



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2021 – 08:06 PM EDT

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 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.

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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 : 2.23.2  
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) : 2.23.2

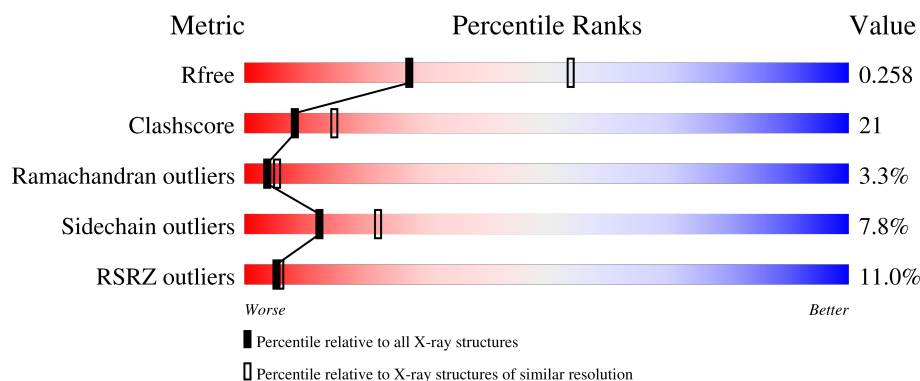
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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))
$R_{free}$	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	<div> <div>9%</div> <div>57%</div> <div>30%</div> <div>5%</div> <div>7%</div> </div>
1	B	555	<div> <div>12%</div> <div>57%</div> <div>32%</div> <div>5%</div> <div>6%</div> </div>

## 2 Entry composition

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

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Metabotropic glutamate receptor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	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:

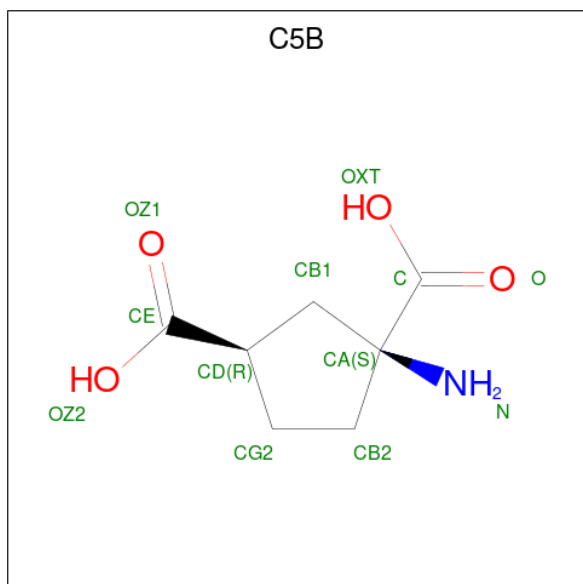
Chain	Residue	Modelled	Actual	Comment	Reference
A	414	GLN	ASN	engineered mutation	UNP P31422
A	439	GLN	ASN	engineered mutation	UNP P31422
A	576	LEU	-	cloning artifact	UNP P31422
A	577	VAL	-	cloning artifact	UNP P31422
A	578	PRO	-	cloning artifact	UNP P31422
A	579	ARG	-	cloning artifact	UNP P31422
B	414	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
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-DICARBOXYLIC ACID (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		

