



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2023 – 07:50 PM EDT

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 X-ray Structure 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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

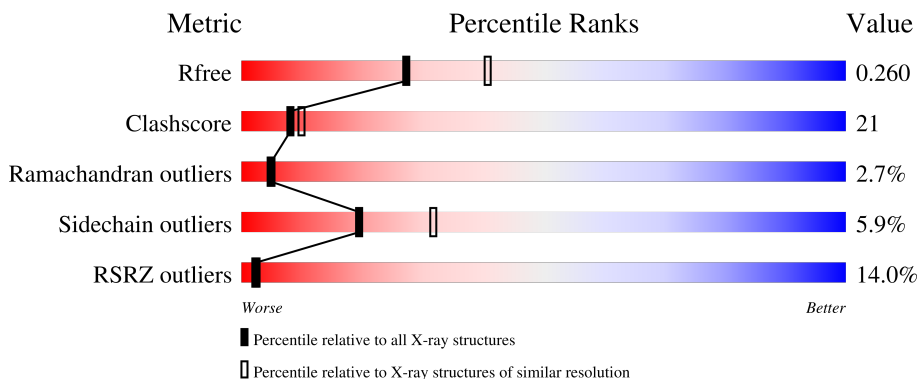
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	
1	B	555	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8656 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
			Total	C	N	O	S			
1	A	518	4118	2606	709	776	27	0	0	0
1	B	520	4137	2620	711	778	28	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

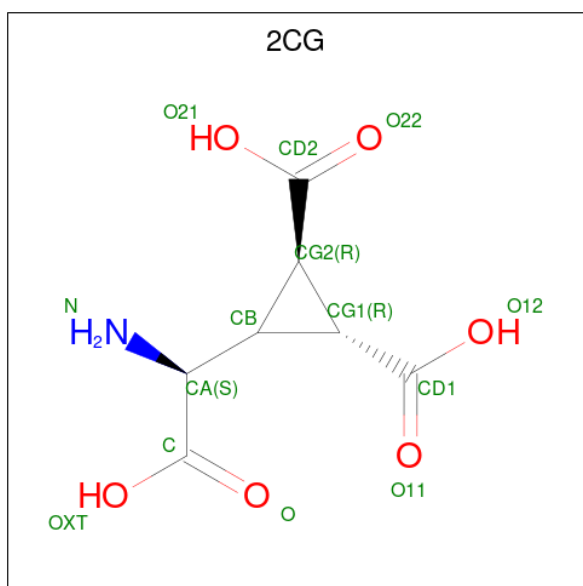
Chain	Residue	Modelled	Actual	Comment	Reference
A	414	GLN	ASN	engineered mutation	UNP P31422
A	439	GLN	ASN	engineered mutation	UNP P31422
A	576	LEU	-	cloning artifact	UNP P31422
A	577	VAL	-	cloning artifact	UNP P31422
A	578	PRO	-	cloning artifact	UNP P31422
A	579	ARG	-	cloning artifact	UNP P31422
B	414	GLN	ASN	engineered mutation	UNP P31422
B	439	GLN	ASN	engineered mutation	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 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 3 is (1R,2R)-3-[(S)-amino(carboxy)methyl]cyclopropane-1,2-dicarboxylic acid (three-letter code: 2CG) (formula: C<sub>7</sub>H<sub>9</sub>NO<sub>6</sub>).



