



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 01:01 pm GMT

PDB ID : 2E4U
Title : Crystal structure of the extracellular region of the group II metabotropic glutamate receptor complexed with L-glutamate
Authors : Muto, T.; Tsuchiya, D.; Morikawa, K.; Jingami, H.
Deposited on : 2006-12-17
Resolution : 2.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

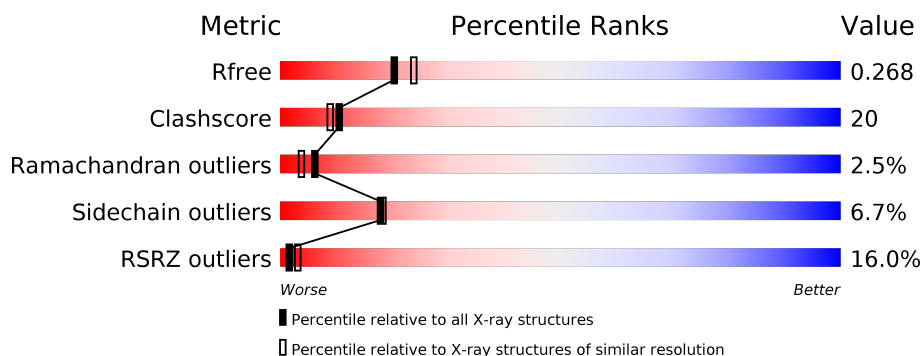
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	111664	1015 (2.36-2.36)
Clashscore	122126	1081 (2.36-2.36)
Ramachandran outliers	120053	1066 (2.36-2.36)
Sidechain outliers	120020	1067 (2.36-2.36)
RSRZ outliers	108989	1002 (2.36-2.36)

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	555	<div> <div>15%</div> <div> <div></div> <div>60%</div> <div>27%</div> <div>5%</div> <div>8%</div> </div> </div>
1	B	555	<div> <div>15%</div> <div> <div></div> <div>61%</div> <div>28%</div> <div>•</div> <div>7%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8463 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 Metabotropic glutamate receptor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	512	Total	C	N	O	S	0	0	0
			4061	2574	692	768	27			
1	B	514	Total	C	N	O	S	0	0	0
			4080	2588	694	770	28			

There are 12 discrepancies between the modelled and reference sequences:

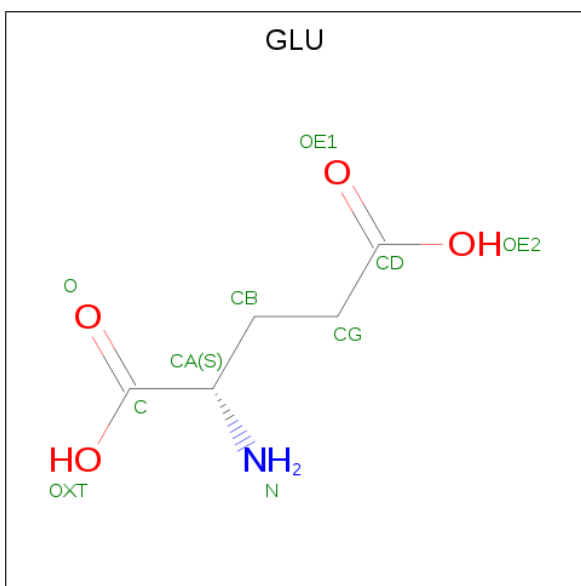
Chain	Residue	Modelled	Actual	Comment	Reference
A	414	GLN	ASN	ENGINEERED	UNP P31422
A	439	GLN	ASN	ENGINEERED	UNP P31422
A	576	LEU	-	CLONING ARTIFACT	UNP P31422
A	577	VAL	-	CLONING ARTIFACT	UNP P31422
A	578	PRO	-	CLONING ARTIFACT	UNP P31422
A	579	ARG	-	CLONING ARTIFACT	UNP P31422
B	414	GLN	ASN	ENGINEERED	UNP P31422
B	439	GLN	ASN	ENGINEERED	UNP P31422
B	576	LEU	-	CLONING ARTIFACT	UNP P31422
B	577	VAL	-	CLONING ARTIFACT	UNP P31422
B	578	PRO	-	CLONING ARTIFACT	UNP P31422
B	579	ARG	-	CLONING ARTIFACT	UNP P31422

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 3 is GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	5	1	4		
3	B	1	Total	C	N	O	0	0
			10	5	1	4		

