



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 10:41 PM GMT

PDB ID : 2E4V
Title : Crystal structure of the extracellular region of the group II metabotropic glutamate receptor complexed with DCG-IV
Authors : Muto, T.; Tsuchiya, D.; Morikawa, K.; Jingami, H.
Deposited on : 2006-12-17
Resolution : 2.40 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

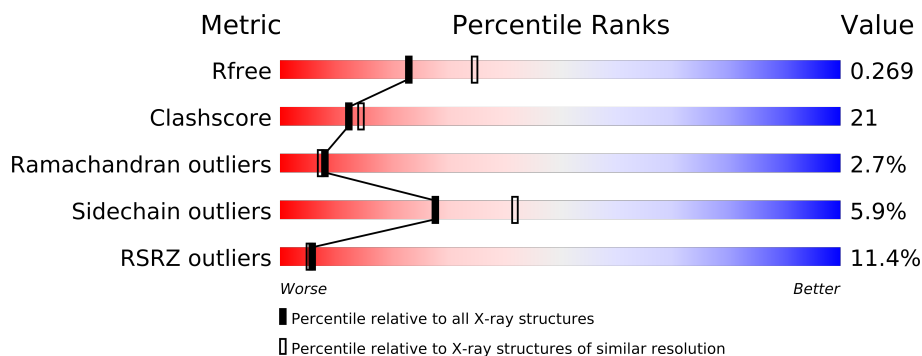
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.40 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	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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. 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	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	NAG	A	801	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8656 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:

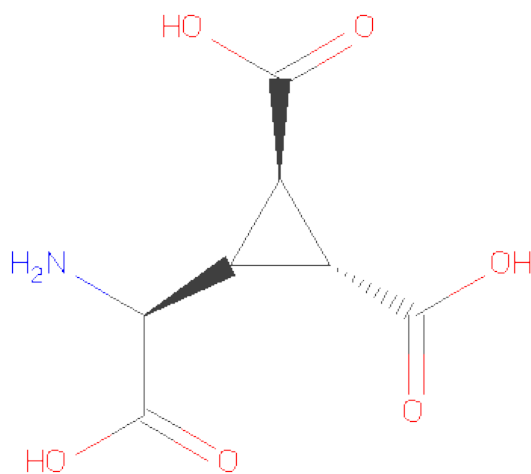
Chain	Residue	Modelled	Actual	Comment	Reference
A	414	GLN	ASN	ENGINEERED	UNP P31422
A	439	GLN	ASN	ENGINEERED	UNP P31422
A	576	LEU	-	CLONING ARTIFACT	UNP P31422
A	577	VAL	-	CLONING ARTIFACT	UNP P31422
A	578	PRO	-	CLONING ARTIFACT	UNP P31422
A	579	ARG	-	CLONING ARTIFACT	UNP P31422
B	414	GLN	ASN	ENGINEERED	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: 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 (1R,2R)-3-[(S)-AMINO(CARBOXY)METHYL]CYCLOPROPANE-1,2-DICARBOXYLICACID (three-letter code: 2CG) (formula: C₇H₉NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	7	1	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	7	1	6		

- Molecule 4 is water.

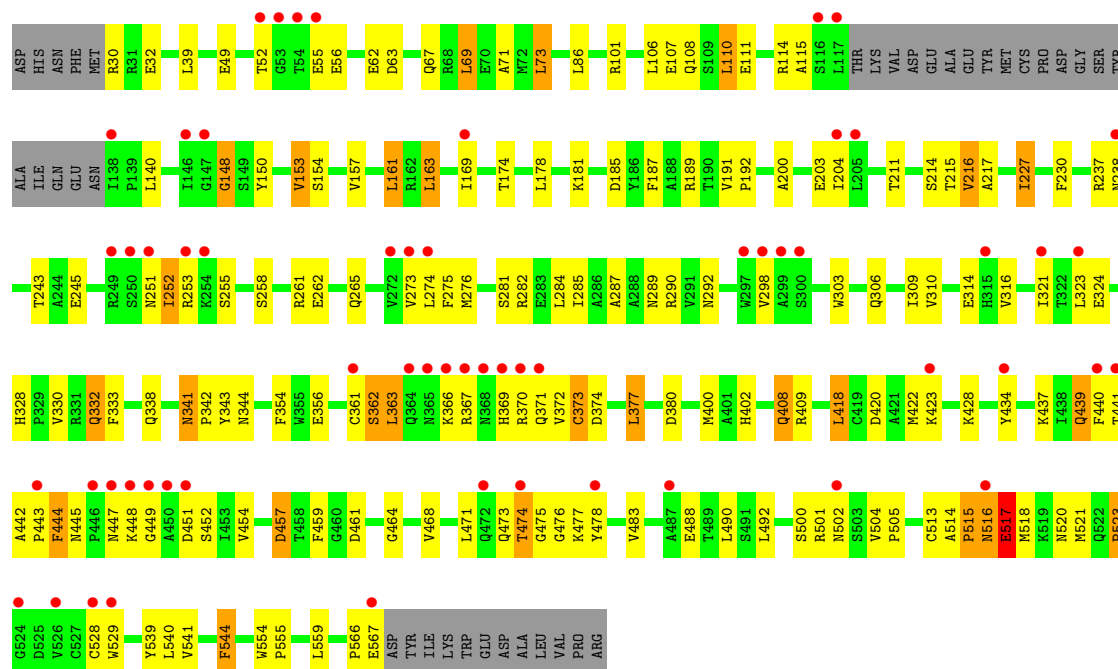
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	193	Total	O	0	0
			193	193		
4	B	152	Total	O	0	0
			152	152		

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.

