



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 10:41 PM GMT

PDB ID : 2E4X  
Title : Crystal structure of the extracellular region of the group II metabotropic glutamate receptor complexed with 1S,3R-ACPD  
Authors : Muto, T.; Tsuchiya, D.; Morikawa, K.; Jingami, H.  
Deposited on : 2006-12-17  
Resolution : 2.75 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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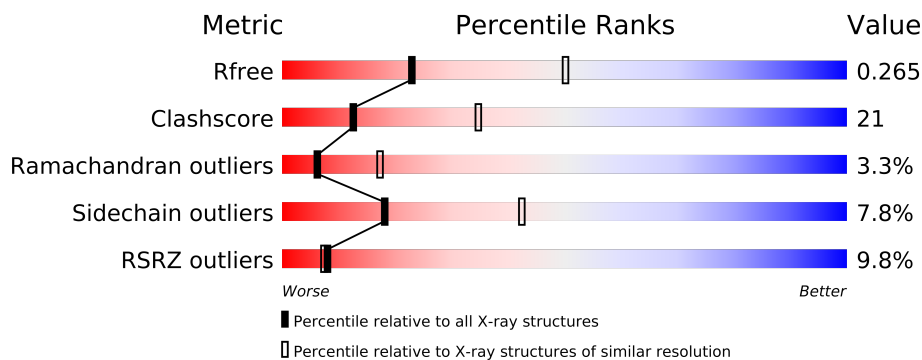
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.75 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))
$R_{free}$	66092	2406 (2.80-2.72)
Clashscore	79885	2995 (2.80-2.72)
Ramachandran outliers	78287	2941 (2.80-2.72)
Sidechain outliers	78261	2944 (2.80-2.72)
RSRZ outliers	66119	2409 (2.80-2.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	555	
1	B	555	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8478 atoms, of which 0 are hydrogen and 0 are deuterium.

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	518	Total	C	N	O	S	0	0	0
			4118	2606	709	776	27			
1	B	520	Total	C	N	O	S	0	0	0
			4137	2620	711	778	28			

There are 12 discrepancies between the modelled and reference sequences:

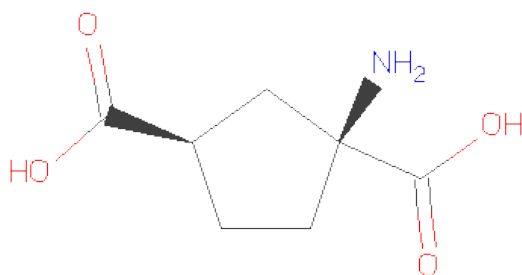
Chain	Residue	Modelled	Actual	Comment	Reference
A	414	GLN	ASN	ENGINEERED	UNP P31422
A	439	GLN	ASN	ENGINEERED	UNP P31422
A	576	LEU	-	CLONING ARTIFACT	UNP P31422
A	577	VAL	-	CLONING ARTIFACT	UNP P31422
A	578	PRO	-	CLONING ARTIFACT	UNP P31422
A	579	ARG	-	CLONING ARTIFACT	UNP P31422
B	414	GLN	ASN	ENGINEERED	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 SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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 (1S,3R)-1-AMINOCYCLOPENTANE-1,3-DICARBOXYLICACID (three-letter code: C5B) (formula: C<sub>7</sub>H<sub>11</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	7	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			12	7	1	4		

- Molecule 4 is water.

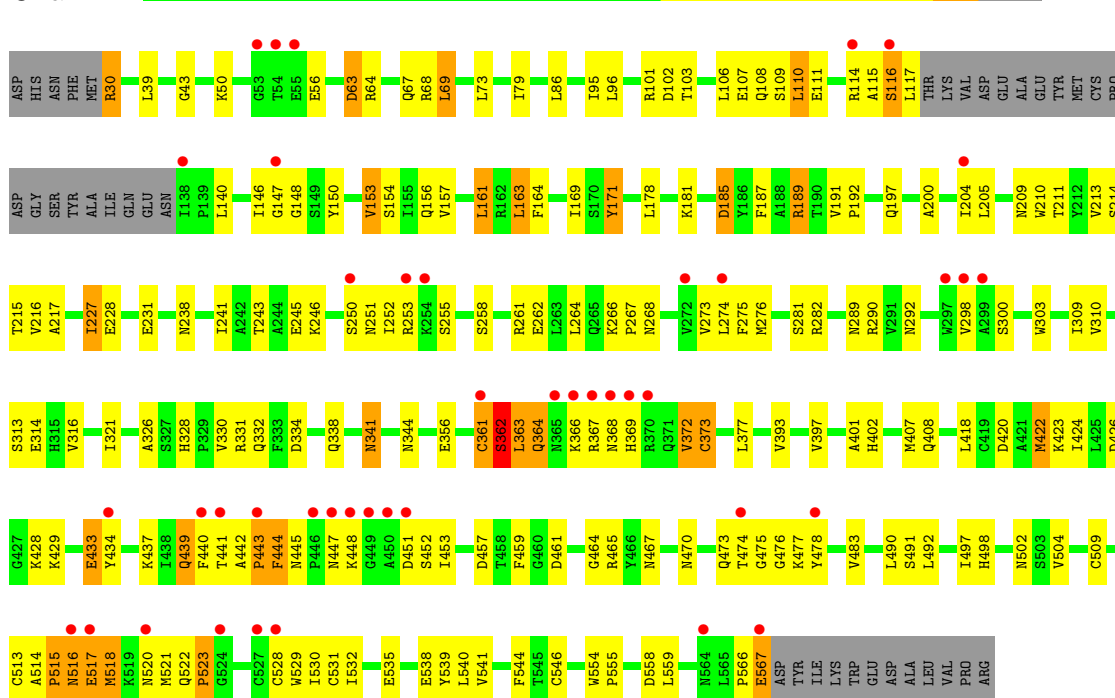
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	93	Total	O	0	0
			93	93		
4	B	78	Total	O	0	0
			78	78		