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

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

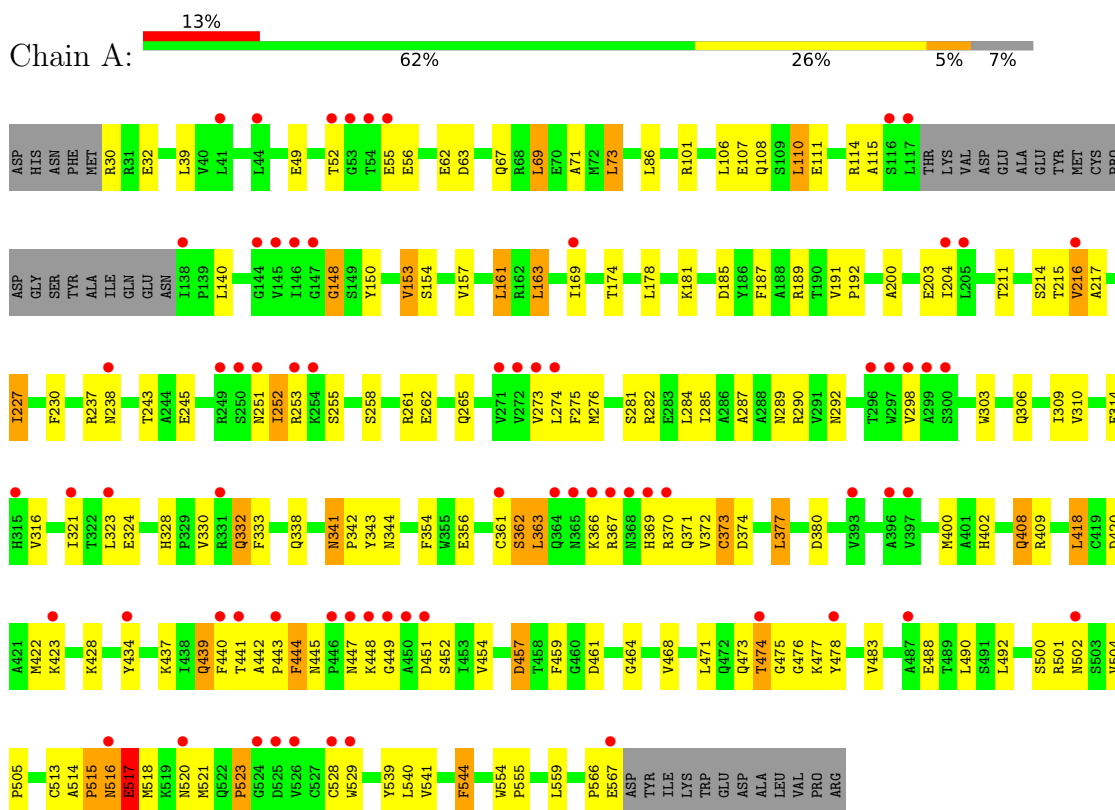
- Molecule 4 is water.

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

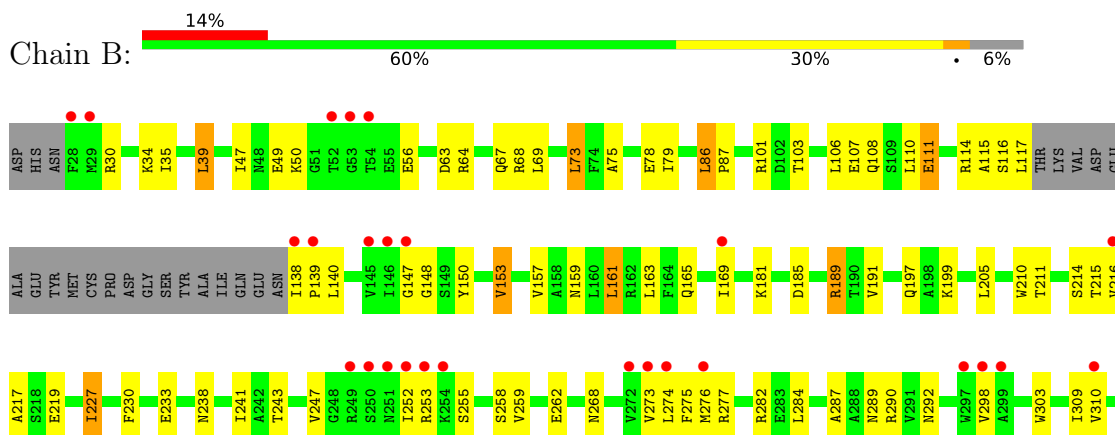
### 3 Residue-property plots [i](#)