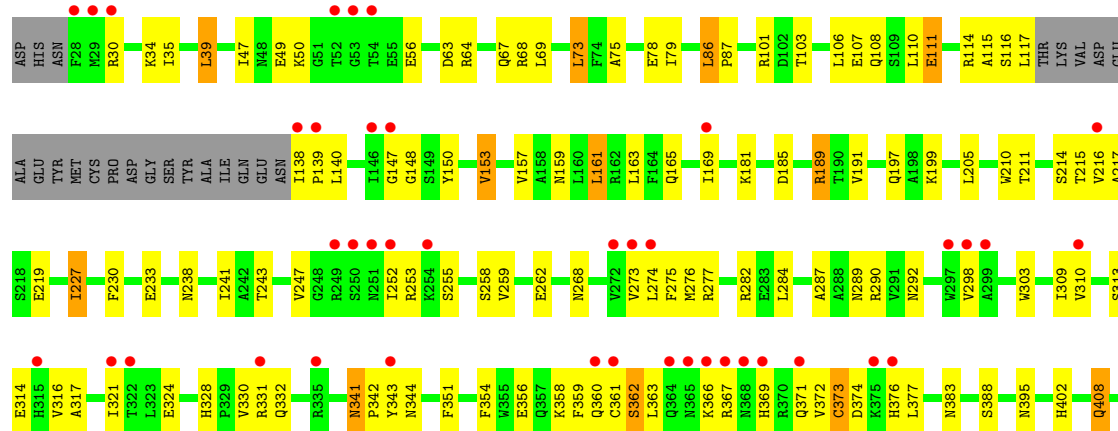
• Molecule 1: Metabotropic glutamate receptor 3

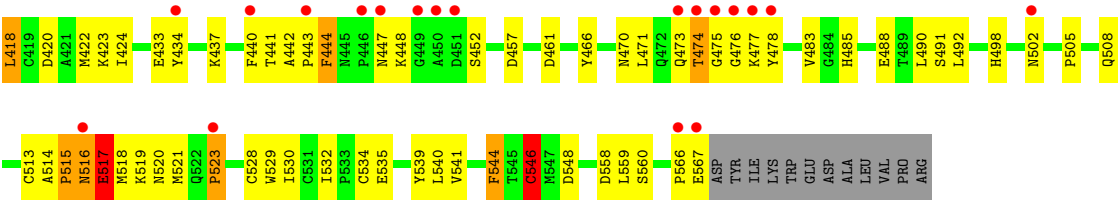
Chain A: 



• 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, α , β , γ	83.78Å 97.36Å 107.74Å 90.00° 92.87° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 29.26 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-2.40) 99.7 (29.26-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.236 , 0.268 0.237 , 0.269	Depositor DCC
R_{free} test set	4806 reflections (7.67%)	DCC
Wilson B-factor (Å ²)	55.3	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.2	EDS
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 67438 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8656	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: 2CG, 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	0/4212	0.67	1/5704 (0.0%)
1	B	0.39	0/4232	0.66	3/5730 (0.1%)
All	All	0.39	0/8444	0.67	4/11434 (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	-5.80	103.57	114.00
1	A	148	GLY	N-CA-C	-5.78	98.66	113.10
1	B	148	GLY	N-CA-C	-5.57	99.17	113.10
1	B	147	GLY	N-CA-C	5.22	126.14	113.10

There are no chirality outliers.

There are no planarity outliers.