### 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.

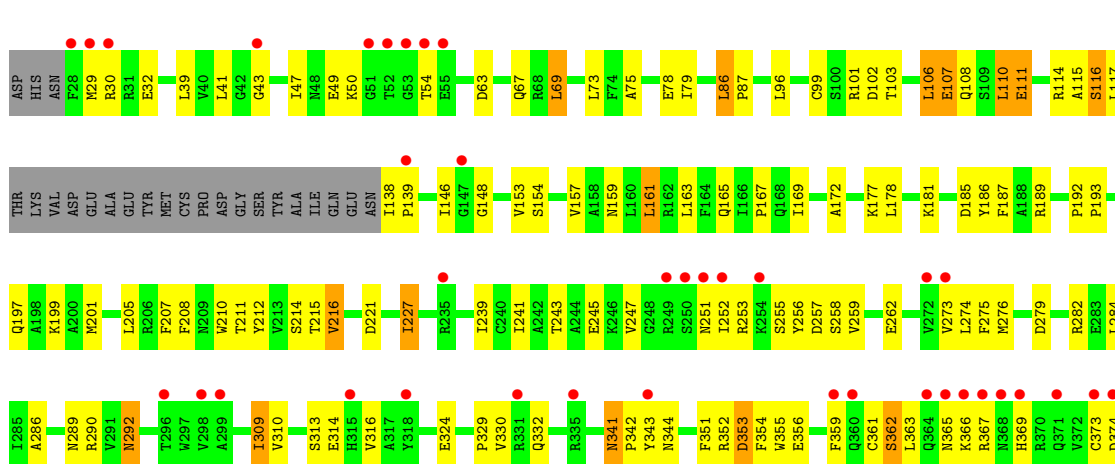
#### • Molecule 1: Metabotropic glutamate receptor 3

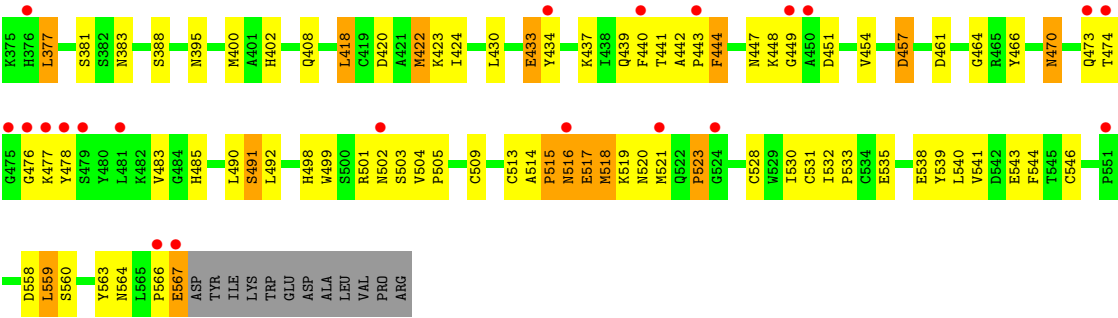
Chain A:



#### • Molecule 1: Metabotropic glutamate receptor 3

Chain B:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.62Å 97.14Å 108.16Å 90.00° 92.92° 90.00°	Depositor
Resolution (Å)	20.00 – 2.75 29.21 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.75) 99.8 (29.21-2.75)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 2.76Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.225 , 0.265 0.227 , 0.265	Depositor DCC
$R_{free}$ test set	3201 reflections (7.66%)	DCC
Wilson B-factor (Å <sup>2</sup> )	65.4	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 45.9	EDS
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 45008 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8478	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, C5B

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	0.42	0/4212	0.68	1/5704 (0.0%)
1	B	0.43	0/4232	0.68	2/5730 (0.0%)
All	All	0.43	0/8444	0.68	3/11434 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	433	GLU	N-CA-C	-5.64	95.77	111.00
1	B	546	CYS	CA-CB-SG	-5.40	104.28	114.00
1	A	433	GLU	N-CA-C	-5.08	97.29	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	171	TYR	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4118	0	3993	174	0
1	B	4137	0	4012	177	0
2	A	14	0	13	1	0
2	B	14	0	13	0	0
3	A	12	0	9	1	0
3	B	12	0	9	0	0
4	A	93	0	0	7	0
4	B	78	0	0	8	0
All	All	8478	0	8049	344	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 21.