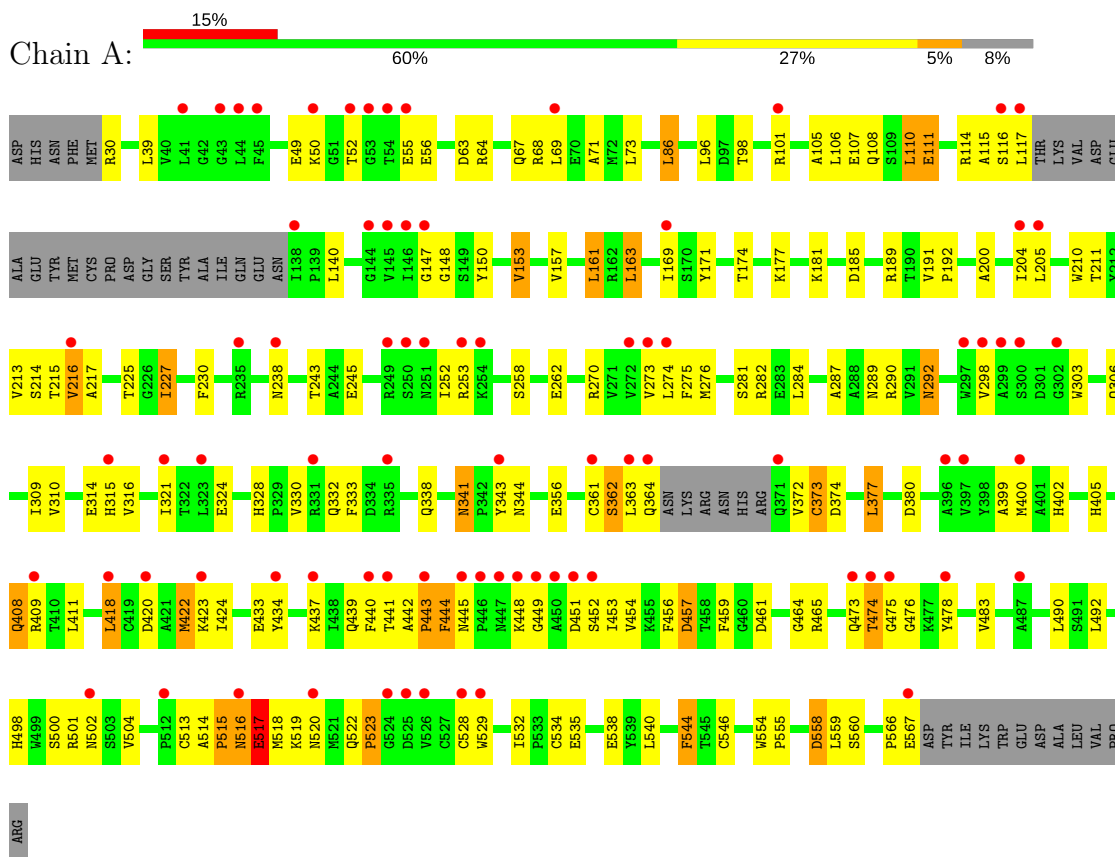
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	157	Total 157	O 157	0	0
4	B	117	Total 117	O 117	0	0

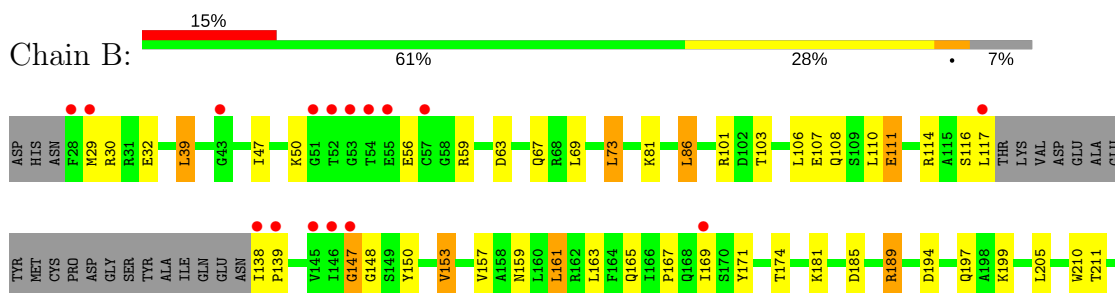
3 Residue-property plots

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: Metabotropic glutamate receptor 3



• Molecule 1: Metabotropic glutamate receptor 3





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.00Å 97.47Å 108.07Å 90.00° 92.95° 90.00°	Depositor
Resolution (Å)	20.00 – 2.35 29.31 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.35) 99.9 (29.31-2.35)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.36Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.238 , 0.267 0.238 , 0.268	Depositor DCC
R_{free} test set	5160 reflections (7.12%)	wwPDB-VP
Wilson B-factor (Å ²)	49.4	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8463	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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: NAG

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	0.40	0/4153	0.67	1/5625 (0.0%)
1	B	0.39	0/4173	0.66	3/5651 (0.1%)
All	All	0.40	0/8326	0.67	4/11276 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	546	CYS	CA-CB-SG	-7.69	100.16	114.00
1	A	148	GLY	N-CA-C	-6.29	97.39	113.10
1	B	148	GLY	N-CA-C	-6.05	97.97	113.10
1	B	147	GLY	N-CA-C	5.05	125.73	113.10

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	4061	0	3934	162	0
1	B	4080	0	3953	159	0
2	A	14	0	13	1	0
2	B	14	0	13	0	0
3	A	10	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	10	0	5	1	0
4	A	157	0	0	16	0
4	B	117	0	0	8	0
All	All	8463	0	7923	319	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 20.