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	165	0
1	B	4137	0	4012	182	0
2	A	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	14	0	13	0	0
3	A	14	0	6	3	0
3	B	14	0	6	2	0
4	A	193	0	0	17	0
4	B	152	0	0	10	0
All	All	8656	0	8043	349	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 (349) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:356:GLU:HA	1:A:361:CYS:HB2	1.35	1.06
1:B:356:GLU:HA	1:B:361:CYS:HB2	1.37	1.04
1:B:30:ARG:HD2	1:B:108:GLN:HE22	1.24	1.01
1:B:402:HIS:HB3	1:B:437:LYS:HE2	1.44	0.98
1:A:420:ASP:HA	1:A:423:LYS:HD3	1.43	0.97
1:A:402:HIS:HB3	1:A:437:LYS:HE2	1.46	0.96
1:B:50:LYS:HE2	1:B:101:ARG:HG2	1.49	0.94
1:A:515:PRO:HG2	1:A:516:ASN:H	1.33	0.93
1:B:341:ASN:HD22	1:B:343:TYR:H	1.12	0.92
1:A:514:ALA:H	1:A:518:MET:HE3	1.36	0.89
1:B:328:HIS:HB2	4:B:2024:HOH:O	1.73	0.89
1:A:400:MET:SD	4:A:1138:HOH:O	2.32	0.88
1:B:540:LEU:HD13	1:B:559:LEU:HD23	1.57	0.86
1:B:514:ALA:HB3	1:B:518:MET:HG3	1.56	0.86
1:A:276:MET:HE3	1:A:281:SER:HA	1.59	0.85
1:B:515:PRO:HG2	1:B:516:ASN:H	1.43	0.83
1:A:514:ALA:HB3	1:A:518:MET:HG3	1.60	0.83
1:B:216:VAL:CG1	1:B:274:LEU:HD22	2.11	0.80
1:A:540:LEU:HD13	1:A:559:LEU:HD23	1.65	0.79
1:A:101:ARG:HD3	4:A:1066:HOH:O	1.83	0.78
1:A:181:LYS:HE2	1:A:459:PHE:O	1.83	0.78
1:B:420:ASP:HA	1:B:423:LYS:HD3	1.64	0.78
1:B:282:ARG:HG2	1:B:282:ARG:HH11	1.48	0.77
1:B:330:VAL:HG13	1:B:444:PHE:HB3	1.66	0.77
1:A:30:ARG:HA	4:A:1129:HOH:O	1.83	0.77
1:B:514:ALA:H	1:B:518:MET:HE3	1.51	0.75
1:B:540:LEU:HG	4:B:2148:HOH:O	1.84	0.75
1:A:418:LEU:HD22	1:A:422:MET:HE3	1.68	0.75
1:A:107:GLU:HB3	4:A:1112:HOH:O	1.85	0.75
1:B:47:ILE:HD12	1:B:69:LEU:HD12	1.69	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:514:ALA:H	1:B:518:MET:CE	2.00	0.74
1:B:440:PHE:CE2	1:B:448:LYS:HB3	2.23	0.74
1:B:314:GLU:HG2	1:B:478:TYR:CD2	2.22	0.73
1:B:310:VAL:HG12	1:B:314:GLU:HG3	1.70	0.73
1:B:50:LYS:HG2	1:B:101:ARG:HG3	1.71	0.72
1:A:330:VAL:HG13	1:A:444:PHE:HB3	1.71	0.72
1:B:258:SER:O	1:B:262:GLU:HG3	1.90	0.72
1:A:282:ARG:HH11	1:A:282:ARG:HG2	1.53	0.72
1:A:216:VAL:HG13	1:A:274:LEU:HD22	1.70	0.72
1:A:314:GLU:HG2	1:A:478:TYR:CD2	2.25	0.72
1:B:362:SER:O	1:B:363:LEU:HD13	1.89	0.71
1:A:258:SER:O	1:A:262:GLU:HG3	1.89	0.71
1:B:274:LEU:HD13	1:B:276:MET:HE2	1.71	0.71
1:A:514:ALA:H	1:A:518:MET:CE	2.03	0.71
1:A:157:VAL:HG12	1:A:161:LEU:HD22	1.71	0.71
1:B:252:ILE:HG22	1:B:253:ARG:H	1.54	0.71
1:A:211:THR:HG23	1:A:238:ASN:O	1.91	0.70
1:B:310:VAL:CG1	1:B:314:GLU:HA	2.22	0.70
1:A:169:ILE:HG12	1:A:434:TYR:OH	1.91	0.70
1:B:341:ASN:ND2	1:B:343:TYR:H	1.90	0.69
1:A:402:HIS:CB	1:A:437:LYS:HE2	2.22	0.69
1:A:328:HIS:HB2	4:A:1080:HOH:O	1.93	0.69
1:B:216:VAL:HG12	1:B:274:LEU:CD2	2.23	0.69
1:A:442:ALA:O	1:A:444:PHE:N	2.25	0.69
1:A:374:ASP:HB3	1:A:377:LEU:HD22	1.75	0.68
1:A:515:PRO:CG	1:A:516:ASN:H	2.07	0.67
1:B:473:GLN:HE21	1:B:476:GLY:CA	2.07	0.67
1:B:216:VAL:HG12	1:B:274:LEU:HD22	1.75	0.66
1:A:361:CYS:O	1:A:362:SER:HB2	1.95	0.66
1:A:56:GLU:HG2	1:A:101:ARG:HH22	1.61	0.66
1:A:338:GLN:OE1	1:A:380:ASP:HA	1.95	0.66
3:B:2001:2CG:HA	3:B:2001:2CG:O21	1.96	0.66
1:A:367:ARG:HB2	1:A:369:HIS:NE2	2.11	0.66
1:A:287:ALA:HA	1:A:290:ARG:NH1	2.12	0.65
1:A:310:VAL:HG12	1:A:314:GLU:HA	1.78	0.65
1:B:103:THR:O	1:B:107:GLU:HG2	1.96	0.65
1:A:310:VAL:CG1	1:A:314:GLU:HA	2.27	0.65
1:B:47:ILE:CD1	1:B:69:LEU:HD12	2.26	0.65
1:A:440:PHE:CE2	1:A:448:LYS:HB3	2.32	0.65
1:B:217:ALA:HB2	1:B:227:ILE:HG13	1.78	0.65
1:B:169:ILE:HG12	1:B:434:TYR:OH	1.97	0.65
1:B:442:ALA:O	1:B:444:PHE:N	2.30	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:374:ASP:HB3	1:A:377:LEU:CD2	2.28	0.64
1:A:452:SER:HA	4:A:1144:HOH:O	1.98	0.64
1:B:69:LEU:HD23	1:B:69:LEU:C	2.19	0.63
1:B:341:ASN:HD22	1:B:343:TYR:N	1.91	0.63
1:B:56:GLU:HG2	1:B:101:ARG:HH22	1.64	0.62
1:B:539:TYR:CZ	1:B:541:VAL:HG22	2.34	0.62
1:B:63:ASP:O	1:B:67:GLN:HB2	2.00	0.62
1:B:253:ARG:HG2	1:B:290:ARG:NH2	2.15	0.61
1:B:483:VAL:O	1:B:492:LEU:HB2	2.00	0.61
1:B:473:GLN:HE21	1:B:476:GLY:HA2	1.65	0.61
1:A:370:ARG:HG2	1:A:370:ARG:HH11	1.66	0.61
1:B:289:ASN:HA	1:B:316:VAL:HG21	1.82	0.61
1:A:341:ASN:ND2	1:A:344:ASN:H	1.99	0.61
1:A:115:ALA:HB1	1:A:140:LEU:O	2.01	0.60
1:B:157:VAL:HG12	1:B:161:LEU:HD22	1.81	0.60
1:A:332:GLN:HG3	4:A:1120:HOH:O	2.00	0.60
1:B:418:LEU:HD22	1:B:422:MET:HE3	1.83	0.60
1:B:473:GLN:NE2	1:B:476:GLY:HA2	2.17	0.60
1:A:515:PRO:O	1:A:517:GLU:N	2.34	0.60
1:A:366:LYS:HG2	1:A:367:ARG:H	1.66	0.60
1:B:366:LYS:HG2	1:B:367:ARG:H	1.67	0.60
1:A:216:VAL:HA	1:A:245:GLU:O	2.02	0.60
1:B:540:LEU:HD13	1:B:559:LEU:CD2	2.31	0.60
1:A:253:ARG:HG2	1:A:290:ARG:NH2	2.16	0.59
1:A:216:VAL:CG1	1:A:274:LEU:HD22	2.32	0.59
1:A:252:ILE:HG22	1:A:253:ARG:H	1.67	0.59
1:B:330:VAL:HG13	1:B:444:PHE:CB	2.33	0.59
1:B:287:ALA:HA	1:B:290:ARG:NH1	2.18	0.59
1:A:362:SER:O	1:A:363:LEU:HD13	2.03	0.59
1:A:341:ASN:HD22	1:A:343:TYR:H	1.50	0.58
1:A:110:LEU:O	1:A:114:ARG:HG3	2.03	0.58
1:A:473:GLN:NE2	1:A:476:GLY:HA2	2.18	0.58
1:B:362:SER:OG	1:B:366:LYS:HD3	2.04	0.58
1:B:374:ASP:HB3	1:B:377:LEU:CD2	2.33	0.58
1:A:418:LEU:HD22	1:A:422:MET:CE	2.32	0.58
1:A:372:VAL:HG22	1:A:373:CYS:N	2.18	0.58
1:A:306:GLN:NE2	1:A:309:ILE:HD11	2.19	0.58
1:A:523:PRO:HD3	1:A:529:TRP:HA	1.86	0.58
1:A:363:LEU:HD22	1:A:363:LEU:N	2.19	0.57
1:B:515:PRO:CG	1:B:516:ASN:H	2.16	0.57