All (344) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:420:ASP:HA	1:A:423:LYS:HD3	1.31	1.13
1:B:356:GLU:HA	1:B:361:CYS:HB2	1.35	1.08
1:A:356:GLU:HA	1:A:361:CYS:HB2	1.30	1.07
1:B:216:VAL:HG13	1:B:274:LEU:HD23	1.39	1.04
1:A:402:HIS:HB3	1:A:437:LYS:HE2	1.41	0.98
1:A:328:HIS:HB2	4:A:1055:HOH:O	1.65	0.96
1:B:402:HIS:HB3	1:B:437:LYS:HE2	1.47	0.95
1:B:514:ALA:H	1:B:518:MET:HE3	1.31	0.95
1:B:514:ALA:HB3	1:B:518:MET:HG3	1.48	0.93
1:A:515:PRO:HG2	1:A:516:ASN:H	1.35	0.90
1:A:514:ALA:HB3	1:A:518:MET:HG3	1.56	0.87
1:B:330:VAL:HG13	1:B:444:PHE:HB3	1.57	0.86
1:B:490:LEU:HD12	1:B:491:SER:H	1.41	0.85
1:A:114:ARG:HG2	1:B:114:ARG:HH21	1.43	0.82
1:A:366:LYS:HG2	1:A:367:ARG:H	1.46	0.80
1:A:341:ASN:ND2	1:A:344:ASN:H	1.80	0.78
1:B:216:VAL:HG13	1:B:274:LEU:CD2	2.14	0.78
1:B:30:ARG:HD2	1:B:108:GLN:HE22	1.49	0.77
1:B:366:LYS:HG2	1:B:367:ARG:H	1.50	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:514:ALA:H	1:A:518:MET:HE3	1.50	0.76
1:B:440:PHE:CE2	1:B:448:LYS:HB3	2.21	0.76
1:A:330:VAL:HG13	1:A:444:PHE:HB3	1.67	0.76
1:B:515:PRO:HG2	1:B:516:ASN:H	1.51	0.76
1:A:107:GLU:HB3	4:A:1075:HOH:O	1.87	0.74
1:B:50:LYS:HG3	1:B:101:ARG:HD3	1.71	0.73
1:B:516:ASN:HB2	1:B:517:GLU:OE2	1.88	0.73
1:B:420:ASP:HA	1:B:423:LYS:HD3	1.70	0.72
1:A:367:ARG:HB2	1:A:369:HIS:CD2	2.25	0.72
1:B:341:ASN:HD22	1:B:343:TYR:H	1.37	0.71
1:B:47:ILE:HD12	1:B:69:LEU:HD12	1.73	0.70
1:B:362:SER:O	1:B:363:LEU:HD13	1.91	0.70
1:B:251:ASN:HD22	1:B:255:SER:HB3	1.56	0.70
1:B:483:VAL:O	1:B:492:LEU:HB2	1.91	0.70
1:B:258:SER:O	1:B:262:GLU:HG3	1.91	0.70
1:B:352:ARG:HG3	4:B:2053:HOH:O	1.92	0.70
1:A:114:ARG:NH2	1:B:114:ARG:HG2	2.06	0.69
1:A:101:ARG:HD3	4:A:1046:HOH:O	1.92	0.69
1:A:367:ARG:HB2	1:A:369:HIS:NE2	2.07	0.69
1:B:341:ASN:HD22	1:B:341:ASN:C	1.96	0.69
1:B:514:ALA:H	1:B:518:MET:CE	2.04	0.68
1:A:217:ALA:HB2	1:A:227:ILE:HG13	1.76	0.68
1:B:215:THR:OG1	1:B:241:ILE:HD11	1.92	0.68
1:A:540:LEU:HD12	1:A:546:CYS:SG	2.33	0.68
1:B:165:GLN:HG3	4:B:2031:HOH:O	1.94	0.67
1:A:181:LYS:HE2	1:A:459:PHE:O	1.95	0.67
1:B:341:ASN:ND2	1:B:344:ASN:H	1.92	0.67
1:B:442:ALA:O	1:B:444:PHE:N	2.28	0.66
1:A:372:VAL:HG22	1:A:373:CYS:N	2.11	0.66
1:A:50:LYS:HE3	4:A:1046:HOH:O	1.93	0.66
1:B:289:ASN:HA	1:B:316:VAL:HG21	1.78	0.66
1:A:341:ASN:C	1:A:341:ASN:HD22	1.99	0.66
1:B:199:LYS:HD3	4:B:2045:HOH:O	1.96	0.66
1:A:420:ASP:O	1:A:423:LYS:HB2	1.97	0.65
1:A:192:PRO:HG3	1:A:464:GLY:HA2	1.79	0.65
1:B:473:GLN:HE21	1:B:476:GLY:CA	2.10	0.65
1:A:514:ALA:HB2	1:A:518:MET:HE2	1.78	0.65
1:A:181:LYS:HE3	1:A:187:PHE:O	1.97	0.65
1:B:252:ILE:HG22	1:B:253:ARG:H	1.62	0.65
1:A:30:ARG:HH11	1:A:30:ARG:HA	1.60	0.65
1:B:440:PHE:HE2	1:B:448:LYS:HB3	1.62	0.65
1:A:473:GLN:HA	1:A:477:LYS:O	1.98	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:366:LYS:HG2	1:A:367:ARG:N	2.11	0.64
1:B:314:GLU:HG2	1:B:478:TYR:CD2	2.33	0.64
1:A:442:ALA:O	1:A:444:PHE:N	2.31	0.64
1:B:205:LEU:HD22	1:B:210:TRP:HE3	1.63	0.64
1:A:440:PHE:CE2	1:A:448:LYS:HB3	2.33	0.63
1:B:169:ILE:HG12	1:B:434:TYR:OH	1.98	0.63
1:A:69:LEU:HD22	1:A:69:LEU:O	1.99	0.62
1:A:515:PRO:CG	1:A:516:ASN:H	2.08	0.62
1:A:114:ARG:HG2	1:B:114:ARG:NH2	2.15	0.62
1:B:341:ASN:ND2	1:B:343:TYR:H	1.97	0.62
1:A:473:GLN:HE21	1:A:476:GLY:CA	2.13	0.62
1:B:177:LYS:HD2	1:B:221:ASP:OD2	1.99	0.62
1:A:372:VAL:HG22	1:A:373:CYS:H	1.63	0.61
1:A:332:GLN:HB2	4:A:1081:HOH:O	2.00	0.61
1:B:282:ARG:HG2	1:B:282:ARG:HH11	1.66	0.61
1:A:253:ARG:HG2	1:A:290:ARG:NH2	2.15	0.61
1:B:535:GLU:HA	1:B:535:GLU:OE2	2.00	0.61
1:A:185:ASP:OD2	1:A:185:ASP:N	2.31	0.61
1:B:201:MET:CE	1:B:273:VAL:HG13	2.31	0.61
1:A:64:ARG:O	1:A:68:ARG:HD2	2.00	0.61
1:B:558:ASP:O	1:B:559:LEU:HB2	2.01	0.61
1:B:252:ILE:HG22	1:B:253:ARG:N	2.16	0.60
1:A:169:ILE:HG12	1:A:434:TYR:OH	2.02	0.60
1:B:63:ASP:O	1:B:67:GLN:HB2	2.01	0.60
1:A:566:PRO:O	1:A:567:GLU:HB2	1.99	0.60