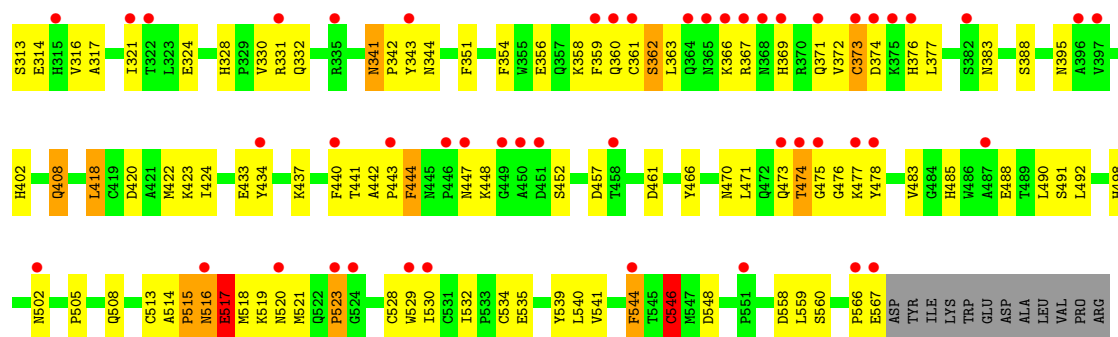
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.24 (at 2.39Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.236 , 0.268 0.227 , 0.260	Depositor DCC
$R_{free}$ test set	4806 reflections (7.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.3	Xtrriage
Anisotropy	0.262	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 54.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.027 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8656	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtrriage'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.*

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

<sup>2</sup>Theoretical 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: 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 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	4118	0	3993	165	0
1	B	4137	0	4012	182	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
3	A	14	0	6	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 21.