1:A:252:ILE:HD12	1:A:252:ILE:H	1.69	0.57
1:B:523:PRO:HD2	1:B:528:CYS:O	2.04	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:395:ASN:OD1	1:B:441:THR:HG23	2.05	0.57
1:B:521:MET:HB2	1:B:530:ILE:HG13	1.87	0.57
1:B:540:LEU:HD12	1:B:546:CYS:SG	2.44	0.57
1:B:215:THR:OG1	1:B:241:ILE:HD11	2.03	0.57
1:B:548:ASP:HB2	4:B:2080:HOH:O	2.05	0.57
1:A:215:THR:HG22	1:A:273:VAL:HB	1.87	0.56
1:A:420:ASP:O	1:A:423:LYS:HB2	2.06	0.56
1:A:367:ARG:HB2	1:A:369:HIS:CD2	2.41	0.56
1:B:165:GLN:HG2	4:B:2043:HOH:O	2.06	0.55
1:A:289:ASN:HA	1:A:316:VAL:HG21	1.89	0.55
1:B:490:LEU:HD12	1:B:491:SER:H	1.72	0.55
1:B:217:ALA:HB2	1:B:227:ILE:CG1	2.36	0.55
1:A:539:TYR:CZ	1:A:541:VAL:HG22	2.42	0.55
1:A:372:VAL:HG22	1:A:373:CYS:H	1.70	0.55
1:A:366:LYS:HG2	1:A:367:ARG:N	2.22	0.54
3:A:1001:2CG:HA	3:A:1001:2CG:O21	2.04	0.54
1:B:440:PHE:HE2	1:B:448:LYS:HB3	1.72	0.54
1:A:150:TYR:HB2	1:A:153:VAL:HG13	1.89	0.54
1:B:181:LYS:HE2	1:B:181:LYS:HA	1.90	0.54
1:B:408:GLN:HB2	1:B:422:MET:HE1	1.89	0.54
1:B:366:LYS:HG2	1:B:367:ARG:N	2.23	0.54
1:B:366:LYS:HE2	1:B:369:HIS:CD2	2.43	0.53
1:B:408:GLN:HB2	1:B:422:MET:CE	2.39	0.53
1:A:523:PRO:HD2	1:A:528:CYS:O	2.09	0.53
1:A:330:VAL:HG13	1:A:444:PHE:CB	2.39	0.53
1:B:252:ILE:HG22	1:B:253:ARG:N	2.23	0.53
1:A:169:ILE:CG1	1:A:434:TYR:OH	2.56	0.53
3:B:2001:2CG:CA	3:B:2001:2CG:O21	2.56	0.53
1:B:332:GLN:HG3	4:B:2025:HOH:O	2.09	0.53
1:A:515:PRO:HG2	1:A:516:ASN:N	2.13	0.53
1:B:424:ILE:O	1:B:424:ILE:HG13	2.08	0.53
1:A:554:TRP:CG	1:A:555:PRO:HD2	2.43	0.52
1:A:216:VAL:CG1	1:A:274:LEU:CD2	2.88	0.52
1:B:50:LYS:HG2	1:B:101:ARG:CG	2.38	0.52
1:B:282:ARG:NH1	1:B:282:ARG:HG2	2.20	0.51
1:A:408:GLN:HB2	1:A:422:MET:CE	2.40	0.51
1:B:211:THR:O	1:B:211:THR:HG22	2.08	0.51
1:B:50:LYS:CE	1:B:101:ARG:HG2	2.30	0.51
1:A:370:ARG:HG2	1:A:370:ARG:NH1	2.25	0.51
1:A:189:ARG:HG3	1:A:191:VAL:O	2.10	0.51
1:B:215:THR:HG22	1:B:273:VAL:HB	1.91	0.51
1:A:189:ARG:HD3	1:A:461:ASP:OD1	2.10	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:211:THR:HG23	1:B:238:ASN:O	2.11	0.51
1:B:441:THR:O	1:B:442:ALA:C	2.48	0.51
1:A:440:PHE:HE2	1:A:448:LYS:HB3	1.76	0.51
1:B:255:SER:O	1:B:259:VAL:HG23	2.11	0.51
1:B:363:LEU:HD22	1:B:363:LEU:N	2.26	0.50
1:B:341:ASN:ND2	1:B:344:ASN:H	2.10	0.50
1:A:303:TRP:HA	1:A:309:ILE:HD13	1.93	0.50
1:A:69:LEU:HD23	1:A:69:LEU:C	2.32	0.50
1:A:473:GLN:HA	1:A:477:LYS:O	2.12	0.50
1:B:515:PRO:O	1:B:517:GLU:N	2.45	0.49
1:B:539:TYR:OH	1:B:541:VAL:HG22	2.11	0.49
1:A:192:PRO:HG3	1:A:464:GLY:HA2	1.94	0.49
1:B:30:ARG:HD2	1:B:108:GLN:NE2	2.09	0.49
1:A:108:GLN:O	1:A:111:GLU:HB2	2.11	0.49
1:A:282:ARG:HG2	1:A:282:ARG:NH1	2.25	0.49
1:A:211:THR:HG22	1:A:211:THR:O	2.12	0.49
1:A:402:HIS:HB3	1:A:437:LYS:CE	2.29	0.49
1:B:367:ARG:HB2	1:B:369:HIS:CD2	2.48	0.49
1:A:217:ALA:HB2	1:A:227:ILE:CG1	2.42	0.49
1:A:513:CYS:HB3	1:A:518:MET:HB2	1.95	0.49
1:B:189:ARG:HD3	1:B:461:ASP:OD1	2.12	0.49
1:A:483:VAL:O	1:A:492:LEU:HB2	2.13	0.49
1:B:519:LYS:HG2	1:B:532:ILE:HB	1.93	0.49
1:B:356:GLU:OE1	1:B:366:LYS:HB2	2.13	0.49
1:A:30:ARG:NH2	1:A:32:GLU:OE1	2.46	0.48
1:A:282:ARG:HD2	1:A:309:ILE:O	2.12	0.48
1:B:34:LYS:O	1:B:35:ILE:HD13	2.13	0.48
1:A:441:THR:O	1:A:442:ALA:C	2.51	0.48
1:A:457:ASP:HB2	1:A:461:ASP:H	1.77	0.48
1:B:268:ASN:HB3	1:B:508:GLN:O	2.14	0.48
1:B:303:TRP:HA	1:B:309:ILE:CD1	2.43	0.48
1:B:351:PHE:O	1:B:354:PHE:HB3	2.12	0.48
1:B:169:ILE:CD1	1:B:434:TYR:CZ	2.95	0.48
1:A:114:ARG:NH2	1:B:114:ARG:HG2	2.27	0.48
1:A:163:LEU:HD11	1:B:159:ASN:HB3	1.95	0.48
1:B:341:ASN:HD21	1:B:343:TYR:HB2	1.79	0.48
1:A:30:ARG:NH2	1:A:111:GLU:OE2	2.47	0.48
1:B:150:TYR:HE2	1:B:277:ARG:HB3	1.79	0.48
1:B:150:TYR:HB2	1:B:153:VAL:HG13	1.95	0.48
1:A:408:GLN:HB2	1:A:422:MET:HE1	1.96	0.47
1:A:252:ILE:N	1:A:252:ILE:HD12	2.29	0.47
1:A:504:VAL:HG13	1:A:504:VAL:O	2.13	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:485:HIS:HB2	4:B:2051:HOH:O	2.13	0.47
1:B:282:ARG:HD2	1:B:309:ILE:O	2.13	0.47
1:B:473:GLN:HA	1:B:477:LYS:O	2.15	0.47
1:B:515:PRO:HG2	1:B:516:ASN:N	2.22	0.47
1:A:69:LEU:CD2	1:A:73:LEU:HD22	2.45	0.47
1:A:323:LEU:HD21	1:A:468:VAL:HG22	1.96	0.47
1:B:367:ARG:HB2	1:B:369:HIS:NE2	2.29	0.47
1:A:341:ASN:HD22	1:A:343:TYR:N	2.13	0.47
1:B:374:ASP:OD2	1:B:376:HIS:HB2	2.15	0.47
1:B:523:PRO:HD3	1:B:529:TRP:HA	1.95	0.47
1:A:492:LEU:N	1:A:492:LEU:HD23	2.30	0.47
1:B:49:GLU:HG3	4:B:2048:HOH:O	2.14	0.47
1:A:473:GLN:HE21	1:A:476:GLY:C	2.18	0.47
1:B:241:ILE:HG22	4:B:2068:HOH:O	2.15	0.46
1:A:63:ASP:O	1:A:67:GLN:HB2	2.15	0.46
1:A:114:ARG:HG2	1:B:114:ARG:HH21	1.80	0.46
1:A:169:ILE:CD1	1:A:434:TYR:OH	2.63	0.46
1:A:516:ASN:C	1:A:517:GLU:HG3	2.36	0.46
1:B:169:ILE:CG1	1:B:434:TYR:OH	2.62	0.46
1:B:362:SER:C	1:B:363:LEU:HD22	2.35	0.46
1:B:558:ASP:OD2	1:B:560:SER:OG	2.33	0.46
1:A:444:PHE:CD2	1:A:444:PHE:N	2.83	0.46
1:A:362:SER:C	1:A:363:LEU:HD22	2.35	0.46
1:A:148:GLY:HA3	1:A:154:SER:OG	2.15	0.46
1:A:49:GLU:HG3	4:A:1134:HOH:O	2.15	0.46
1:B:56:GLU:HG2	1:B:101:ARG:NH2	2.31	0.45
3:A:1001:2CG:CA	3:A:1001:2CG:O21	2.63	0.45
1:A:30:ARG:O	1:A:30:ARG:HG3	2.16	0.45
1:A:303:TRP:HA	1:A:309:ILE:CD1	2.47	0.45
1:A:216:VAL:HG13	1:A:274:LEU:CD2	2.42	0.45
1:A:475:GLY:C	1:A:477:LYS:H	2.19	0.45
1:B:78:GLU:HG3	1:B:444:PHE:CZ	2.51	0.45
1:A:200:ALA:O	1:A:204:ILE:HG13	2.16	0.45
1:B:115:ALA:HB1	1:B:140:LEU:O	2.16	0.45