1:B:539:TYR:CZ	1:B:541:VAL:HG22	2.36	0.60
1:B:367:ARG:HB2	1:B:369:HIS:CD2	2.37	0.60
1:B:49:GLU:HG3	4:B:2035:HOH:O	2.03	0.59
1:B:518:MET:HB3	1:B:531:CYS:HB3	1.85	0.59
1:B:366:LYS:HG2	1:B:367:ARG:N	2.15	0.59
1:B:514:ALA:N	1:B:518:MET:HE3	2.10	0.59
1:A:63:ASP:O	1:A:67:GLN:HB2	2.02	0.59
1:B:78:GLU:HG3	1:B:444:PHE:CZ	2.38	0.59
1:A:216:VAL:HG13	1:A:274:LEU:HD22	1.84	0.58
1:A:216:VAL:HA	1:A:245:GLU:O	2.03	0.58
1:B:148:GLY:HA3	1:B:154:SER:OG	2.03	0.58
1:B:274:LEU:HD22	1:B:276:MET:SD	2.43	0.58
1:A:513:CYS:HB3	1:A:518:MET:HB2	1.86	0.58
1:A:514:ALA:H	1:A:518:MET:CE	2.16	0.58
1:B:535:GLU:HB2	1:B:538:GLU:HG3	1.84	0.58
1:A:483:VAL:O	1:A:492:LEU:HB2	2.03	0.58
1:A:148:GLY:HA3	1:A:154:SER:OG	2.03	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:165:GLN:CG	4:B:2031:HOH:O	2.51	0.57
1:A:163:LEU:HB3	1:B:106:LEU:HD11	1.85	0.57
1:A:56:GLU:HG2	1:A:101:ARG:HH22	1.67	0.57
1:A:341:ASN:HD21	1:A:344:ASN:H	1.51	0.57
1:A:289:ASN:HA	1:A:316:VAL:HG21	1.86	0.57
1:B:178:LEU:HD13	1:B:187:PHE:CZ	2.40	0.57
1:B:367:ARG:HB2	1:B:369:HIS:NE2	2.20	0.56
1:A:330:VAL:HG13	1:A:444:PHE:CB	2.35	0.56
1:A:523:PRO:HD2	1:A:528:CYS:O	2.05	0.56
1:A:157:VAL:HG12	1:A:161:LEU:HD22	1.87	0.56
1:B:157:VAL:HG12	1:B:161:LEU:HD22	1.87	0.56
1:A:441:THR:O	1:A:442:ALA:C	2.43	0.56
1:B:332:GLN:HB2	4:B:2021:HOH:O	2.05	0.56
1:A:361:CYS:O	1:A:362:SER:HB2	2.04	0.56
1:A:516:ASN:HB2	1:A:517:GLU:OE2	2.06	0.56
1:B:441:THR:O	1:B:442:ALA:C	2.43	0.56
1:B:485:HIS:HB2	4:B:2037:HOH:O	2.06	0.56
1:A:43:GLY:HA2	1:A:146:ILE:O	2.05	0.56
1:B:255:SER:O	1:B:259:VAL:HG23	2.06	0.55
1:B:504:VAL:O	1:B:504:VAL:HG13	2.06	0.55
1:B:165:GLN:HG2	1:B:186:TYR:OH	2.06	0.55
1:A:282:ARG:HD2	1:A:309:ILE:O	2.06	0.55
1:B:30:ARG:NH2	1:B:32:GLU:OE1	2.39	0.55
1:A:211:THR:HG23	1:A:238:ASN:O	2.07	0.55
1:B:310:VAL:CG1	1:B:314:GLU:HA	2.37	0.55
1:A:518:MET:HB3	1:A:531:CYS:HB3	1.89	0.55
1:A:521:MET:HB2	1:A:530:ILE:HG13	1.88	0.54
1:B:215:THR:HG22	1:B:273:VAL:HB	1.89	0.54
1:B:513:CYS:HB3	1:B:518:MET:HB2	1.88	0.54
1:A:473:GLN:NE2	1:A:476:GLY:HA2	2.22	0.54
1:A:258:SER:O	1:A:262:GLU:HG3	2.07	0.54
1:B:103:THR:O	1:B:107:GLU:HG2	2.07	0.54
1:B:473:GLN:HA	1:B:477:LYS:O	2.08	0.53
1:A:251:ASN:HD22	1:A:255:SER:HB3	1.73	0.53
1:A:298:VAL:HA	1:A:321:ILE:O	2.08	0.53
1:A:402:HIS:NE2	1:A:439:GLN:HG3	2.23	0.53
1:A:424:ILE:HG13	1:A:424:ILE:O	2.08	0.53
1:B:362:SER:OG	1:B:366:LYS:HD3	2.08	0.53
1:A:114:ARG:HH21	1:B:114:ARG:HG2	1.74	0.53
1:B:341:ASN:HD21	1:B:344:ASN:H	1.56	0.53
1:B:43:GLY:HA2	1:B:146:ILE:O	2.09	0.52
1:A:171:TYR:CG	1:A:393:VAL:HG22	2.44	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:395:ASN:OD1	1:B:441:THR:HG23	2.10	0.52
1:A:363:LEU:HD22	1:A:363:LEU:N	2.25	0.52
1:B:192:PRO:HG3	1:B:464:GLY:HA2	1.91	0.52
1:A:452:SER:HA	4:A:1091:HOH:O	2.10	0.52
1:A:30:ARG:O	1:A:30:ARG:HG3	2.09	0.52
1:B:116:SER:O	1:B:117:LEU:HD12	2.09	0.52
1:A:515:PRO:HG2	1:A:516:ASN:N	2.15	0.52
1:A:504:VAL:HG13	1:A:504:VAL:O	2.09	0.52
1:A:457:ASP:HB2	1:A:461:ASP:H	1.75	0.52
1:B:138:ILE:N	1:B:139:PRO:HD2	2.25	0.51
1:A:217:ALA:HB2	1:A:227:ILE:CG1	2.39	0.51
1:A:473:GLN:HE21	1:A:476:GLY:HA2	1.74	0.51
1:A:189:ARG:HD3	1:A:461:ASP:OD1	2.11	0.51
1:A:334:ASP:O	1:A:338:GLN:HG3	2.10	0.51
1:B:449:GLY:C	1:B:451:ASP:H	2.14	0.51
1:A:363:LEU:O	1:A:364:GLN:HG2	2.10	0.51
1:B:330:VAL:HG13	1:B:444:PHE:CB	2.37	0.51
1:A:253:ARG:HG2	1:A:290:ARG:HH22	1.74	0.51
1:B:521:MET:HB2	1:B:530:ILE:HG13	1.93	0.51
1:A:443:PRO:O	1:A:445:ASN:N	2.44	0.51
1:A:515:PRO:O	1:A:517:GLU:N	2.44	0.50
1:B:193:PRO:HD3	1:B:461:ASP:HB3	1.94	0.50
1:A:540:LEU:HD13	1:A:559:LEU:HD23	1.94	0.50
1:B:169:ILE:CD1	1:B:434:TYR:OH	2.60	0.50
1:B:310:VAL:HG12	1:B:314:GLU:HA	1.94	0.50
1:B:314:GLU:HG2	1:B:478:TYR:CE2	2.47	0.50
1:A:492:LEU:N	1:A:492:LEU:HD23	2.26	0.50
1:A:200:ALA:O	1:A:204:ILE:HG13	2.12	0.50
1:B:541:VAL:O	1:B:541:VAL:HG12	2.11	0.50