All (349) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A: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:514:ALA:HB3	1:B:518:MET:HG3	1.56	0.86
1:B:540:LEU:HD13	1:B:559:LEU:HD23	1.57	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	Interatomic distance (Å)	Clash overlap (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:216:VAL:HG13	1:A:274:LEU:HD22	1.70	0.72
1:A:282:ARG:HG2	1:A:282:ARG:HH11	1.53	0.72
1:A:314:GLU:HG2	1:A:478:TYR:CD2	2.25	0.72
1:A:258:SER:O	1:A:262:GLU:HG3	1.89	0.71
1:B:362:SER:O	1:B:363:LEU:HD13	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:A:442:ALA:O	1:A:444:PHE:N	2.25	0.69
1:B:216:VAL:HG12	1:B:274:LEU:CD2	2.23	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
1:A:367:ARG:HB2	1:A:369:HIS:NE2	2.11	0.66
3:B:2001:2CG:O21	3:B:2001:2CG:HA	1.96	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:169:ILE:HG12	1:B:434:TYR:OH	1.97	0.65
1:B:217:ALA:HB2	1:B:227:ILE:HG13	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:ALA:O	1:B:444:PHE:N	2.30	0.64
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:C	1:B:69:LEU:HD23	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:A:370:ARG:HG2	1:A:370:ARG:HH11	1.66	0.61
1:B:473:GLN:HE21	1:B:476:GLY:HA2	1.65	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:366:LYS:HG2	1:A:367:ARG:H	1.66	0.60
1:A:515:PRO:O	1:A:517:GLU:N	2.34	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:287:ALA:HA	1:B:290:ARG:NH1	2.18	0.59
1:B:330:VAL:HG13	1:B:444:PHE:CB	2.33	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:252:ILE:H	1:A:252:ILE:HD12	1.69	0.57
1:A:363:LEU:N	1:A:363:LEU:HD22	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:PRO:CG	1:B:516:ASN:H	2.16	0.57
1:B:523:PRO:HD2	1:B:528:CYS:O	2.04	0.57
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:215:THR:OG1	1:B:241:ILE:HD11	2.03	0.57
1:B:540:LEU:HD12	1:B:546:CYS:SG	2.44	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:367:ARG:HB2	1:A:369:HIS:CD2	2.41	0.56
1:A:420:ASP:O	1:A:423:LYS:HB2	2.06	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:O21	3:A:1001:2CG:HA	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:A:523:PRO:HD2	1:A:528:CYS:O	2.09	0.53
1:B:408:GLN:HB2	1:B:422:MET:CE	2.39	0.53
1:A:169:ILE:CG1	1:A:434:TYR:OH	2.56	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
3:B:2001:2CG:O21	3:B:2001:2CG:CA	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:A:408:GLN:HB2	1:A:422:MET:CE	2.40	0.51
1:B:211:THR:HG22	1:B:211:THR:O	2.08	0.51
1:B:282:ARG:HG2	1:B:282:ARG:NH1	2.20	0.51
1:A:370:ARG:HG2	1:A:370:ARG:NH1	2.25	0.51
1:B:50:LYS:CE	1:B:101:ARG:HG2	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ARG:HG3	1:A:191:VAL:O	2.10	0.51
1:A:189:ARG:HD3	1:A:461:ASP:OD1	2.10	0.51
1:B:215:THR:HG22	1:B:273:VAL:HB	1.91	0.51
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:N	1:B:363:LEU:HD22	2.26	0.50
1:A:303:TRP:HA	1:A:309:ILE:HD13	1.93	0.50
1:B:341:ASN:ND2	1:B:344:ASN:H	2.10	0.50
1:A:69:LEU:C	1:A:69:LEU:HD23	2.32	0.50
1:A:473:GLN:HA	1:A:477:LYS:O	2.12	0.50
1:A:192:PRO:HG3	1:A:464:GLY:HA2	1.94	0.49