1:A:520:ASN:O	1:A:544:PHE:HB3	2.17	0.45
1:B:523:PRO:C	4:B:2067:HOH:O	2.55	0.45
1:A:52:THR:O	1:A:55:GLU:HG2	2.16	0.45
1:B:214:SER:OG	1:B:243:THR:HG22	2.16	0.45
1:A:203:GLU:HG2	1:A:237:ARG:NH1	2.31	0.45
1:A:251:ASN:HD22	1:A:255:SER:HB3	1.82	0.45
1:A:451:ASP:HA	4:A:1190:HOH:O	2.16	0.45
1:A:473:GLN:NE2	1:A:476:GLY:CA	2.80	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:374:ASP:HB3	1:B:377:LEU:HD22	1.98	0.45
1:B:197:GLN:HB2	1:B:466:TYR:CE2	2.52	0.45
1:B:492:LEU:N	1:B:492:LEU:HD23	2.32	0.44
1:A:473:GLN:HE21	1:A:476:GLY:CA	2.30	0.44
1:A:230:PHE:CZ	1:A:273:VAL:HG21	2.52	0.44
1:B:535:GLU:HA	1:B:535:GLU:OE2	2.17	0.44
1:B:185:ASP:N	1:B:185:ASP:OD2	2.51	0.44
1:B:448:LYS:HA	1:B:452:SER:OG	2.18	0.44
1:B:372:VAL:HG22	1:B:373:CYS:H	1.81	0.44
1:A:298:VAL:HA	1:A:321:ILE:O	2.17	0.44
1:B:310:VAL:HG13	1:B:314:GLU:HA	2.00	0.44
1:B:475:GLY:C	1:B:477:LYS:H	2.21	0.44
1:B:521:MET:O	1:B:529:TRP:HB2	2.17	0.44
1:A:521:MET:O	1:A:529:TRP:HB2	2.17	0.44
1:B:330:VAL:CG1	1:B:444:PHE:HB3	2.42	0.44
1:B:230:PHE:CZ	1:B:273:VAL:HG21	2.53	0.44
1:B:169:ILE:HD11	1:B:434:TYR:CE1	2.53	0.44
1:B:418:LEU:HD22	1:B:422:MET:CE	2.47	0.44
1:A:409:ARG:HH11	1:A:409:ARG:HA	1.82	0.43
1:A:310:VAL:HG11	1:A:471:LEU:HD21	2.00	0.43
1:B:332:GLN:HE21	1:B:332:GLN:HB3	1.54	0.43
1:B:324:GLU:HG2	1:B:388:SER:OG	2.17	0.43
1:A:437:LYS:HE3	1:A:439:GLN:HB3	1.99	0.43
1:B:216:VAL:HG12	1:B:274:LEU:HD23	1.99	0.43
1:B:513:CYS:HB3	1:B:518:MET:HB2	2.00	0.43
1:B:241:ILE:O	1:B:241:ILE:HG23	2.19	0.43
1:A:276:MET:CE	1:A:281:SER:HA	2.38	0.43
1:B:515:PRO:CG	1:B:516:ASN:N	2.81	0.43
1:B:199:LYS:HE2	1:B:233:GLU:OE2	2.18	0.43
1:A:408:GLN:HG2	4:A:1173:HOH:O	2.17	0.43
1:A:408:GLN:HE21	1:A:409:ARG:HA	1.84	0.43
1:B:517:GLU:O	1:B:534:CYS:N	2.46	0.43
1:B:157:VAL:CG1	1:B:161:LEU:HD22	2.47	0.43
1:A:174:THR:C	1:A:189:ARG:NH2	2.72	0.43
1:B:189:ARG:HG3	1:B:191:VAL:O	2.18	0.43
1:A:185:ASP:N	1:A:185:ASP:OD2	2.42	0.43
1:B:514:ALA:H	1:B:518:MET:HE2	1.80	0.43
1:A:341:ASN:C	1:A:341:ASN:HD22	2.21	0.43
1:B:558:ASP:OD2	1:B:560:SER:CB	2.67	0.43
1:B:282:ARG:NH1	1:B:282:ARG:CG	2.77	0.43
1:A:445:ASN:ND2	4:A:1080:HOH:O	2.52	0.43
1:B:108:GLN:O	1:B:111:GLU:HB2	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:282:ARG:CG	1:A:282:ARG:NH1	2.81	0.43
1:B:298:VAL:HA	1:B:321:ILE:O	2.18	0.43
1:B:331:ARG:NH1	1:B:331:ARG:HG3	2.34	0.43
1:A:363:LEU:HD12	4:A:1086:HOH:O	2.18	0.42
1:B:30:ARG:NH1	1:B:111:GLU:OE2	2.45	0.42
1:B:69:LEU:CD2	1:B:73:LEU:HD22	2.49	0.42
1:B:39:LEU:HA	1:B:39:LEU:HD12	1.89	0.42
1:A:428:LYS:NZ	4:A:1017:HOH:O	2.51	0.42
1:A:62:GLU:HB3	1:A:354:PHE:HE1	1.84	0.42
1:B:361:CYS:HB3	1:B:362:SER:H	1.33	0.42
1:A:110:LEU:HD12	1:A:110:LEU:HA	1.94	0.42
1:B:169:ILE:CD1	1:B:434:TYR:OH	2.67	0.42
1:A:227:ILE:HD13	1:A:227:ILE:HA	1.83	0.42
1:A:285:ILE:HD13	1:A:285:ILE:HA	1.92	0.42
1:B:73:LEU:HD12	1:B:73:LEU:HA	1.91	0.42
1:B:313:SER:N	1:B:314:GLU:OE1	2.53	0.42
1:B:520:ASN:O	1:B:544:PHE:HB3	2.19	0.42
1:B:219:GLU:HG3	1:B:247:VAL:O	2.18	0.42
1:B:341:ASN:HB2	1:B:342:PRO:HD2	2.00	0.42
1:A:441:THR:HG22	4:A:1042:HOH:O	2.20	0.42
1:A:69:LEU:HD23	1:A:69:LEU:O	2.20	0.42
1:B:437:LYS:HA	1:B:437:LYS:HD2	1.77	0.42
1:B:314:GLU:HG2	1:B:478:TYR:CE2	2.55	0.42
1:A:341:ASN:HB2	1:A:342:PRO:HD2	2.02	0.42
1:B:64:ARG:O	1:B:68:ARG:HD2	2.20	0.42
1:B:359:PHE:O	1:B:360:GLN:HB2	2.20	0.41
1:A:71:ALA:HA	1:A:333:PHE:CE1	2.54	0.41
1:A:169:ILE:CD1	1:A:434:TYR:CZ	3.04	0.41
1:A:449:GLY:C	1:A:451:ASP:H	2.23	0.41
1:B:56:GLU:HA	1:B:101:ARG:NH2	2.35	0.41
1:A:115:ALA:CB	1:A:140:LEU:O	2.68	0.41
1:B:116:SER:O	1:B:117:LEU:HD12	2.20	0.41
1:B:69:LEU:HD23	1:B:73:LEU:HD22	2.01	0.41
1:A:169:ILE:HG12	1:A:434:TYR:CZ	2.55	0.41
1:A:473:GLN:O	1:A:474:THR:C	2.59	0.41
1:B:181:LYS:CA	1:B:181:LYS:HE2	2.50	0.41
1:B:211:THR:CG2	1:B:211:THR:O	2.68	0.41
1:A:442:ALA:C	1:A:444:PHE:N	2.73	0.41
1:A:314:GLU:N	1:A:314:GLU:OE1	2.38	0.41
3:A:1001:2CG:O	3:A:1001:2CG:O21	2.38	0.41
1:B:86:LEU:N	1:B:87:PRO:CD	2.83	0.41
1:B:341:ASN:ND2	1:B:343:TYR:HD1	2.18	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:558:ASP:O	1:B:559:LEU:HB2	2.19	0.41
1:B:558:ASP:OD2	1:B:560:SER:HB3	2.21	0.41
1:A:544:PHE:N	1:A:544:PHE:CD1	2.89	0.41
1:A:214:SER:OG	1:A:243:THR:HG22	2.21	0.41
1:B:169:ILE:HD11	1:B:434:TYR:CZ	2.56	0.41
1:A:504:VAL:HA	1:A:505:PRO:HD3	1.92	0.41
1:B:442:ALA:C	1:B:444:PHE:N	2.74	0.41
1:B:165:GLN:CG	4:B:2043:HOH:O	2.64	0.41
1:B:205:LEU:CD2	1:B:210:TRP:HE3	2.33	0.41
1:B:317:ALA:O	1:B:471:LEU:HD23	2.21	0.41
1:A:261:ARG:O	1:A:265:GLN:HG3	2.21	0.41
1:B:358:LYS:NZ	1:B:383:ASN:O	2.53	0.40
1:B:75:ALA:O	1:B:79:ILE:HG13	2.20	0.40
1:A:324:GLU:HG3	4:A:1143:HOH:O	2.21	0.40
1:B:138:ILE:N	1:B:139:PRO:HD2	2.36	0.40
1:A:69:LEU:C	1:A:69:LEU:CD2	2.89	0.40
1:B:359:PHE:HB2	1:B:361:CYS:SG	2.62	0.40
1:B:473:GLN:O	1:B:474:THR:C	2.60	0.40
1:B:408:GLN:CB	1:B:422:MET:HE1	2.51	0.40
1:B:341:ASN:HD22	1:B:341:ASN:C	2.25	0.40
1:A:30:ARG:HD2	4:A:1129:HOH:O	2.22	0.40
1:A:490:LEU:HG	1:A:492:LEU:CD2	2.52	0.40
1:A:237:ARG:NH1	4:A:1030:HOH:O	2.54	0.40
1:A:500:SER:O	1:A:501:ARG:CB	2.68	0.40
1:A:178:LEU:HD13	1:A:187:PHE:CZ	2.57	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%)	464 (90%)	37 (7%)	13 (2%)	9	8
1	B	516/555 (93%)	455 (88%)	46 (9%)	15 (3%)	7	6
All	All	1030/1110 (93%)	919 (89%)	83 (8%)	28 (3%)	8	7

