0/1/1/1
3	NAG	C	397	2	-	0/6/23/26	0/1/1/1
3	NAG	C	398	2	1/1/6/7	0/6/23/26	0/1/1/1
3	NAG	D	396	2	-	0/6/23/26	0/1/1/1
3	NAG	D	397	2	1/1/6/7	0/6/23/26	0/1/1/1
3	NAG	D	398	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	398	NAG	C2-N2-C7	-4.57	117.17	123.04
3	B	394	NAG	C4-C3-C2	-3.79	105.34	111.23
3	A	397	NAG	C2-N2-C7	-2.80	119.44	123.04
3	C	397	NAG	C2-N2-C7	-2.63	119.66	123.04
3	B	394	NAG	C6-C5-C4	-2.38	107.13	113.02
3	D	397	NAG	C2-N2-C7	-2.32	120.06	123.04
3	D	397	NAG	C1-O5-C5	-2.18	109.49	112.25
3	B	396	NAG	C6-C5-C4	-2.04	107.97	113.02
3	B	398	NAG	C1-O5-C5	2.02	114.81	112.25
3	B	394	NAG	O5-C5-C6	2.12	111.95	107.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	398	NAG	C1-O5-C5	2.24	115.09	112.25
3	B	394	NAG	C8-C7-N2	2.28	120.48	116.11
3	B	397	NAG	O5-C5-C6	2.29	112.30	107.35
3	B	396	NAG	C1-O5-C5	2.51	115.44	112.25
3	B	394	NAG	O3-C3-C2	2.56	114.19	109.11
3	A	397	NAG	C1-O5-C5	3.21	116.32	112.25
3	D	397	NAG	C4-C3-C2	3.71	117.00	111.23
3	A	398	NAG	C1-O5-C5	4.26	117.66	112.25
3	B	394	NAG	C1-O5-C5	4.82	118.36	112.25
3	C	398	NAG	C1-O5-C5	5.10	118.72	112.25
3	A	396	NAG	C1-O5-C5	5.44	119.15	112.25
3	B	395	NAG	C1-O5-C5	6.04	119.91	112.25

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	398	NAG	C1
3	D	397	NAG	C1

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	397	NAG	5	0
3	B	396	NAG	1	0
5	B	400	GOL	2	0
3	C	398	NAG	1	0
3	D	397	NAG	1	1

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	372/393 (94%)	-0.07	18 (4%) 34 28	10, 35, 92, 165	0
1	B	381/393 (96%)	-0.10	17 (4%) 37 31	9, 35, 92, 179	0
2	C	372/395 (94%)	-0.10	12 (3%) 51 43	17, 39, 79, 114	0
2	D	373/395 (94%)	-0.14	12 (3%) 51 43	18, 40, 81, 114	0
All	All	1498/1576 (95%)	-0.10	59 (3%) 43 36	9, 37, 85, 179	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	39	PRO	5.9
1	B	382	ALA	4.7
1	A	275	ALA	4.5
1	A	111	TYR	4.4
2	D	349	THR	4.4
1	B	15	THR	4.2
1	A	38	VAL	4.2
1	B	16	VAL	4.0
1	B	38	VAL	4.0
1	B	241	ASP	3.9
1	A	109	LEU	3.8
1	B	176	ASP	3.8
1	B	39	PRO	3.8
1	A	15	THR	3.6
2	D	280	LEU	3.4
1	A	106	THR	3.3
2	C	283	GLY	3.2
1	B	107	PRO	3.2
1	A	276	SER	3.2
1	B	381	ASN	3.1
1	B	110	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	108	ARG	3.1
1	B	109	LEU	3.1
2	D	147	ASP	2.9
1	A	16	VAL	2.9
1	A	274	GLU	2.8
1	A	373	TYR	2.8
2	D	282	ASP	2.7
2	D	176	ASP	2.7
2	D	278	SER	2.7
2	C	349	THR	2.6
2	C	38	THR	2.5
1	A	37	GLU	2.5
1	A	110	GLN	2.5
2	C	280	LEU	2.5
2	C	278	SER	2.5
2	C	175	ALA	2.5
2	C	177	THR	2.5
1	B	367	ARG	2.4
2	D	175	ALA	2.4
1	B	177	SER	2.4
2	D	240	TYR	2.4
2	C	3	HIS	2.3
1	B	108	ARG	2.3
1	A	375	ASN	2.3
2	D	267	MET	2.2
1	B	14	GLN	2.2
1	B	179	ASP	2.2
2	D	320	LYS	2.2
2	C	281	LEU	2.2
2	C	148	SER	2.2
1	B	363	ARG	2.2
1	A	14	GLN	2.2
1	A	273	CYS	2.1
2	C	176	ASP	2.1
2	D	191	LYS	2.1
2	C	213	ASN	2.0
1	A	35	ILE	2.0
2	D	381	ASN	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 [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
3	NAG	C	398	14/15	0.87	0.39	6.74	48,102,132,132	0
3	NAG	B	398	14/15	0.71	0.44	4.87	96,116,145,150	0
3	NAG	D	397	14/15	0.86	0.36	3.23	82,106,131,142	0
3	NAG	B	397	14/15	0.90	0.30	2.92	42,62,90,94	0
3	NAG	A	398	14/15	0.88	0.34	1.88	64,88,105,109	0
4	CL	B	399	1/1	0.97	0.22	1.44	46,46,46,46	0
3	NAG	B	395	14/15	0.92	0.19	1.34	32,55,85,85	0
3	NAG	A	394	14/15	0.86	0.29	1.22	47,94,114,124	0
3	NAG	C	397	14/15	0.88	0.30	0.97	40,64,78,79	0
3	NAG	D	398	14/15	0.88	0.31	0.85	60,83,100,100	0
3	NAG	D	396	14/15	0.82	0.27	0.65	66,81,98,109	0
3	NAG	A	396	14/15	0.89	0.27	0.58	54,67,85,92	0
3	NAG	A	397	14/15	0.86	0.28	0.16	60,75,94,101	0
3	NAG	B	396	14/15	0.89	0.18	-0.15	32,64,81,83	0
3	NAG	C	396	14/15	0.91	0.22	-0.24	43,106,133,135	0
5	GOL	B	400	6/6	0.88	0.18	-0.46	25,49,68,82	0
3	NAG	A	395	14/15	0.96	0.14	-0.90	26,39,62,75	0
4	CL	C	399	1/1	0.93	0.08	-	53,53,53,53	0
3	NAG	B	394	14/15	0.86	0.28	-	58,103,132,142	0

6.5 Other polymers [i](#)

There are no such residues in this entry.