1:B:205:LEU:CD2	1:B:210:TRP:HE3	2.24	0.49
1:B:78:GLU:HG3	1:B:444:PHE:HZ	1.76	0.49
1:B:473:GLN:O	1:B:473:GLN:NE2	2.45	0.49
1:A:535:GLU:HB2	1:A:538:GLU:HG3	1.94	0.49
1:A:114:ARG:CZ	1:B:114:ARG:HG2	2.43	0.49
1:B:356:GLU:OE1	1:B:366:LYS:HB2	2.11	0.49
1:B:341:ASN:HB2	1:B:342:PRO:HD2	1.93	0.49
1:B:251:ASN:HD22	1:B:255:SER:CB	2.25	0.49
1:B:289:ASN:CA	1:B:316:VAL:HG21	2.41	0.49
1:A:326:ALA:HB3	1:A:465:ARG:HB2	1.95	0.49
1:B:214:SER:OG	1:B:243:THR:HG22	2.12	0.49
1:A:56:GLU:HG2	1:A:101:ARG:NH2	2.28	0.49
1:A:150:TYR:HB2	1:A:153:VAL:HG13	1.95	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:554:TRP:CG	1:A:555:PRO:HD2	2.47	0.49
1:B:286:ALA:O	1:B:290:ARG:HG3	2.13	0.48
1:B:169:ILE:CG1	1:B:434:TYR:OH	2.61	0.48
1:A:310:VAL:HG12	1:A:314:GLU:HA	1.93	0.48
1:A:116:SER:O	1:A:117:LEU:HD12	2.13	0.48
1:B:457:ASP:HB2	1:B:461:ASP:H	1.77	0.48
1:B:351:PHE:O	1:B:354:PHE:HB3	2.14	0.48
1:A:515:PRO:CG	1:A:516:ASN:N	2.74	0.48
1:B:341:ASN:HD22	1:B:343:TYR:N	2.08	0.48
1:B:566:PRO:O	1:B:567:GLU:HB2	2.13	0.48
1:B:324:GLU:HG2	1:B:388:SER:OG	2.14	0.48
1:A:440:PHE:HE2	1:A:448:LYS:HB3	1.76	0.48
1:A:214:SER:OG	1:A:243:THR:HG22	2.14	0.47
1:A:252:ILE:HG22	1:A:253:ARG:H	1.79	0.47
1:B:519:LYS:HG2	1:B:532:ILE:HB	1.95	0.47
1:B:86:LEU:N	1:B:87:PRO:CD	2.78	0.47
1:B:444:PHE:CD2	1:B:444:PHE:N	2.80	0.47
1:A:473:GLN:NE2	1:A:476:GLY:CA	2.77	0.47
1:B:563:TYR:HD1	1:B:564:ASN:O	1.97	0.47
1:A:522:GLN:HA	1:A:522:GLN:HE21	1.80	0.47
1:B:99:CYS:O	1:B:101:ARG:HG3	2.15	0.47
1:A:79:ILE:HD13	1:A:401:ALA:HB2	1.96	0.47
1:B:523:PRO:HD2	1:B:528:CYS:O	2.15	0.47
1:B:341:ASN:C	1:B:341:ASN:ND2	2.65	0.47
1:A:540:LEU:CD1	1:A:546:CYS:SG	3.02	0.47
1:B:181:LYS:HE2	1:B:181:LYS:HA	1.97	0.47
1:A:108:GLN:O	1:A:111:GLU:HB2	2.15	0.47
1:A:516:ASN:C	1:A:517:GLU:HG3	2.34	0.47
1:B:518:MET:HA	1:B:533:PRO:HA	1.97	0.46
1:A:197:GLN:OE1	1:A:300:SER:HB2	2.15	0.46
1:A:115:ALA:HB1	1:A:140:LEU:O	2.15	0.46
1:B:355:TRP:CZ2	1:B:359:PHE:HE1	2.34	0.46
1:A:178:LEU:O	1:A:181:LYS:NZ	2.49	0.46
1:A:372:VAL:CG2	1:A:373:CYS:N	2.78	0.46
1:A:443:PRO:C	1:A:445:ASN:H	2.19	0.46
1:B:108:GLN:O	1:B:111:GLU:HB2	2.16	0.46
1:A:457:ASP:HB3	1:A:459:PHE:H	1.81	0.46
1:B:558:ASP:OD2	1:B:560:SER:HB3	2.16	0.46
1:A:215:THR:HG22	1:A:273:VAL:HB	1.98	0.46
1:B:227:ILE:HD13	1:B:227:ILE:HA	1.83	0.46
1:B:241:ILE:HG23	1:B:241:ILE:O	2.16	0.46
1:A:96:LEU:HD13	1:A:108:GLN:HB3	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:75:ALA:O	1:B:79:ILE:HG13	2.16	0.46
1:B:566:PRO:HB2	1:B:567:GLU:OE1	2.16	0.46
1:B:515:PRO:O	1:B:517:GLU:N	2.49	0.45
1:A:473:GLN:HE21	1:A:476:GLY:C	2.19	0.45
1:B:418:LEU:HD13	1:B:422:MET:HB2	1.97	0.45
1:A:276:MET:HE3	1:A:281:SER:HA	1.98	0.45
1:A:310:VAL:CG1	1:A:314:GLU:HA	2.46	0.45
1:B:185:ASP:N	1:B:185:ASP:OD2	2.49	0.45
1:B:558:ASP:OD2	1:B:560:SER:CB	2.65	0.45
1:B:366:LYS:CG	1:B:367:ARG:H	2.25	0.45
1:A:169:ILE:CD1	1:A:434:TYR:OH	2.64	0.45
1:A:314:GLU:HG2	1:A:478:TYR:CD2	2.51	0.45
1:B:284:LEU:C	1:B:284:LEU:HD13	2.37	0.45
1:A:428:LYS:NZ	4:A:1011:HOH:O	2.50	0.45
1:B:473:GLN:NE2	1:B:476:GLY:HA2	2.32	0.45
1:B:253:ARG:HG2	1:B:290:ARG:NH2	2.31	0.45
1:B:309:ILE:HG22	1:B:310:VAL:HG23	1.98	0.45
1:A:110:LEU:O	1:A:114:ARG:HG3	2.16	0.45
1:A:274:LEU:HD13	1:A:276:MET:HE2	1.98	0.45
1:A:169:ILE:CG1	1:A:434:TYR:OH	2.65	0.45
1:B:424:ILE:O	1:B:424:ILE:HG13	2.17	0.45
1:B:96:LEU:HD13	1:B:108:GLN:HB3	1.98	0.44
1:A:372:VAL:CG2	1:A:373:CYS:H	2.30	0.44
1:A:558:ASP:O	1:A:559:LEU:HB2	2.17	0.44
1:B:359:PHE:HE2	1:B:383:ASN:HD22	1.65	0.44
1:B:197:GLN:HB2	1:B:466:TYR:CE2	2.53	0.44
1:B:211:THR:O	1:B:211:THR:HG22	2.18	0.44
1:A:361:CYS:HB3	1:A:362:SER:H	1.23	0.44
1:A:362:SER:O	1:A:363:LEU:HD13	2.18	0.44
1:B:115:ALA:C	1:B:117:LEU:H	2.21	0.44
1:B:352:ARG:HH11	1:B:352:ARG:HG2	1.83	0.44
1:A:209:ASN:ND2	2:A:801:NAG:H82	2.32	0.44
1:A:216:VAL:CG1	1:A:274:LEU:HD22	2.47	0.44