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	362	SER
1	A	443	PRO
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	A	444	PHE
1	A	474	THR
1	A	502	ASN
1	A	517	GLU
1	B	517	GLU
1	B	523	PRO
1	A	371	GLN
1	A	488	GLU
1	B	444	PHE
1	B	447	ASN
1	B	474	THR
1	B	488	GLU
1	A	447	ASN
1	A	515	PRO
1	B	371	GLN
1	B	433	GLU
1	B	515	PRO
1	A	566	PRO
1	B	566	PRO
1	B	505	PRO

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%)	419 (94%)	28 (6%)	25	38
1	B	449/481 (93%)	424 (94%)	25 (6%)	30	45
All	All	896/962 (93%)	843 (94%)	53 (6%)	28	42

All (53) 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	153	VAL
1	A	161	LEU
1	A	163	LEU
1	A	216	VAL
1	A	227	ILE
1	A	252	ILE
1	A	275	PHE
1	A	284	LEU
1	A	292	ASN
1	A	332	GLN
1	A	341	ASN
1	A	363	LEU
1	A	373	CYS
1	A	377	LEU
1	A	408	GLN
1	A	418	LEU
1	A	439	GLN
1	A	454	VAL
1	A	457	ASP
1	A	517	GLU
1	A	544	PHE
1	A	567	GLU
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	227	ILE
1	B	275	PHE
1	B	284	LEU
1	B	292	ASN