All (319) 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:B:30:ARG:HD2	1:B:108:GLN:HE22	1.18	1.05
1:B:165:GLN:HG3	4:B:846:HOH:O	1.57	1.02
1:A:356:GLU:HA	1:A:361:CYS:HB2	1.49	0.95
1:B:514:ALA:H	1:B:518:MET:HE3	1.31	0.94
1:A:515:PRO:HG2	1:A:516:ASN:H	1.34	0.92
1:A:420:ASP:HA	1:A:423:LYS:HD3	1.52	0.91
1:A:514:ALA:H	1:A:518:MET:HE3	1.34	0.91
1:A:402:HIS:HB3	1:A:437:LYS:HE2	1.52	0.90
1:B:356:GLU:HA	1:B:361:CYS:HB2	1.50	0.90
1:B:402:HIS:HB3	1:B:437:LYS:HE2	1.57	0.85
1:B:514:ALA:HB3	1:B:518:MET:HG3	1.57	0.85
1:A:514:ALA:HB3	1:A:518:MET:HG3	1.62	0.82
1:B:515:PRO:HG2	1:B:516:ASN:H	1.47	0.80
1:A:181:LYS:HE2	1:A:459:PHE:O	1.80	0.80
1:A:30:ARG:HA	4:A:937:HOH:O	1.82	0.80
1:B:328:HIS:HB2	4:B:827:HOH:O	1.84	0.77
1:B:47:ILE:HD12	1:B:69:LEU:HD12	1.64	0.77
1:A:157:VAL:HG12	1:A:161:LEU:HD22	1.67	0.76
1:B:341:ASN:HD22	1:B:343:TYR:H	1.28	0.76
1:B:216:VAL:HG13	1:B:274:LEU:HD23	1.67	0.76
1:A:101:ARG:HD3	4:A:870:HOH:O	1.86	0.75
1:A:276:MET:HE3	1:A:281:SER:HA	1.68	0.75
1:A:107:GLU:HB3	4:A:917:HOH:O	1.86	0.74
1:B:86:LEU:H	1:B:405:HIS:HD1	1.33	0.74
1:A:216:VAL:HG13	1:A:274:LEU:HD23	1.69	0.74
1:B:282:ARG:HG2	1:B:282:ARG:HH11	1.51	0.74
1:B:103:THR:O	1:B:107:GLU:HG2	1.87	0.73
1:A:216:VAL:HG13	1:A:274:LEU:CD2	2.18	0.73
1:B:420:ASP:HA	1:B:423:LYS:HD3	1.71	0.72
1:A:50:LYS:HE3	4:A:870:HOH:O	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:HIS:NE2	1:A:409:ARG:NE	2.37	0.72
1:B:287:ALA:HA	1:B:290:ARG:NH1	2.05	0.72
1:A:400:MET:SD	4:A:947:HOH:O	2.47	0.71
1:B:310:VAL:CG1	1:B:314:GLU:HA	2.20	0.71
1:A:56:GLU:HG2	1:A:101:ARG:HH22	1.55	0.71
1:B:514:ALA:H	1:B:518:MET:CE	2.01	0.71
1:B:310:VAL:HG12	1:B:314:GLU:HA	1.72	0.70
1:A:442:ALA:O	1:A:444:PHE:N	2.25	0.69
1:B:258:SER:O	1:B:262:GLU:HG3	1.92	0.69
1:A:310:VAL:HG12	1:A:314:GLU:HA	1.72	0.69
1:A:282:ARG:HH11	1:A:282:ARG:HG2	1.58	0.68
1:A:341:ASN:HD22	1:A:343:TYR:H	1.42	0.68
1:B:252:ILE:HG22	1:B:253:ARG:H	1.59	0.67
1:A:211:THR:HG23	1:A:238:ASN:O	1.95	0.67
1:B:442:ALA:O	1:B:444:PHE:N	2.28	0.67
1:A:519:LYS:HD2	1:A:546:CYS:SG	2.34	0.67
1:B:30:ARG:HD2	1:B:108:GLN:NE2	2.02	0.67
1:B:483:VAL:O	1:B:492:LEU:HB2	1.95	0.66
1:A:287:ALA:HA	1:A:290:ARG:NH1	2.10	0.66
1:B:540:LEU:HD12	1:B:546:CYS:SG	2.35	0.66
1:A:523:PRO:HD2	1:A:528:CYS:O	1.96	0.66
1:B:157:VAL:HG12	1:B:161:LEU:HD22	1.77	0.66
1:A:405:HIS:NE2	1:A:409:ARG:CZ	2.58	0.66
1:A:515:PRO:CG	1:A:516:ASN:H	2.08	0.66
1:B:215:THR:OG1	1:B:241:ILE:HD11	1.96	0.66
1:A:252:ILE:HG22	1:A:253:ARG:H	1.61	0.66
1:B:473:GLN:HE21	1:B:476:GLY:CA	2.08	0.65
1:A:402:HIS:CB	1:A:437:LYS:HE2	2.26	0.65
1:B:330:VAL:HG13	1:B:444:PHE:HB3	1.79	0.64
1:B:362:SER:O	1:B:363:LEU:HD13	1.98	0.64
1:A:258:SER:O	1:A:262:GLU:HG3	1.97	0.64
1:A:558:ASP:OD1	1:A:560:SER:HB3	1.98	0.63
1:B:50:LYS:HG3	1:B:101:ARG:HD3	1.79	0.63
1:A:514:ALA:H	1:A:518:MET:CE	2.08	0.63
1:A:330:VAL:HG13	1:A:444:PHE:HB3	1.81	0.63
1:B:409:ARG:HD3	4:B:834:HOH:O	1.97	0.63
1:B:473:GLN:HE21	1:B:476:GLY:HA2	1.64	0.63
1:B:289:ASN:HA	1:B:316:VAL:HG21	1.81	0.62
1:B:216:VAL:HG13	1:B:274:LEU:CD2	2.28	0.62
1:B:47:ILE:CD1	1:B:69:LEU:HD12	2.29	0.62
1:A:328:HIS:HB2	4:A:885:HOH:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:GLN:HE21	1:A:476:GLY:CA	2.13	0.62
1:B:374:ASP:HB3	1:B:377:LEU:HD22	1.80	0.61
1:A:473:GLN:HE21	1:A:476:GLY:HA2	1.66	0.61
1:A:169:ILE:HG12	1:A:434:TYR:OH	2.00	0.61
1:B:169:ILE:HD13	1:B:434:TYR:OH	2.00	0.61
1:B:451:ASP:OD1	1:B:453:ILE:HG12	1.99	0.61
1:B:523:PRO:HD2	1:B:528:CYS:O	1.99	0.61
1:B:181:LYS:HE2	1:B:181:LYS:HA	1.83	0.61