1:A:164:PHE:N	1:A:164:PHE:CD1	2.85	0.44
1:A:282:ARG:CD	1:A:309:ILE:HA	2.48	0.44
1:A:490:LEU:HG	1:A:492:LEU:HD22	2.00	0.43
1:B:207:PHE:HD2	1:B:208:PHE:CD1	2.36	0.43
1:B:514:ALA:CB	1:B:518:MET:HG3	2.35	0.43
1:A:213:VAL:O	1:A:241:ILE:HA	2.18	0.43
1:A:437:LYS:HA	1:A:437:LYS:HD2	1.79	0.43
1:B:490:LEU:HD12	1:B:491:SER:N	2.19	0.43
1:B:473:GLN:HE21	1:B:476:GLY:HA2	1.80	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:208:PHE:CE2	1:B:499:TRP:HZ2	2.37	0.43
1:B:157:VAL:CG1	1:B:161:LEU:HD22	2.47	0.43
1:B:107:GLU:O	1:B:110:LEU:HB2	2.18	0.43
1:A:147:GLY:HA2	1:A:171:TYR:CE2	2.53	0.43
1:B:205:LEU:HD22	1:B:210:TRP:CE3	2.49	0.43
1:A:69:LEU:HD22	1:A:69:LEU:C	2.37	0.43
1:B:102:ASP:OD2	1:B:103:THR:N	2.50	0.43
1:A:310:VAL:HG12	1:A:310:VAL:O	2.17	0.43
1:B:54:THR:HB	4:B:2012:HOH:O	2.18	0.43
1:A:268:ASN:ND2	1:A:509:CYS:O	2.51	0.43
1:B:257:ASP:OD2	1:B:290:ARG:NH1	2.52	0.43
1:A:490:LEU:HG	1:A:492:LEU:CD2	2.48	0.43
1:B:138:ILE:N	1:B:139:PRO:CD	2.81	0.43
1:B:352:ARG:HG2	1:B:352:ARG:NH1	2.34	0.43
1:A:146:ILE:HG13	1:A:397:VAL:HG22	2.01	0.43
1:A:102:ASP:HB2	1:A:156:GLN:HG3	2.01	0.43
1:B:374:ASP:HB3	1:B:377:LEU:HD22	2.00	0.42
1:A:227:ILE:HG22	1:A:228:GLU:N	2.33	0.42
1:B:437:LYS:HA	1:B:437:LYS:HD2	1.68	0.42
1:B:41:LEU:CD2	1:B:400:MET:HG2	2.49	0.42
1:A:252:ILE:HG22	1:A:253:ARG:N	2.35	0.42
1:A:520:ASN:HB3	1:A:544:PHE:CD2	2.55	0.42
1:A:539:TYR:CZ	1:A:541:VAL:HG22	2.54	0.42
1:A:227:ILE:O	1:A:231:GLU:HG3	2.19	0.42
1:B:282:ARG:HH11	1:B:282:ARG:CG	2.33	0.42
1:B:440:PHE:CD2	1:B:448:LYS:HD3	2.54	0.42
1:A:69:LEU:HD23	1:A:95:ILE:HG21	2.01	0.42
1:A:341:ASN:ND2	1:A:341:ASN:C	2.70	0.42
1:B:211:THR:HG23	1:B:239:ILE:HA	2.02	0.42
1:B:377:LEU:HA	1:B:377:LEU:HD13	1.71	0.42
1:B:212:TYR:HB2	1:B:509:CYS:N	2.35	0.42
1:A:266:LYS:N	1:A:267:PRO:CD	2.82	0.42
1:A:451:ASP:OD1	1:A:453:ILE:HG12	2.20	0.42
1:A:367:ARG:O	1:A:369:HIS:N	2.49	0.42
1:B:167:PRO:HG3	1:B:430:LEU:HD23	2.02	0.42
1:A:407:MET:HG2	1:A:422:MET:SD	2.60	0.42
1:B:501:ARG:O	1:B:503:SER:N	2.52	0.42
1:B:310:VAL:HG12	1:B:310:VAL:O	2.20	0.41
1:A:523:PRO:HD3	1:A:529:TRP:HA	2.02	0.41
1:B:216:VAL:HG22	1:B:276:MET:SD	2.60	0.41
1:A:530:ILE:HD12	1:A:532:ILE:HD11	2.02	0.41
1:A:444:PHE:CD2	1:A:444:PHE:N	2.85	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:181:LYS:HD3	1:A:181:LYS:HA	1.83	0.41
1:A:282:ARG:HH11	1:A:282:ARG:HG2	1.85	0.41
1:B:341:ASN:HD21	1:B:343:TYR:HB2	1.86	0.41
1:B:520:ASN:HB3	1:B:544:PHE:CD2	2.54	0.41
1:B:353:ASP:N	1:B:353:ASP:OD1	2.50	0.41
1:A:261:ARG:O	1:A:264:LEU:N	2.53	0.41
1:B:470:ASN:HB2	1:B:483:VAL:HG11	2.02	0.41
1:A:289:ASN:CA	1:A:316:VAL:HG21	2.51	0.41
1:A:163:LEU:HD11	1:B:159:ASN:HB3	2.02	0.41
1:A:326:ALA:HA	1:A:467:ASN:ND2	2.35	0.41
1:B:86:LEU:HA	1:B:86:LEU:HD12	1.91	0.41
1:B:418:LEU:HD13	1:B:422:MET:CB	2.51	0.41
1:A:470:ASN:OD1	1:A:497:ILE:HG23	2.21	0.41
1:B:365:ASN:OD1	1:B:365:ASN:O	2.39	0.41
1:B:492:LEU:N	1:B:492:LEU:HD23	2.35	0.41
1:A:558:ASP:C	1:A:558:ASP:OD2	2.57	0.41
1:A:252:ILE:O	1:A:253:ARG:C	2.59	0.41
1:A:116:SER:C	1:A:117:LEU:HD12	2.42	0.41
1:B:363:LEU:N	1:B:363:LEU:HD22	2.36	0.40
1:A:102:ASP:OD2	1:A:103:THR:N	2.55	0.40
1:A:246:LYS:O	1:A:246:LYS:HG3	2.21	0.40
1:A:189:ARG:HG3	1:A:191:VAL:O	2.21	0.40
1:B:41:LEU:HD22	1:B:400:MET:HG2	2.03	0.40
1:A:475:GLY:C	1:A:477:LYS:H	2.25	0.40
1:A:64:ARG:HD3	3:A:1001:C5B:OZ1	2.22	0.40
1:A:426:ASP:OD2	1:A:429:LYS:HD3	2.21	0.40
1:B:216:VAL:HA	1:B:245:GLU:O	2.22	0.40
1:B:169:ILE:HD13	1:B:434:TYR:OH	2.22	0.40
1:A:109:SER:C	1:A:111:GLU:N	2.73	0.40
1:A:205:LEU:CD2	1:A:210:TRP:HE3	2.35	0.40
1:B:247:VAL:HG11	1:B:256:TYR:CE2	2.56	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	514/555 (93%)	446 (87%)	51 (10%)	17 (3%)	6	17
1	B	516/555 (93%)	443 (86%)	56 (11%)	17 (3%)	6	17
All	All	1030/1110 (93%)	889 (86%)	107 (10%)	34 (3%)	6	17