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Mol	Chain	Res	Type
1	B	341	ASN
1	B	373	CYS
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	544	PHE
1	B	546	CYS
1	B	567	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	251	ASN
1	A	292	ASN
1	A	306	GLN
1	A	332	GLN
1	A	341	ASN
1	A	365	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	332	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	2CG	A	1001	-	14,14,14	0.88	0	21,21,21	2.10	7 (33%)
2	NAG	A	801	1	12,14,15	0.51	0	15,19,21	0.71	0
3	2CG	B	2001	-	14,14,14	0.89	0	21,21,21	2.14	8 (38%)
2	NAG	B	802	1	12,14,15	0.44	0	15,19,21	0.76	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	2CG	A	1001	-	-	0/16/25/25	0/0/1/1
2	NAG	A	801	1	-	0/6/23/26	0/1/1/1
3	2CG	B	2001	-	-	0/16/25/25	0/0/1/1
2	NAG	B	802	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2001	2CG	CG1-CG2-CD2	-4.60	108.55	117.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	2CG	CG1-CG2-CD2	-4.47	108.80	117.27
3	B	2001	2CG	CG2-CG1-CD1	-4.03	109.65	117.27
3	A	1001	2CG	CG2-CG1-CD1	-3.93	109.82	117.27
3	A	1001	2CG	CG1-CB-CA	-3.47	109.59	120.08
3	B	2001	2CG	CG1-CB-CA	-3.44	109.69	120.08
3	A	1001	2CG	CB-CG1-CD1	-3.13	110.13	116.88
3	B	2001	2CG	CB-CG1-CD1	-3.05	110.30	116.88
3	A	1001	2CG	OXT-C-CA	2.68	119.38	112.98
3	A	1001	2CG	CG2-CB-CA	-2.45	112.68	120.08
3	B	2001	2CG	C-CA-N	-2.38	105.54	109.60
3	B	2001	2CG	CG2-CB-CA	-2.30	113.13	120.08
3	B	2001	2CG	OXT-C-CA	2.28	118.41	112.98
3	B	2001	2CG	O21-CD2-CG2	2.23	121.16	114.06
3	A	1001	2CG	O21-CD2-CG2	2.04	120.54	114.06