1:B:352:ARG:HG3	4:B:879:HOH:O	2.01	0.59
1:A:30:ARG:O	1:A:30:ARG:HG3	2.02	0.59
1:B:276:MET:HE1	1:B:281:SER:HA	1.85	0.59
1:A:341:ASN:ND2	1:A:344:ASN:H	2.00	0.59
1:B:485:HIS:HB2	4:B:856:HOH:O	2.02	0.58
1:A:362:SER:C	1:A:363:LEU:HD22	2.24	0.58
1:A:408:GLN:HA	1:A:422:MET:HE2	1.85	0.58
1:A:310:VAL:CG1	1:A:314:GLU:HA	2.34	0.58
1:A:216:VAL:HA	1:A:245:GLU:O	2.04	0.58
1:A:189:ARG:HD3	1:A:461:ASP:OD1	2.04	0.57
1:A:483:VAL:O	1:A:492:LEU:HB2	2.04	0.57
1:B:169:ILE:CD1	1:B:434:TYR:OH	2.53	0.57
1:B:330:VAL:HG13	1:B:444:PHE:CB	2.34	0.57
1:A:452:SER:HA	4:A:953:HOH:O	2.03	0.57
1:A:515:PRO:O	1:A:517:GLU:N	2.37	0.57
1:B:434:TYR:HH	1:B:456:PHE:HZ	1.46	0.57
1:A:274:LEU:HD13	1:A:276:MET:HE1	1.87	0.57
1:A:457:ASP:HB2	1:A:461:ASP:H	1.69	0.56
1:B:215:THR:HG22	1:B:273:VAL:HB	1.86	0.56
1:B:395:ASN:OD1	1:B:441:THR:HG23	2.04	0.56
1:B:490:LEU:HD12	1:B:491:SER:H	1.71	0.56
1:B:69:LEU:HD23	1:B:69:LEU:C	2.25	0.56
1:B:362:SER:C	1:B:363:LEU:HD22	2.26	0.56
1:B:519:LYS:HG2	1:B:532:ILE:HB	1.88	0.56
1:B:56:GLU:HG2	1:B:101:ARG:HH22	1.69	0.56
1:B:408:GLN:HB2	1:B:422:MET:HE1	1.87	0.55
1:B:434:TYR:OH	1:B:456:PHE:CZ	2.55	0.55
1:A:110:LEU:O	1:A:114:ARG:HG3	2.06	0.55
1:A:372:VAL:HG22	1:A:373:CYS:N	2.22	0.55
1:B:169:ILE:CD1	1:B:434:TYR:CZ	2.89	0.55
1:B:174:THR:HG1	3:B:702:GLU:N	2.03	0.55
1:B:56:GLU:HG2	1:B:101:ARG:NH2	2.21	0.55
1:B:253:ARG:HG2	1:B:290:ARG:NH2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:GLN:NE2	1:A:476:GLY:HA2	2.21	0.55
1:A:56:GLU:HG2	1:A:101:ARG:NH2	2.20	0.55
1:B:515:PRO:CG	1:B:516:ASN:H	2.18	0.55
1:B:211:THR:O	1:B:211:THR:HG22	2.07	0.55
1:B:441:THR:O	1:B:442:ALA:C	2.45	0.55
1:A:252:ILE:HD12	1:A:252:ILE:H	1.72	0.54
1:A:282:ARG:HD2	1:A:309:ILE:O	2.07	0.54
1:A:192:PRO:HG3	1:A:464:GLY:HA2	1.89	0.54
1:B:418:LEU:HD22	1:B:422:MET:HE3	1.88	0.54
1:B:473:GLN:NE2	1:B:476:GLY:HA2	2.23	0.54
1:A:215:THR:HG22	1:A:273:VAL:HB	1.90	0.54
1:A:332:GLN:HG2	4:A:888:HOH:O	2.08	0.54
1:A:515:PRO:HG2	1:A:516:ASN:N	2.13	0.54
1:A:330:VAL:HG13	1:A:444:PHE:CB	2.38	0.54
1:A:513:CYS:HB3	1:A:518:MET:HB2	1.90	0.54
1:B:517:GLU:O	1:B:534:CYS:N	2.39	0.53
1:A:408:GLN:HB2	1:A:422:MET:HE1	1.91	0.53
1:A:205:LEU:HD22	1:A:210:TRP:HE3	1.73	0.53
1:A:441:THR:O	1:A:442:ALA:C	2.46	0.53
1:B:216:VAL:HG22	1:B:276:MET:SD	2.49	0.53
1:B:341:ASN:HD22	1:B:343:TYR:N	2.03	0.53
1:B:341:ASN:ND2	1:B:344:ASN:H	2.06	0.53
1:A:374:ASP:HB3	1:A:377:LEU:HD22	1.91	0.53
1:A:473:GLN:HG3	1:A:478:TYR:CE1	2.43	0.53
1:A:519:LYS:HG2	1:A:532:ILE:HB	1.91	0.53
1:A:534:CYS:SG	1:A:540:LEU:HD11	2.49	0.53
1:B:63:ASP:O	1:B:67:GLN:HB2	2.09	0.53
1:B:399:ALA:HB1	1:B:434:TYR:HE1	1.73	0.53
1:A:332:GLN:HB2	4:A:927:HOH:O	2.09	0.53
1:A:289:ASN:HA	1:A:316:VAL:HG21	1.91	0.52
1:B:252:ILE:HG22	1:B:253:ARG:N	2.22	0.52
1:B:473:GLN:HG3	1:B:478:TYR:CE1	2.44	0.52
1:B:515:PRO:O	1:B:517:GLU:N	2.43	0.52
1:A:492:LEU:N	1:A:492:LEU:HD23	2.24	0.52
1:B:424:ILE:O	1:B:424:ILE:HG13	2.09	0.52
1:A:114:ARG:HG2	1:B:114:ARG:HH21	1.75	0.52
1:A:169:ILE:CD1	1:A:434:TYR:OH	2.59	0.51
2:A:801:NAG:H82	4:A:849:HOH:O	2.10	0.51
1:B:408:GLN:HB2	1:B:422:MET:CE	2.41	0.51
1:B:69:LEU:CD2	1:B:73:LEU:HD22	2.41	0.51
1:A:64:ARG:O	1:A:68:ARG:HD2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:THR:O	1:A:55:GLU:HG2	2.11	0.50
1:A:451:ASP:OD1	1:A:453:ILE:HG12	2.12	0.50
1:B:434:TYR:OH	1:B:456:PHE:HZ	1.92	0.50
1:B:303:TRP:HA	1:B:309:ILE:CD1	2.41	0.50
1:B:169:ILE:HD11	1:B:434:TYR:CZ	2.47	0.50
1:A:253:ARG:HG2	1:A:290:ARG:NH2	2.26	0.50
1:A:303:TRP:HA	1:A:309:ILE:CD1	2.41	0.50
1:A:540:LEU:HD13	1:A:559:LEU:HD23	1.94	0.50