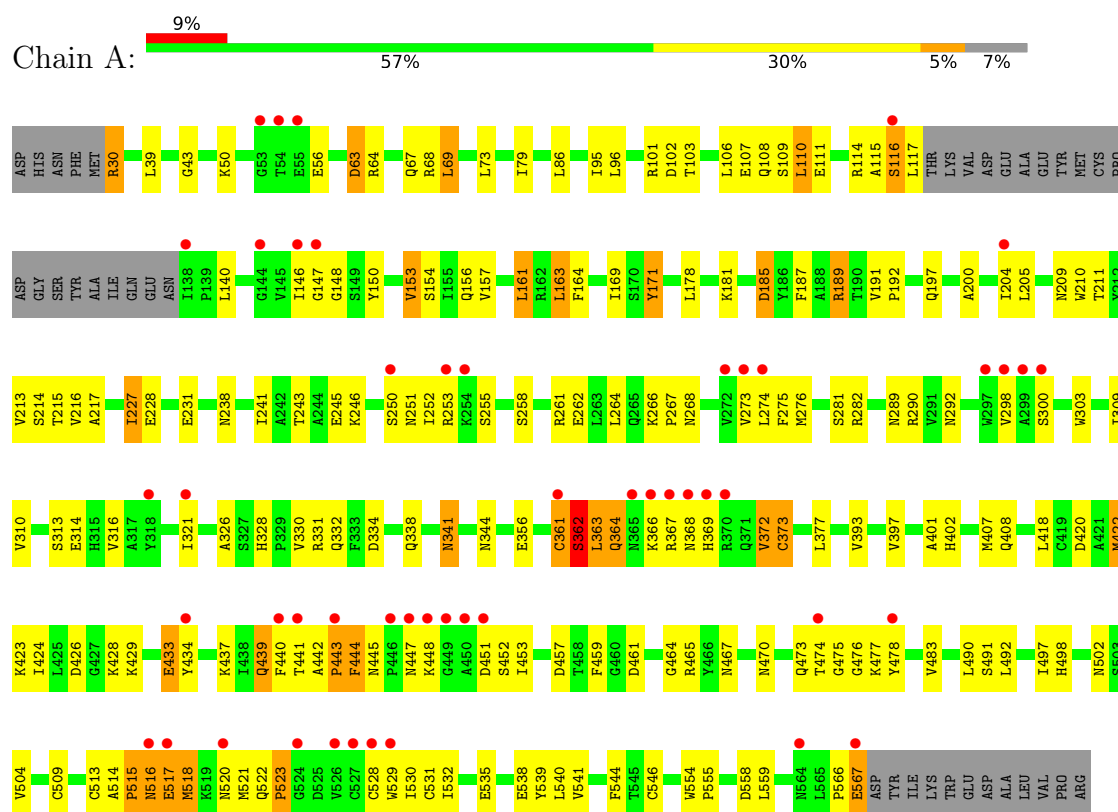
- Molecule 4 is water.