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, 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	518/555 (93%)	0.61	59 (11%) 6 5	31, 60, 100, 136	0
1	B	520/555 (93%)	0.57	60 (11%) 5 5	29, 62, 102, 136	0
All	All	1038/1110 (93%)	0.59	119 (11%) 6 5	29, 61, 101, 136	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	516	ASN	12.2
1	B	368	ASN	11.1
1	A	368	ASN	10.0
1	A	516	ASN	9.2
1	B	28	PHE	8.4
1	B	567	GLU	8.0
1	B	250	SER	7.9
1	A	250	SER	7.7
1	A	365	ASN	7.7
1	B	366	LYS	7.5
1	B	367	ARG	7.4
1	A	367	ARG	7.2
1	A	369	HIS	7.1
1	B	369	HIS	7.0
1	B	29	MET	7.0
1	A	370	ARG	6.9
1	A	449	GLY	6.4
1	B	443	PRO	5.9
1	B	474	THR	5.8
1	B	566	PRO	5.7
1	A	443	PRO	5.4
1	A	446	PRO	5.2
1	A	116	SER	4.9
1	A	54	THR	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	449	GLY	4.8
1	B	478	TYR	4.8
1	B	52	THR	4.7
1	A	448	LYS	4.7
1	A	450	ALA	4.6
1	A	451	ASP	4.6
1	A	474	THR	4.5
1	A	366	LYS	4.4
1	B	364	GLN	4.4
1	B	249	ARG	4.4
1	A	447	ASN	4.3
1	A	478	TYR	4.3
1	B	450	ALA	4.1
1	B	365	ASN	4.1
1	A	361	CYS	4.0
1	A	524	GLY	3.9
1	B	273	VAL	3.9
1	B	251	ASN	3.9
1	A	272	VAL	3.9
1	B	343	TYR	3.9
1	B	53	GLY	3.7
1	A	53	GLY	3.6
1	B	54	THR	3.6
1	B	440	PHE	3.6
1	A	147	GLY	3.5
1	A	138	ILE	3.4
1	B	272	VAL	3.3
1	B	299	ALA	3.3
1	A	434	TYR	3.2
1	B	475	GLY	3.2
1	A	299	ALA	3.2
1	A	249	ARG	3.1
1	B	315	HIS	3.1
1	A	52	THR	3.1
1	A	274	LEU	3.1
1	A	204	ILE	3.1
1	A	146	ILE	3.0
1	B	331	ARG	2.9
1	B	298	VAL	2.9
1	B	477	LYS	2.9
1	A	440	PHE	2.8
1	A	251	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	487	ALA	2.7
1	B	297	TRP	2.7
1	A	55	GLU	2.7
1	B	446	PRO	2.7
1	A	273	VAL	2.6
1	A	300	SER	2.6
1	B	375	LYS	2.6
1	B	361	CYS	2.6
1	A	529	TRP	2.6
1	B	447	ASN	2.6
1	A	323	LEU	2.6
1	B	371	GLN	2.6
1	B	434	TYR	2.6
1	B	252	ILE	2.5
1	B	139	PRO	2.5
1	A	254	LYS	2.5
1	B	254	LYS	2.5
1	B	335	ARG	2.4
1	B	146	ILE	2.4
1	B	274	LEU	2.4
1	A	297	TRP	2.4
1	A	423	LYS	2.4
1	A	502	ASN	2.4
1	B	321	ILE	2.4
1	A	528	CYS	2.4
1	B	322	THR	2.4
1	A	321	ILE	2.4
1	A	371	GLN	2.3
1	A	253	ARG	2.3
1	B	310	VAL	2.3
1	A	117	LEU	2.3
1	A	169	ILE	2.3
1	A	567	GLU	2.3
1	B	360	GLN	2.2
1	A	441	THR	2.2
1	B	523	PRO	2.2
1	A	205	LEU	2.2
1	A	364	GLN	2.2
1	A	238	ASN	2.2
1	B	473	GLN	2.1
1	A	298	VAL	2.1
1	B	502	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	451	ASP	2.1
1	B	376	HIS	2.1
1	B	476	GLY	2.1
1	B	216	VAL	2.1
1	B	147	GLY	2.1
1	B	169	ILE	2.1
1	A	315	HIS	2.0
1	B	138	ILE	2.0
1	B	30	ARG	2.0
1	A	526	VAL	2.0
1	A	472	GLN	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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NAG	A	801	14/15	0.22	5.77	89,92,95,96	0
2	NAG	B	802	14/15	0.20	1.87	88,91,95,95	0
3	2CG	B	2001	14/14	0.20	0.60	38,42,45,46	0
3	2CG	A	1001	14/14	0.21	0.29	35,40,42,46	0

6.5 Other polymers ⓘ

There are no such residues in this entry.