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	362	SER
1	A	443	PRO
1	A	444	PHE
1	A	474	THR
1	A	502	ASN
1	A	516	ASN
1	A	523	PRO
1	B	362	SER
1	B	443	PRO
1	B	502	ASN
1	B	516	ASN
1	B	523	PRO
1	A	368	ASN
1	B	474	THR
1	B	543	GLU
1	A	447	ASN
1	B	116	SER
1	B	292	ASN
1	B	447	ASN
1	B	505	PRO
1	A	116	SER
1	A	250	SER
1	A	313	SER
1	A	364	GLN
1	B	313	SER
1	B	444	PHE
1	B	515	PRO
1	A	361	CYS
1	A	433	GLU
1	A	515	PRO
1	B	329	PRO
1	B	172	ALA
1	B	433	GLU
1	A	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	447/481 (93%)	415 (93%)	32 (7%)	21	47
1	B	449/481 (93%)	411 (92%)	38 (8%)	15	38
All	All	896/962 (93%)	826 (92%)	70 (8%)	18	42

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	39	LEU
1	A	63	ASP
1	A	69	LEU
1	A	73	LEU
1	A	86	LEU
1	A	106	LEU
1	A	110	LEU
1	A	153	VAL
1	A	161	LEU
1	A	163	LEU
1	A	185	ASP
1	A	189	ARG
1	A	227	ILE
1	A	275	PHE
1	A	292	ASN
1	A	303	TRP
1	A	331	ARG
1	A	341	ASN
1	A	362	SER
1	A	363	LEU
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	491	SER
1	A	498	HIS