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:108:GLN:O	1:A:111:GLU:HB2	2.11	0.49
1:A:211:THR:HG22	1:A:211:THR:O	2.12	0.49
1:A:282:ARG:HG2	1:A:282:ARG:NH1	2.25	0.49
1:B:30:ARG:HD2	1:B:108:GLN:NE2	2.09	0.49
1:A:402:HIS:HB3	1:A:437:LYS:CE	2.29	0.49
1:A:217:ALA:HB2	1:A:227:ILE:CG1	2.42	0.49
1:B:367:ARG:HB2	1:B:369:HIS:CD2	2.48	0.49
1:A:483:VAL:O	1:A:492:LEU:HB2	2.13	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: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:A:114:ARG:NH2	1:B:114:ARG:HG2	2.27	0.48
1:B:169:ILE:CD1	1:B:434:TYR:CZ	2.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:TYR:HB2	1:B:153:VAL:HG13	1.95	0.48
1:A:252:ILE:HD12	1:A:252:ILE:N	2.29	0.47
1:A:408:GLN:HB2	1:A:422:MET:HE1	1.96	0.47
1:A:504:VAL:O	1:A:504:VAL:HG13	2.13	0.47
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: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:515:PRO:HG2	1:B:516:ASN:N	2.22	0.47
1:A:341:ASN:HD22	1:A:343:TYR:N	2.13	0.47
1:B:367:ARG:HB2	1:B:369:HIS:NE2	2.29	0.47
1:A:492:LEU:HD23	1:A:492:LEU:N	2.30	0.47
1:B:49:GLU:HG3	4:B:2048:HOH:O	2.14	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:473:GLN:HE21	1:A:476:GLY:C	2.18	0.47
1:A:63:ASP:O	1:A:67:GLN:HB2	2.15	0.46
1:B:241:ILE:HG22	4:B:2068:HOH:O	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:N	1:A:444:PHE:CD2	2.83	0.46
1:A:49:GLU:HG3	4:A:1134:HOH:O	2.15	0.46
1:A:148:GLY:HA3	1:A:154:SER:OG	2.15	0.46
1:A:362:SER:C	1:A:363:LEU:HD22	2.35	0.46
3:A:1001:2CG:O21	3:A:1001:2CG:CA	2.63	0.45
1:B:56:GLU:HG2	1:B:101:ARG:NH2	2.31	0.45
1:A:30:ARG:HG3	1:A:30:ARG:O	2.16	0.45
1:A:216:VAL:HG13	1:A:274:LEU:CD2	2.42	0.45
1:A:303:TRP:HA	1:A:309:ILE:CD1	2.47	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:A:520:ASN:O	1:A:544:PHE:HB3	2.17	0.45
1:B:115:ALA:HB1	1:B:140:LEU:O	2.16	0.45
1:A:52:THR:O	1:A:55:GLU:HG2	2.16	0.45
1:B:523:PRO:C	4:B:2067:HOH:O	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:214:SER:OG	1:B:243:THR:HG22	2.16	0.45
1:A:473:GLN:NE2	1:A:476:GLY:CA	2.80	0.45
1:B:197:GLN:HB2	1:B:466:TYR:CE2	2.52	0.45
1:B:374:ASP:HB3	1:B:377:LEU:HD22	1.98	0.45
1:A:230:PHE:CZ	1:A:273:VAL:HG21	2.52	0.44
1:A:473:GLN:HE21	1:A:476:GLY:CA	2.30	0.44
1:B:492:LEU:N	1:B:492:LEU:HD23	2.32	0.44
1:B:185:ASP:OD2	1:B:185:ASP:N	2.51	0.44
1:B:535:GLU:OE2	1:B:535:GLU:HA	2.17	0.44
1:B:448:LYS:HA	1:B:452:SER:OG	2.18	0.44
1:A:298:VAL:HA	1:A:321:ILE:O	2.17	0.44
1:B:372:VAL:HG22	1:B:373:CYS:H	1.81	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:230:PHE:CZ	1:B:273:VAL:HG21	2.53	0.44
1:B:330:VAL:CG1	1:B:444:PHE:HB3	2.42	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:310:VAL:HG11	1:A:471:LEU:HD21	2.00	0.43
1:A:409:ARG:HA	1:A:409:ARG:HH11	1.82	0.43
1:B:324:GLU:HG2	1:B:388:SER:OG	2.17	0.43
1:B:332:GLN:HE21	1:B:332:GLN:HB3	1.54	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:241:ILE:HG23	1:B:241:ILE:O	2.19	0.43
1:B:513:CYS:HB3	1:B:518:MET:HB2	2.00	0.43
1:A:276:MET:CE	1:A:281:SER:HA	2.38	0.43
1:B:199:LYS:HE2	1:B:233:GLU:OE2	2.18	0.43
1:B:515:PRO:CG	1:B:516:ASN:N	2.81	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:A:174:THR:C	1:A:189:ARG:NH2	2.72	0.43