1:A:108:GLN:O	1:A:111:GLU:HB2	2.11	0.50
1:B:374:ASP:HB3	1:B:377:LEU:CD2	2.42	0.50
1:A:298:VAL:HA	1:A:321:ILE:O	2.12	0.49
1:A:185:ASP:OD2	1:A:185:ASP:N	2.46	0.49
1:A:252:ILE:HG22	1:A:253:ARG:N	2.25	0.49
1:B:317:ALA:O	1:B:471:LEU:HD23	2.13	0.49
1:A:189:ARG:HG3	1:A:191:VAL:O	2.12	0.49
1:A:515:PRO:CG	1:A:516:ASN:N	2.73	0.49
1:A:169:ILE:CG1	1:A:434:TYR:OH	2.60	0.49
1:A:200:ALA:O	1:A:204:ILE:HG13	2.13	0.49
1:A:211:THR:O	1:A:211:THR:HG22	2.12	0.49
1:A:49:GLU:HG3	4:A:942:HOH:O	2.13	0.49
1:A:399:ALA:HB1	1:A:434:TYR:HE1	1.77	0.49
1:A:516:ASN:C	1:A:517:GLU:HG3	2.33	0.48
1:A:554:TRP:CG	1:A:555:PRO:HD2	2.48	0.48
1:B:214:SER:OG	1:B:243:THR:HG22	2.13	0.48
1:B:282:ARG:NH1	1:B:282:ARG:HG2	2.24	0.48
1:B:400:MET:CE	1:B:400:MET:HA	2.43	0.48
1:B:150:TYR:HB2	1:B:153:VAL:HG13	1.95	0.48
1:A:163:LEU:HD11	1:B:159:ASN:HB3	1.96	0.48
1:B:310:VAL:HG12	1:B:310:VAL:O	2.14	0.48
1:A:338:GLN:OE1	1:A:380:ASP:HA	2.13	0.48
1:A:434:TYR:OH	1:A:456:PHE:CZ	2.65	0.48
1:B:30:ARG:NH2	1:B:32:GLU:OE1	2.47	0.48
1:B:492:LEU:N	1:B:492:LEU:HD23	2.29	0.48
1:B:189:ARG:HD3	1:B:461:ASP:OD1	2.13	0.47
1:B:211:THR:HG23	1:B:238:ASN:O	2.14	0.47
1:B:108:GLN:O	1:B:111:GLU:HB2	2.13	0.47
1:B:274:LEU:HD13	1:B:276:MET:HE2	1.95	0.47
1:B:448:LYS:HA	1:B:452:SER:OG	2.14	0.47
1:A:504:VAL:HG13	1:A:504:VAL:O	2.14	0.47
1:A:520:ASN:O	1:A:544:PHE:HB3	2.14	0.47
1:B:150:TYR:HE2	1:B:277:ARG:HB3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:LYS:HE2	1:B:181:LYS:CA	2.45	0.47
1:A:341:ASN:HD22	1:A:343:TYR:N	2.08	0.47
1:A:63:ASP:O	1:A:67:GLN:HB2	2.15	0.47
1:B:514:ALA:N	1:B:518:MET:HE3	2.14	0.47
1:A:276:MET:CE	1:A:281:SER:HA	2.43	0.47
1:B:138:ILE:N	1:B:139:PRO:HD2	2.30	0.47
1:A:217:ALA:HB2	1:A:227:ILE:CG1	2.44	0.46
1:A:363:LEU:HD22	1:A:363:LEU:N	2.29	0.46
1:B:282:ARG:HD2	1:B:309:ILE:O	2.15	0.46
1:A:356:GLU:OE1	1:A:363:LEU:HD23	2.15	0.46
1:A:169:ILE:HD13	1:A:434:TYR:OH	2.15	0.46
1:A:522:GLN:NE2	1:A:528:CYS:O	2.49	0.46
1:B:284:LEU:O	1:B:284:LEU:HD22	2.16	0.46
1:B:341:ASN:HD22	1:B:341:ASN:C	2.18	0.46
1:B:521:MET:HB2	1:B:530:ILE:HG13	1.97	0.46
1:A:147:GLY:HA2	1:A:171:TYR:CE2	2.50	0.46
1:B:434:TYR:CZ	1:B:456:PHE:CZ	3.04	0.46
1:B:504:VAL:O	1:B:504:VAL:HG13	2.15	0.46
1:A:420:ASP:O	1:A:423:LYS:HB2	2.15	0.46
1:A:157:VAL:CG1	1:A:161:LEU:HD22	2.43	0.46
1:A:116:SER:C	1:A:117:LEU:HD12	2.36	0.46
1:A:402:HIS:HB3	1:A:437:LYS:CE	2.32	0.46
1:B:324:GLU:HG2	1:B:388:SER:OG	2.16	0.46
1:B:341:ASN:ND2	1:B:343:TYR:H	2.05	0.45
1:B:276:MET:CE	1:B:281:SER:HA	2.46	0.45
1:B:437:LYS:HA	1:B:437:LYS:HD2	1.69	0.45
1:A:115:ALA:HB1	1:A:140:LEU:O	2.16	0.45
1:A:440:PHE:CE1	1:A:448:LYS:HG2	2.51	0.45
1:A:252:ILE:N	1:A:252:ILE:HD12	2.32	0.45
1:A:310:VAL:HG12	1:A:310:VAL:O	2.15	0.45
1:A:535:GLU:HB2	1:A:538:GLU:HG3	1.99	0.45
1:A:217:ALA:HB2	1:A:227:ILE:HG13	1.99	0.45
1:B:521:MET:O	1:B:529:TRP:HB2	2.16	0.45
1:B:408:GLN:CB	1:B:422:MET:HE1	2.47	0.45
1:B:539:TYR:CZ	1:B:541:VAL:HG22	2.52	0.45
1:A:282:ARG:HG2	1:A:282:ARG:NH1	2.28	0.45
1:A:534:CYS:SG	1:A:540:LEU:CD1	3.05	0.45
1:A:292:ASN:HD21	1:A:315:HIS:HE1	1.65	0.44
1:B:540:LEU:CD1	1:B:546:CYS:SG	3.04	0.44
1:A:523:PRO:HD3	1:A:529:TRP:HA	1.98	0.44
1:A:324:GLU:HG3	4:A:952:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:ASP:O	1:A:377:LEU:HD22	2.17	0.44
1:A:96:LEU:HD13	1:A:108:GLN:HB3	1.98	0.44
1:B:501:ARG:O	1:B:503:SER:N	2.50	0.44
1:B:116:SER:C	1:B:117:LEU:HD12	2.38	0.44
1:B:199:LYS:HD3	4:B:865:HOH:O	2.17	0.44
1:A:86:LEU:HD13	1:A:405:HIS:HB2	1.99	0.44
1:B:157:VAL:CG1	1:B:161:LEU:HD22	2.47	0.44