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Mol	Chain	Res	Type
1	A	517	GLU
1	A	518	MET
1	A	567	GLU
1	B	29	MET
1	B	39	LEU
1	B	69	LEU
1	B	73	LEU
1	B	86	LEU
1	B	106	LEU
1	B	107	GLU
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	279	ASP
1	B	292	ASN
1	B	309	ILE
1	B	341	ASN
1	B	353	ASP
1	B	373	CYS
1	B	377	LEU
1	B	381	SER
1	B	408	GLN
1	B	418	LEU
1	B	422	MET
1	B	439	GLN
1	B	454	VAL
1	B	457	ASP
1	B	470	ASN
1	B	491	SER
1	B	498	HIS
1	B	517	GLU
1	B	518	MET
1	B	540	LEU
1	B	559	LEU
1	B	567	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	251	ASN
1	A	292	ASN
1	A	341	ASN
1	A	365	ASN
1	A	473	GLN
1	A	485	HIS
1	A	522	GLN
1	B	108	GLN
1	B	251	ASN
1	B	268	ASN
1	B	292	ASN
1	B	306	GLN
1	B	341	ASN
1	B	365	ASN
1	B	369	HIS
1	B	408	GLN
1	B	473	GLN
1	B	522	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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	C5B	A	1001	-	12,12,12	0.90	0	18,18,18	1.43	2 (11%)
2	NAG	A	801	1	12,14,15	0.53	0	15,19,21	0.66	0
3	C5B	B	2001	-	12,12,12	1.00	1 (8%)	18,18,18	1.41	2 (11%)
2	NAG	B	802	1	12,14,15	0.49	0	15,19,21	0.69	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	C5B	A	1001	-	-	0/10/21/21	0/1/1/1
2	NAG	A	801	1	-	0/6/23/26	0/1/1/1
3	C5B	B	2001	-	-	0/10/21/21	0/1/1/1
2	NAG	B	802	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2001	C5B	CD-CE	2.12	1.54	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	C5B	CB2-CA-CB1	3.41	108.45	102.75
3	B	2001	C5B	CB2-CA-CB1	3.33	108.34	102.75
3	B	2001	C5B	OXT-C-CA	2.44	119.44	113.70
3	A	1001	C5B	OXT-C-CA	2.42	119.39	113.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	518/555 (93%)	0.60	43 (8%)	11 11	33, 66, 105, 141	0
1	B	520/555 (93%)	0.64	59 (11%)	6 5	35, 68, 107, 141	0
All	All	1038/1110 (93%)	0.62	102 (9%)	8 7	33, 67, 106, 141	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	368	ASN	10.4
1	B	516	ASN	8.2
1	A	516	ASN	7.7
1	A	368	ASN	7.7
1	B	567	GLU	7.5
1	B	367	ARG	7.2
1	B	366	LYS	6.8
1	B	365	ASN	6.7
1	A	369	HIS	6.6
1	B	28	PHE	6.4
1	B	369	HIS	6.4
1	A	449	GLY	6.4
1	A	367	ARG	6.1
1	A	366	LYS	5.9
1	B	474	THR	5.5
1	A	250	SER	5.4
1	A	450	ALA	5.3
1	A	365	ASN	5.3
1	B	250	SER	5.2
1	B	449	GLY	5.2
1	A	443	PRO	4.8
1	B	450	ALA	4.8
1	B	52	THR	4.7
1	B	251	ASN	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	29	MET	4.3
1	B	343	TYR	4.3
1	B	54	THR	4.2
1	A	370	ARG	4.1
1	A	478	TYR	4.0
1	A	55	GLU	3.9
1	A	446	PRO	3.9
1	B	477	LYS	3.8
1	B	478	TYR	3.8
1	A	361	CYS	3.7
1	B	440	PHE	3.7
1	B	331	ARG	3.7
1	A	524	GLY	3.6
1	B	566	PRO	3.6
1	A	474	THR	3.6
1	B	475	GLY	3.6
1	B	443	PRO	3.5
1	B	373	CYS	3.5
1	B	315	HIS	3.4
1	A	53	GLY	3.4
1	B	298	VAL	3.4
1	A	54	THR	3.3
1	B	139	PRO	3.3
1	A	254	LYS	3.3
1	A	448	LYS	3.3
1	B	249	ARG	3.1
1	A	299	ALA	3.1
1	B	364	GLN	3.0
1	A	138	ILE	2.9
1	B	476	GLY	2.9
1	B	299	ALA	2.9
1	A	441	THR	2.8
1	B	273	VAL	2.8
1	B	51	GLY	2.8
1	B	30	ARG	2.7
1	B	335	ARG	2.7
1	A	527	CYS	2.7
1	B	252	ILE	2.6
1	B	374	ASP	2.6
1	A	564	ASN	2.6
1	A	298	VAL	2.6
1	A	253	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	551	PRO	2.6
1	A	147	GLY	2.5
1	A	434	TYR	2.5
1	B	359	PHE	2.5
1	B	473	GLN	2.5
1	B	521	MET	2.5
1	A	567	GLU	2.5
1	A	451	ASP	2.4
1	B	254	LYS	2.4
1	B	376	HIS	2.4
1	A	297	TRP	2.4
1	B	53	GLY	2.4
1	B	43	GLY	2.4
1	B	147	GLY	2.4
1	B	272	VAL	2.3
1	A	272	VAL	2.3
1	B	360	GLN	2.3
1	A	274	LEU	2.3
1	A	520	ASN	2.3
1	A	440	PHE	2.2
1	B	235	ARG	2.2
1	B	318	TYR	2.2
1	A	116	SER	2.2
1	B	434	TYR	2.2
1	B	502	ASN	2.1
1	B	524	GLY	2.1
1	B	296	THR	2.1
1	A	204	ILE	2.1
1	B	371	GLN	2.1
1	B	55	GLU	2.1
1	B	481	LEU	2.1
1	A	447	ASN	2.0
1	A	528	CYS	2.0
1	B	479	SER	2.0
1	A	114	ARG	2.0
1	A	517	GLU	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

There are no carbohydrates in this entry.

### 6.4 Ligands

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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	A	801	14/15	0.23	1.80	95,97,100,100	0
3	C5B	B	2001	12/12	0.23	1.08	48,50,51,52	0
3	C5B	A	1001	12/12	0.24	0.97	45,46,51,53	0
2	NAG	B	802	14/15	0.22	0.89	88,95,96,98	0

### 6.5 Other polymers

There are no such residues in this entry.