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

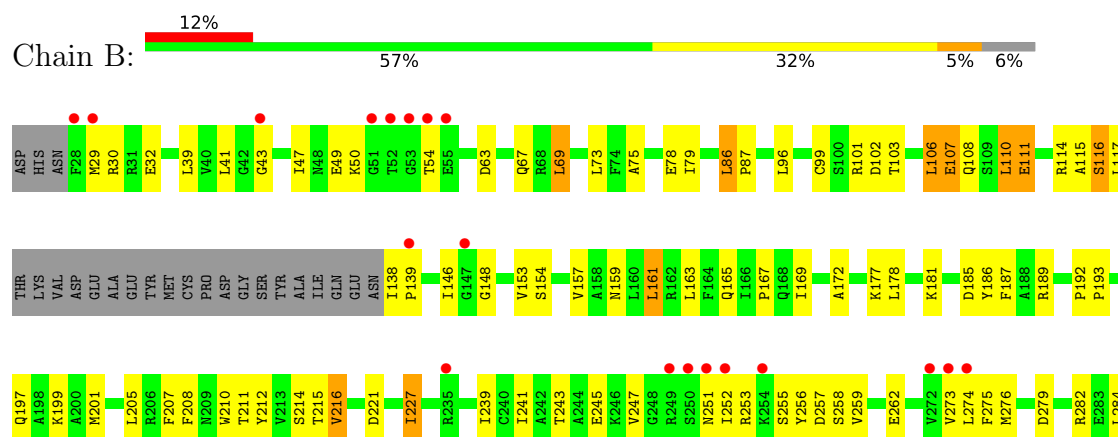
### 3 Residue-property plots

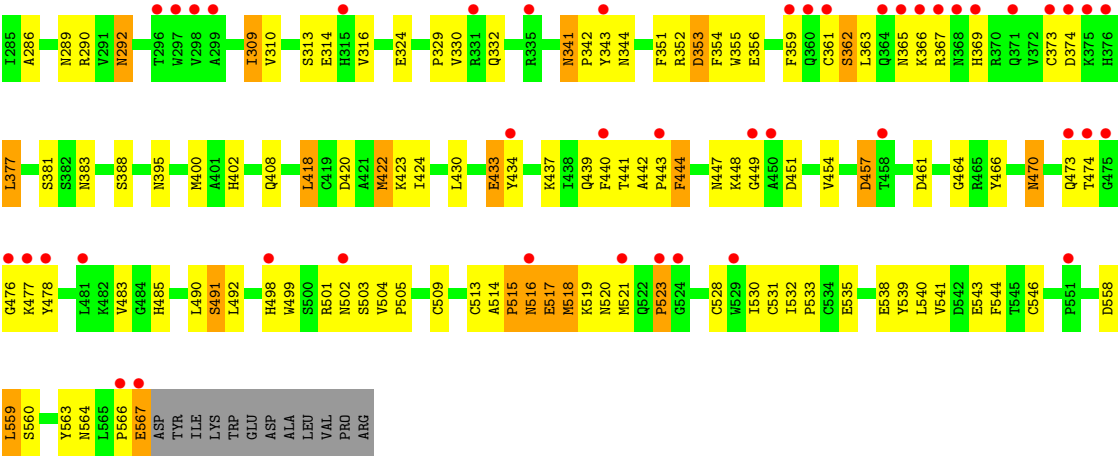
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

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 0.223 , 0.258	Depositor DCC
$R_{free}$ test set	3201 reflections (7.11%)	wwPDB-VP
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> )	0.32 , 70.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	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.

<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: C5B, 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	0.42	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 Too-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 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	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