1:A:163:LEU:HD11	1:B:159:ASN:CB	2.48	0.43
1:A:270:ARG:HH11	1:A:270:ARG:HG2	1.83	0.43
1:A:169:ILE:CD1	1:A:434:TYR:CZ	3.01	0.43
1:B:30:ARG:NH1	1:B:111:GLU:OE2	2.50	0.43
1:B:519:LYS:CG	1:B:532:ILE:HB	2.48	0.43
1:A:177:LYS:HE3	1:A:225:THR:HG21	1.99	0.43
1:B:241:ILE:HG23	1:B:241:ILE:O	2.19	0.43
1:B:268:ASN:HB3	1:B:508:GLN:O	2.17	0.43
1:A:443:PRO:C	1:A:445:ASN:H	2.22	0.43
1:A:98:THR:HB	1:A:105:ALA:HB2	2.00	0.43
1:B:217:ALA:HB2	1:B:227:ILE:HG13	2.00	0.43
1:B:361:CYS:HB3	1:B:362:SER:H	1.35	0.43
1:A:424:ILE:HG13	1:A:424:ILE:O	2.19	0.43
1:A:230:PHE:CZ	1:A:273:VAL:HG21	2.54	0.42
1:A:362:SER:O	1:A:363:LEU:HD13	2.18	0.42
1:A:372:VAL:HG22	1:A:373:CYS:H	1.84	0.42
1:B:185:ASP:N	1:B:185:ASP:OD2	2.49	0.42
1:A:169:ILE:HG12	1:A:434:TYR:CZ	2.54	0.42
1:B:194:ASP:OD1	1:B:197:GLN:NE2	2.52	0.42
1:B:230:PHE:CZ	1:B:273:VAL:HG21	2.54	0.42
1:A:214:SER:OG	1:A:243:THR:HG22	2.20	0.42
1:A:30:ARG:CG	1:A:30:ARG:O	2.67	0.42
1:A:363:LEU:O	1:A:364:GLN:HG2	2.19	0.42
1:B:69:LEU:CD2	1:B:69:LEU:C	2.88	0.42
1:A:341:ASN:C	1:A:341:ASN:HD22	2.21	0.42
1:A:500:SER:O	1:A:501:ARG:CB	2.67	0.42
1:B:377:LEU:HA	1:B:377:LEU:HD13	1.90	0.42
1:B:255:SER:O	1:B:259:VAL:HG23	2.19	0.42
1:B:261:ARG:HB3	1:B:261:ARG:HH11	1.84	0.42
1:B:449:GLY:C	1:B:451:ASP:H	2.23	0.42
1:A:408:GLN:HB2	1:A:422:MET:CE	2.48	0.42
1:A:418:LEU:HD22	1:A:422:MET:HE3	2.02	0.42
1:B:341:ASN:HB2	1:B:342:PRO:HD2	1.99	0.42
1:B:363:LEU:N	1:B:363:LEU:HD22	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:VAL:HA	1:B:245:GLU:O	2.20	0.42
1:B:374:ASP:C	1:B:376:HIS:H	2.23	0.42
1:A:434:TYR:CZ	1:A:456:PHE:CZ	3.08	0.42
1:A:465:ARG:CZ	4:A:955:HOH:O	2.67	0.42
1:A:150:TYR:HB2	1:A:153:VAL:HG13	2.00	0.42
1:A:449:GLY:C	1:A:451:ASP:H	2.23	0.41
1:B:199:LYS:HE2	1:B:233:GLU:OE2	2.20	0.41
1:A:544:PHE:N	1:A:544:PHE:CD1	2.88	0.41
1:B:39:LEU:HA	1:B:39:LEU:HD12	1.92	0.41
1:B:69:LEU:HD23	1:B:73:LEU:HD22	2.01	0.41
1:B:147:GLY:HA2	1:B:171:TYR:CE2	2.55	0.41
1:B:199:LYS:HG2	1:B:233:GLU:CD	2.41	0.41
1:B:544:PHE:N	1:B:544:PHE:CD1	2.88	0.41
1:A:306:GLN:NE2	1:A:309:ILE:HD11	2.36	0.41
1:B:359:PHE:HB2	1:B:361:CYS:SG	2.60	0.41
1:B:251:ASN:HD22	1:B:255:SER:HB3	1.85	0.41
1:B:167:PRO:HG3	1:B:430:LEU:HD23	2.01	0.41
1:A:86:LEU:H	1:A:405:HIS:HD1	1.67	0.41
1:A:473:GLN:O	1:A:474:THR:C	2.59	0.41
1:A:473:GLN:O	1:A:475:GLY:N	2.53	0.41
1:B:282:ARG:NH1	1:B:282:ARG:CG	2.78	0.41
1:B:351:PHE:O	1:B:354:PHE:HB3	2.20	0.41
1:B:522:GLN:NE2	1:B:528:CYS:O	2.54	0.41
1:A:115:ALA:HB3	4:A:830:HOH:O	2.19	0.41
1:B:59:ARG:HG3	4:B:849:HOH:O	2.20	0.41
1:A:169:ILE:HG13	4:A:947:HOH:O	2.20	0.41
1:B:520:ASN:O	1:B:544:PHE:HB3	2.21	0.41
1:A:71:ALA:HA	1:A:333:PHE:CE1	2.56	0.41
1:B:205:LEU:HD22	1:B:210:TRP:HE3	1.85	0.41
1:A:473:GLN:HG3	1:A:478:TYR:CZ	2.56	0.41
1:B:69:LEU:O	1:B:69:LEU:HD23	2.21	0.41
1:A:174:THR:C	1:A:189:ARG:NH2	2.75	0.40
1:A:227:ILE:HD13	1:A:227:ILE:HA	1.90	0.40
1:B:515:PRO:CG	1:B:516:ASN:N	2.83	0.40
1:B:517:GLU:OE1	1:B:518:MET:HG2	2.21	0.40
1:A:205:LEU:HD13	1:A:213:VAL:HG11	2.02	0.40
1:B:210:TRP:CD2	1:B:271:VAL:HG21	2.56	0.40
1:B:211:THR:HG22	1:B:527:CYS:SG	2.61	0.40
1:A:445:ASN:ND2	4:A:885:HOH:O	2.54	0.40
1:B:81:LYS:HG3	4:B:899:HOH:O	2.20	0.40
1:A:411:LEU:HD12	1:A:422:MET:HG3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:LEU:HG	1:A:492:LEU:CD2	2.51	0.40
1:B:516:ASN:C	1:B:517:GLU:HG3	2.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	506/555 (91%)	452 (89%)	43 (8%)	11 (2%)	7	5
1	B	508/555 (92%)	455 (90%)	39 (8%)	14 (3%)	5	3
All	All	1014/1110 (91%)	907 (89%)	82 (8%)	25 (2%)	6	4