1:A:185:ASP:OD2	1:A:185:ASP:N	2.42	0.43
1:B:157:VAL:CG1	1:B:161:LEU:HD22	2.47	0.43
1:B:189:ARG:HG3	1:B:191:VAL:O	2.18	0.43
1:B:517:GLU:O	1:B:534:CYS:N	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:ASN:HD22	1:A:341:ASN:C	2.21	0.43
1:B:514:ALA:H	1:B:518:MET:HE2	1.80	0.43
1:A:445:ASN:ND2	4:A:1080:HOH:O	2.52	0.43
1:B:282:ARG:NH1	1:B:282:ARG:CG	2.77	0.43
1:B:558:ASP:OD2	1:B:560:SER:CB	2.67	0.43
1:A:282:ARG:NH1	1:A:282:ARG:CG	2.81	0.43
1:B:108:GLN:O	1:B:111:GLU:HB2	2.18	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:62:GLU:HB3	1:A:354:PHE:HE1	1.84	0.42
1:A:363:LEU:HD12	4:A:1086:HOH:O	2.18	0.42
1:A:428:LYS:NZ	4:A:1017:HOH:O	2.51	0.42
1:B:30:ARG:NH1	1:B:111:GLU:OE2	2.45	0.42
1:B:39:LEU:HD12	1:B:39:LEU:HA	1.89	0.42
1:B:69:LEU:CD2	1:B:73:LEU:HD22	2.49	0.42
1:A:110:LEU:HD12	1:A:110:LEU:HA	1.94	0.42
1:B:361:CYS:HB3	1:B:362:SER:H	1.33	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:219:GLU:HG3	1:B:247:VAL:O	2.18	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:341:ASN:HB2	1:B:342:PRO:HD2	2.00	0.42
1:A:69:LEU:HD23	1:A:69:LEU:O	2.20	0.42
1:A:441:THR:HG22	4:A:1042:HOH:O	2.20	0.42
1:B:437:LYS:HD2	1:B:437:LYS:HA	1.77	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:314:GLU:HG2	1:B:478:TYR:CE2	2.55	0.42
1:A:71:ALA:HA	1:A:333:PHE:CE1	2.54	0.41
1:B:359:PHE:O	1:B:360:GLN:HB2	2.20	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:A:115:ALA:CB	1:A:140:LEU:O	2.68	0.41
1:B:56:GLU:HA	1:B:101:ARG:NH2	2.35	0.41
1:B:116:SER:O	1:B:117:LEU:HD12	2.20	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:69:LEU:HD23	1:B:73:LEU:HD22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:LYS:HE2	1:B:181:LYS:CA	2.50	0.41
1:B:211:THR:O	1:B:211:THR:CG2	2.68	0.41
1:A:314:GLU:OE1	1:A:314:GLU:N	2.38	0.41
1:A:442:ALA:C	1:A:444:PHE:N	2.73	0.41
3:A:1001:2CG:O21	3:A:1001:2CG:O	2.38	0.41
1:B:86:LEU:N	1:B:87:PRO:CD	2.83	0.41
1:A:214:SER:OG	1:A:243:THR:HG22	2.21	0.41
1:A:544:PHE:CD1	1:A:544:PHE:N	2.89	0.41
1:B:341:ASN:ND2	1:B:343:TYR:HD1	2.18	0.41
1:B:558:ASP:OD2	1:B:560:SER:HB3	2.21	0.41
1:B:558:ASP:O	1:B:559:LEU:HB2	2.19	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:A:261:ARG:O	1:A:265:GLN:HG3	2.21	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:B:442:ALA:C	1:B:444:PHE:N	2.74	0.41
1:A:324:GLU:HG3	4:A:1143:HOH:O	2.21	0.40
1:B:75:ALA:O	1:B:79:ILE:HG13	2.20	0.40
1:B:138:ILE:N	1:B:139:PRO:HD2	2.36	0.40
1:B:358:LYS:NZ	1:B:383:ASN:O	2.53	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:408:GLN:CB	1:B:422:MET:HE1	2.51	0.40
1:B:473:GLN:O	1:B:474:THR:C	2.60	0.40
1:A:30:ARG:HD2	4:A:1129:HOH:O	2.22	0.40
1:B:341:ASN:HD22	1:B:341:ASN:C	2.25	0.40
1:A:178:LEU:HD13	1:A:187:PHE:CZ	2.57	0.40
1:A:237:ARG:NH1	4:A:1030:HOH:O	2.54	0.40
1:A:490:LEU:HG	1:A:492:LEU:CD2	2.52	0.40
1:A:500:SER:O	1:A:501:ARG:CB	2.68	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	514/555 (93%)	464 (90%)	37 (7%)	13 (2%)	5	6
1	B	516/555 (93%)	455 (88%)	46 (9%)	15 (3%)	4	4
All	All	1030/1110 (93%)	919 (89%)	83 (8%)	28 (3%)	5	5

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 [i](#)

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%)	18	28
1	B	449/481 (93%)	424 (94%)	25 (6%)	21	34
All	All	896/962 (93%)	843 (94%)	53 (6%)	19	32

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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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
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

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

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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

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Mol	Chain	Res	Type
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 [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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	$\# Z  > 2$
2	NAG	B	802	1	14,14,15	0.59	0	17,19,21	0.63	0
2	NAG	A	801	1	14,14,15	0.65	0	17,19,21	0.63	0
3	2CG	A	1001	-	12,14,14	1.07	0	16,21,21	2.04	4 (25%)
3	2CG	B	2001	-	12,14,14	1.08	0	16,21,21	2.06	4 (25%)

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
2	NAG	B	802	1	-	4/6/23/26	0/1/1/1
2	NAG	A	801	1	-	3/6/23/26	0/1/1/1
3	2CG	A	1001	-	-	8/16/25/25	0/1/1/1
3	2CG	B	2001	-	-	7/16/25/25	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2001	2CG	CG1-CG2-CD2	-4.48	108.55	118.04
3	A	1001	2CG	CG1-CG2-CD2	-4.37	108.80	118.04
3	B	2001	2CG	CG2-CG1-CD1	-3.96	109.65	118.04
3	A	1001	2CG	CG2-CG1-CD1	-3.88	109.82	118.04
3	A	1001	2CG	CB-CG1-CD1	-2.78	110.13	117.09
3	B	2001	2CG	CB-CG1-CD1	-2.72	110.30	117.09
3	B	2001	2CG	O21-CD2-CG2	2.41	121.16	114.01
3	A	1001	2CG	O21-CD2-CG2	2.20	120.54	114.01

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	NAG	C8-C7-N2-C2
2	A	801	NAG	O7-C7-N2-C2
2	B	802	NAG	C8-C7-N2-C2
2	B	802	NAG	O7-C7-N2-C2
3	A	1001	2CG	O11-CD1-CG1-CB
3	A	1001	2CG	O12-CD1-CG1-CB
3	A	1001	2CG	O11-CD1-CG1-CG2
3	A	1001	2CG	O12-CD1-CG1-CG2
3	A	1001	2CG	O21-CD2-CG2-CB
3	A	1001	2CG	O22-CD2-CG2-CB
3	B	2001	2CG	O11-CD1-CG1-CB
3	B	2001	2CG	O12-CD1-CG1-CB
3	B	2001	2CG	O11-CD1-CG1-CG2
3	B	2001	2CG	O12-CD1-CG1-CG2
3	A	1001	2CG	O21-CD2-CG2-CG1

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Mol	Chain	Res	Type	Atoms
3	B	2001	2CG	O21-CD2-CG2-CG1
3	B	2001	2CG	O22-CD2-CG2-CG1
2	B	802	NAG	C4-C5-C6-O6
2	B	802	NAG	O5-C5-C6-O6
3	A	1001	2CG	O22-CD2-CG2-CG1
2	A	801	NAG	C4-C5-C6-O6
3	B	2001	2CG	OXT-C-CA-N