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	443	PRO
1	A	474	THR
1	A	502	ASN
1	A	516	ASN
1	A	523	PRO
1	B	443	PRO
1	B	502	ASN
1	B	516	ASN
1	B	523	PRO
1	A	362	SER
1	A	444	PHE
1	A	517	GLU
1	B	362	SER
1	B	474	THR
1	B	517	GLU
1	B	433	GLU

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Mol	Chain	Res	Type
1	B	444	PHE
1	A	515	PRO
1	B	447	ASN
1	B	505	PRO
1	B	515	PRO
1	A	433	GLU
1	B	566	PRO
1	A	566	PRO
1	B	372	VAL

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	441/481 (92%)	412 (93%)	29 (7%)	18	19
1	B	443/481 (92%)	413 (93%)	30 (7%)	17	18
All	All	884/962 (92%)	825 (93%)	59 (7%)	18	18

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	69	LEU
1	A	73	LEU
1	A	86	LEU
1	A	106	LEU
1	A	110	LEU
1	A	111	GLU
1	A	153	VAL
1	A	161	LEU
1	A	163	LEU
1	A	216	VAL
1	A	227	ILE
1	A	275	PHE
1	A	284	LEU

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Mol	Chain	Res	Type
1	A	292	ASN
1	A	341	ASN
1	A	373	CYS
1	A	377	LEU
1	A	408	GLN
1	A	418	LEU
1	A	422	MET
1	A	439	GLN
1	A	454	VAL
1	A	457	ASP
1	A	498	HIS
1	A	517	GLU
1	A	544	PHE
1	A	558	ASP
1	A	567	GLU
1	B	29	MET
1	B	39	LEU
1	B	73	LEU
1	B	86	LEU
1	B	106	LEU
1	B	110	LEU
1	B	111	GLU
1	B	153	VAL
1	B	161	LEU
1	B	163	LEU
1	B	189	ARG
1	B	216	VAL
1	B	227	ILE
1	B	275	PHE
1	B	284	LEU
1	B	292	ASN
1	B	341	ASN
1	B	373	CYS
1	B	377	LEU
1	B	400	MET
1	B	408	GLN
1	B	418	LEU
1	B	457	ASP
1	B	470	ASN
1	B	498	HIS
1	B	517	GLU
1	B	540	LEU

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Mol	Chain	Res	Type
1	B	544	PHE
1	B	546	CYS
1	B	567	GLU

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	251	ASN
1	A	292	ASN
1	A	306	GLN
1	A	341	ASN
1	A	408	GLN
1	A	473	GLN
1	A	522	GLN
1	B	108	GLN
1	B	251	ASN
1	B	292	ASN
1	B	306	GLN
1	B	338	GLN
1	B	341	ASN
1	B	408	GLN
1	B	473	GLN
1	B	522	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 ⓘ

4 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	GLU	A	701	-	1,9,9	0.43	0	1,11,11	0.06	0
2	NAG	A	801	1	14,14,15	0.68	0	17,19,21	0.60	0
3	GLU	B	702	-	1,9,9	0.04	0	1,11,11	0.08	0
2	NAG	B	802	1	14,14,15	0.56	0	17,19,21	0.62	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	GLU	A	701	-	-	0/3/9/9	0/0/0/0
2	NAG	A	801	1	-	0/6/23/26	0/1/1/1
3	GLU	B	702	-	-	0/3/9/9	0/0/0/0
2	NAG	B	802	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	NAG	1	0
3	B	702	GLU	1	0

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 ⓘ

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	512/555 (92%)	0.90	82 (16%) ⓘ ⓘ	28, 55, 90, 108	0
1	B	514/555 (92%)	0.89	82 (15%) ⓘ ⓘ	26, 56, 92, 108	0
All	All	1026/1110 (92%)	0.89	164 (15%) ⓘ ⓘ	26, 56, 91, 108	0