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	2CG	3	0
3	B	2001	2CG	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.73	70 (13%) <b>3</b> <b>2</b>	31, 60, 100, 136	0
1	B	520/555 (93%)	0.67	75 (14%) <b>2</b> <b>2</b>	29, 62, 102, 136	0
All	All	1038/1110 (93%)	0.70	145 (13%) <b>2</b> <b>2</b>	29, 61, 101, 136	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	516	ASN	13.0
1	A	368	ASN	11.2
1	B	368	ASN	11.1
1	A	516	ASN	9.9
1	A	250	SER	9.2
1	B	250	SER	8.5
1	B	369	HIS	8.4
1	A	365	ASN	8.1
1	B	367	ARG	7.9
1	B	28	PHE	7.8
1	A	367	ARG	7.6
1	B	366	LYS	7.5
1	B	29	MET	7.5
1	B	567	GLU	7.3
1	A	369	HIS	7.1
1	A	370	ARG	7.1
1	A	449	GLY	6.7
1	B	474	THR	6.6
1	A	446	PRO	6.3
1	A	116	SER	6.1
1	A	443	PRO	6.0
1	B	443	PRO	5.8
1	B	566	PRO	5.6
1	A	451	ASP	5.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	366	LYS	5.5
1	A	448	LYS	5.3
1	A	450	ALA	5.2
1	A	447	ASN	5.1
1	B	449	GLY	5.0
1	A	524	GLY	5.0
1	A	272	VAL	4.9
1	A	54	THR	4.8
1	B	52	THR	4.8
1	A	474	THR	4.7
1	A	478	TYR	4.6
1	B	273	VAL	4.5
1	B	343	TYR	4.5
1	B	272	VAL	4.5
1	B	249	ARG	4.5
1	B	54	THR	4.4
1	B	365	ASN	4.4
1	B	478	TYR	4.4
1	B	450	ALA	4.3
1	B	364	GLN	4.2
1	A	361	CYS	4.2
1	A	274	LEU	4.1
1	B	251	ASN	4.1
1	A	147	GLY	4.0
1	B	475	GLY	3.9
1	A	299	ALA	3.8
1	B	299	ALA	3.8
1	B	53	GLY	3.6
1	A	146	ILE	3.5
1	A	273	VAL	3.5
1	B	440	PHE	3.5
1	A	55	GLU	3.5
1	A	249	ARG	3.5
1	A	254	LYS	3.5
1	A	53	GLY	3.4
1	B	315	HIS	3.4
1	B	298	VAL	3.3
1	B	477	LYS	3.3
1	A	434	TYR	3.3
1	A	251	ASN	3.3
1	B	297	TRP	3.2
1	B	274	LEU	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	331	ARG	3.2
1	A	298	VAL	3.1
1	A	529	TRP	3.1
1	B	146	ILE	3.0
1	B	254	LYS	3.0
1	A	52	THR	3.0
1	B	361	CYS	3.0
1	A	253	ARG	3.0
1	A	300	SER	3.0
1	A	423	LYS	3.0
1	A	297	TRP	3.0
1	A	487	ALA	2.9
1	B	371	GLN	2.9
1	B	310	VAL	2.8
1	A	204	ILE	2.8
1	B	360	GLN	2.8
1	A	205	LEU	2.8
1	B	523	PRO	2.7
1	A	138	ILE	2.7
1	A	117	LEU	2.7
1	A	525	ASP	2.7
1	B	139	PRO	2.7
1	B	322	THR	2.7
1	A	145	VAL	2.7
1	B	376	HIS	2.7
1	B	434	TYR	2.7
1	A	526	VAL	2.7
1	B	502	ASN	2.7
1	B	530	ILE	2.6
1	B	335	ARG	2.6
1	B	147	GLY	2.6
1	A	364	GLN	2.6
1	B	447	ASN	2.6
1	B	446	PRO	2.6
1	A	528	CYS	2.5
1	B	473	GLN	2.5
1	A	321	ILE	2.5
1	A	216	VAL	2.5
1	A	323	LEU	2.5
1	A	169	ILE	2.4
1	B	375	LYS	2.4
1	B	524	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	252	ILE	2.4
1	B	145	VAL	2.4
1	A	238	ASN	2.4
1	A	440	PHE	2.4
1	B	529	TRP	2.4
1	A	331	ARG	2.4
1	A	271	VAL	2.4
1	B	359	PHE	2.3
1	B	551	PRO	2.3
1	B	169	ILE	2.3
1	B	373	CYS	2.3
1	B	374	ASP	2.3
1	A	502	ASN	2.3
1	B	397	VAL	2.2
1	B	321	ILE	2.2
1	A	396	ALA	2.2
1	B	216	VAL	2.2
1	B	138	ILE	2.2
1	A	441	THR	2.2
1	B	487	ALA	2.2
1	A	393	VAL	2.1
1	B	451	ASP	2.1
1	A	397	VAL	2.1
1	A	44	LEU	2.1
1	A	315	HIS	2.1
1	A	144	GLY	2.1
1	A	296	THR	2.1
1	A	567	GLU	2.1
1	B	253	ARG	2.1
1	A	520	ASN	2.1
1	B	458	THR	2.1
1	A	41	LEU	2.1
1	B	276	MET	2.1
1	B	382	SER	2.0
1	B	396	ALA	2.0
1	B	520	ASN	2.0
1	B	544	PHE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 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	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	B	802	14/15	0.84	0.20	88,91,95,95	0
2	NAG	A	801	14/15	0.85	0.24	89,92,95,96	0
3	2CG	B	2001	14/14	0.94	0.22	38,42,45,46	0
3	2CG	A	1001	14/14	0.96	0.22	35,40,42,46	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.