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	516	ASN	11.8
1	A	250	SER	11.6
1	A	516	ASN	10.8
1	B	250	SER	10.0
1	B	28	PHE	9.3
1	A	449	GLY	9.2
1	B	474	THR	8.9
1	B	567	GLU	8.0
1	A	450	ALA	8.0
1	B	443	PRO	7.9
1	B	29	MET	7.4
1	A	443	PRO	7.2
1	A	446	PRO	7.0
1	B	364	GLN	6.2
1	B	249	ARG	5.9
1	B	566	PRO	5.6
1	B	52	THR	5.5
1	B	54	THR	5.5
1	B	449	GLY	5.5
1	A	116	SER	5.5
1	A	447	ASN	5.1
1	B	343	TYR	5.1
1	A	474	THR	5.0
1	A	448	LYS	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	54	THR	4.8
1	A	451	ASP	4.8
1	A	55	GLU	4.8
1	B	53	GLY	4.7
1	A	274	LEU	4.5
1	A	299	ALA	4.5
1	A	524	GLY	4.4
1	A	440	PHE	4.4
1	B	299	ALA	4.2
1	B	475	GLY	4.2
1	A	53	GLY	4.2
1	A	147	GLY	4.1
1	A	272	VAL	4.1
1	A	364	GLN	4.0
1	B	446	PRO	4.0
1	A	434	TYR	4.0
1	A	361	CYS	4.0
1	B	272	VAL	4.0
1	A	478	TYR	4.0
1	B	117	LEU	4.0
1	A	273	VAL	4.0
1	A	146	ILE	3.9
1	A	117	LEU	3.9
1	B	521	MET	3.9
1	B	440	PHE	3.9
1	A	298	VAL	3.8
1	B	274	LEU	3.8
1	B	298	VAL	3.8
1	A	249	ARG	3.7
1	B	146	ILE	3.7
1	B	139	PRO	3.7
1	B	376	HIS	3.6
1	B	450	ALA	3.6
1	A	254	LYS	3.6
1	A	502	ASN	3.6
1	B	373	CYS	3.6
1	A	253	ARG	3.6
1	A	529	TRP	3.6
1	B	252	ILE	3.6
1	B	523	PRO	3.6
1	A	409	ARG	3.5
1	B	530	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	372	VAL	3.3
1	B	51	GLY	3.3
1	B	315	HIS	3.3
1	A	204	ILE	3.3
1	B	273	VAL	3.3
1	B	331	ARG	3.3
1	B	434	TYR	3.3
1	B	478	TYR	3.2
1	B	254	LYS	3.2
1	A	297	TRP	3.2
1	B	297	TRP	3.2
1	B	55	GLU	3.2
1	B	310	VAL	3.1
1	B	447	ASN	3.1
1	A	138	ILE	3.1
1	B	473	GLN	3.1
1	A	52	THR	3.0
1	A	321	ILE	3.0
1	A	526	VAL	3.0
1	B	251	ASN	3.0
1	A	475	GLY	3.0
1	B	216	VAL	3.0
1	A	323	LEU	2.9
1	A	487	ALA	2.9
1	A	145	VAL	2.9
1	B	322	THR	2.9
1	B	363	LEU	2.9
1	A	205	LEU	2.8
1	B	520	ASN	2.8
1	B	375	LYS	2.8
1	B	477	LYS	2.8
1	B	145	VAL	2.8
1	A	41	LEU	2.8
1	A	441	THR	2.7
1	A	331	ARG	2.7
1	B	360	GLN	2.7
1	B	321	ILE	2.7
1	A	371	GLN	2.7
1	A	423	LYS	2.7
1	A	315	HIS	2.7
1	A	169	ILE	2.6
1	B	487	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	397	VAL	2.6
1	A	397	VAL	2.6
1	A	512	PRO	2.6
1	A	567	GLU	2.6
1	B	335	ARG	2.6
1	B	551	PRO	2.6
1	B	524	GLY	2.6
1	B	502	ASN	2.6
1	A	44	LEU	2.5
1	B	57	CYS	2.5
1	B	318	TYR	2.5
1	A	452	SER	2.5
1	A	144	GLY	2.5
1	A	238	ASN	2.5
1	B	361	CYS	2.5
1	A	445	ASN	2.5
1	B	235	ARG	2.4
1	B	544	PHE	2.4
1	A	300	SER	2.4
1	A	216	VAL	2.4
1	A	343	TYR	2.4
1	B	371	GLN	2.4
1	B	147	GLY	2.4
1	B	359	PHE	2.4
1	A	363	LEU	2.3
1	A	251	ASN	2.3
1	A	335	ARG	2.3
1	B	320	ALA	2.3
1	B	458	THR	2.3
1	A	400	MET	2.3
1	B	253	ARG	2.3
1	A	473	GLN	2.2
1	A	528	CYS	2.2
1	A	302	GLY	2.2
1	B	43	GLY	2.2
1	B	323	LEU	2.2
1	A	235	ARG	2.2
1	A	437	LYS	2.2
1	B	374	ASP	2.2
1	A	50	LYS	2.2
1	A	43	GLY	2.2
1	A	396	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	138	ILE	2.1
1	B	169	ILE	2.1
1	A	101	ARG	2.1
1	A	525	ASP	2.1
1	B	271	VAL	2.1
1	B	400	MET	2.1
1	B	382	SER	2.1
1	A	45	PHE	2.1
1	B	451	ASP	2.0
1	A	69	LEU	2.0
1	A	420	ASP	2.0
1	A	418	LEU	2.0
1	A	520	ASN	2.0
1	B	281	SER	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. 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	B-factors(\AA^2)	Q<0.9
2	NAG	B	802	14/15	0.80	0.24	82,87,90,91	0
2	NAG	A	801	14/15	0.81	0.17	85,87,90,90	0
3	GLU	B	702	10/10	0.93	0.24	33,37,39,40	0
3	GLU	A	701	10/10	0.99	0.23	33,36,38,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.