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 (344) 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: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	Interatomic distance (Å)	Clash overlap (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:251:ASN:HD22	1:B:255:SER:HB3	1.56	0.70
1:B:362:SER:O	1:B:363:LEU:HD13	1.91	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:A:217:ALA:HB2	1:A:227:ILE:HG13	1.76	0.68
1:B:514:ALA:H	1:B:518:MET:CE	2.04	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:A:181:LYS:HE2	1:A:459:PHE:O	1.95	0.67
1:B:165:GLN:HG3	4:B:2031:HOH:O	1.94	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:181:LYS:HE3	1:A:187:PHE:O	1.97	0.65
1:A:514:ALA:HB2	1:A:518:MET:HE2	1.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:GLN:HA	1:A:477:LYS:O	1.98	0.64
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:O	1:A:69:LEU:HD22	1.99	0.62
1:A:114:ARG:HG2	1:B:114:ARG:NH2	2.15	0.62
1:A:515:PRO:CG	1:A:516:ASN:H	2.08	0.62
1:A:473:GLN:HE21	1:A:476:GLY:CA	2.13	0.62
1:B:341:ASN:ND2	1:B:343:TYR:H	1.97	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:A:253:ARG:HG2	1:A:290:ARG:NH2	2.15	0.61
1:B:282:ARG:HG2	1:B:282:ARG:HH11	1.66	0.61
1:B:535:GLU:OE2	1:B:535:GLU:HA	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:A:483:VAL:O	1:A:492:LEU:HB2	2.03	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:274:LEU:HD22	1:B:276:MET:SD	2.43	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:535:GLU:HB2	1:B:538:GLU:HG3	1.84	0.58
1:A:148:GLY:HA3	1:A:154:SER:OG	2.03	0.58
1:A:163:LEU:HB3	1:B:106:LEU:HD11	1.85	0.57
1:B:165:GLN:CG	4:B:2031:HOH:O	2.51	0.57
1:A:56:GLU:HG2	1:A:101:ARG:HH22	1.67	0.57
1:A:289:ASN:HA	1:A:316:VAL:HG21	1.86	0.57
1:A:341:ASN:HD21	1:A:344:ASN:H	1.51	0.57
1:B:178:LEU:HD13	1:B:187:PHE:CZ	2.40	0.57
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:B:367:ARG:HB2	1:B:369:HIS:NE2	2.20	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:A:282:ARG:HD2	1:A:309:ILE:O	2.06	0.55
1:B:165:GLN:HG2	1:B:186:TYR:OH	2.06	0.55
1:A:211:THR:HG23	1:A:238:ASN:O	2.07	0.55
1:B:30:ARG:NH2	1:B:32:GLU:OE1	2.39	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:258:SER:O	1:A:262:GLU:HG3	2.07	0.54
1:A:473:GLN:NE2	1:A:476:GLY:HA2	2.22	0.54
1:B:103:THR:O	1:B:107:GLU:HG2	2.07	0.54
1:A:251:ASN:HD22	1:A:255:SER:HB3	1.73	0.53
1:B:473:GLN:HA	1:B:477:LYS:O	2.08	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:O	1:A:424:ILE:HG13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:SER:OG	1:B:366:LYS:HD3	2.08	0.53
1:A:171:TYR:CG	1:A:393:VAL:HG22	2.44	0.52
1:B:43:GLY:HA2	1:B:146:ILE:O	2.09	0.52
1:B:395:ASN:OD1	1:B:441:THR:HG23	2.10	0.52
1:A:363:LEU:N	1:A:363:LEU:HD22	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:HG3	1:A:30:ARG:O	2.09	0.52
1:B:116:SER:O	1:B:117:LEU:HD12	2.09	0.52
1:A:504:VAL:O	1:A:504:VAL:HG13	2.09	0.52
1:A:515:PRO:HG2	1:A:516:ASN:N	2.15	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:A:253:ARG:HG2	1:A:290:ARG:HH22	1.74	0.51
1:B:330:VAL:HG13	1:B:444:PHE:CB	2.37	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:A:492:LEU:HD23	1:A:492:LEU:N	2.26	0.50
1:B:314:GLU:HG2	1:B:478:TYR:CE2	2.47	0.50
1:A:200:ALA:O	1:A:204:ILE:HG13	2.12	0.50
1:B:541:VAL:HG12	1:B:541:VAL:O	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:A:535:GLU:HB2	1:A:538:GLU:HG3	1.94	0.49
1:B:473:GLN:O	1:B:473:GLN:NE2	2.45	0.49
1:A:114:ARG:CZ	1:B:114:ARG:HG2	2.43	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:ASN:HB2	1:B:342:PRO:HD2	1.93	0.49
1:B:356:GLU:OE1	1:B:366:LYS:HB2	2.11	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
1:A:554:TRP:CG	1:A:555:PRO:HD2	2.47	0.49
1:A:310:VAL:HG12	1:A:314:GLU:HA	1.93	0.48
1:B:169:ILE:CG1	1:B:434:TYR:OH	2.61	0.48
1:B:286:ALA:O	1:B:290:ARG:HG3	2.13	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:324:GLU:HG2	1:B:388:SER:OG	2.14	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: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:A:473:GLN:NE2	1:A:476:GLY:CA	2.77	0.47
1:A:522:GLN:HE21	1:A:522:GLN:HA	1.80	0.47
1:B:444:PHE:N	1:B:444:PHE:CD2	2.80	0.47
1:B:563:TYR:HD1	1:B:564:ASN:O	1.97	0.47
1:A:79:ILE:HD13	1:A:401:ALA:HB2	1.96	0.47
1:B:99:CYS:O	1:B:101:ARG:HG3	2.15	0.47
1:B:523:PRO:HD2	1:B:528:CYS:O	2.15	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:B:341:ASN:C	1:B:341:ASN:ND2	2.65	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:115:ALA:HB1	1:A:140:LEU:O	2.15	0.46
1:A:197:GLN:OE1	1:A:300:SER:HB2	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:A:215:THR:HG22	1:A:273:VAL:HB	1.98	0.46
1:A:457:ASP:HB3	1:A:459:PHE:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:GLN:O	1:B:111:GLU:HB2	2.16	0.46
1:B:558:ASP:OD2	1:B:560:SER:HB3	2.16	0.46
1:B:227:ILE:HD13	1:B:227:ILE:HA	1.83	0.46
1:A:96:LEU:HD13	1:A:108:GLN:HB3	1.97	0.46
1:B:75:ALA:O	1:B:79:ILE:HG13	2.16	0.46
1:B:241:ILE:HG23	1:B:241:ILE:O	2.16	0.46
1:B:566:PRO:HB2	1:B:567:GLU:OE1	2.16	0.46
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:B:515:PRO:O	1:B:517:GLU:N	2.49	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: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:B:366:LYS:CG	1:B:367:ARG:H	2.25	0.45
1:A:428:LYS:NZ	4:A:1011:HOH:O	2.50	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:B:473:GLN:NE2	1:B:476:GLY:HA2	2.32	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:A:372:VAL:CG2	1:A:373:CYS:H	2.30	0.44
1:B:96:LEU:HD13	1:B:108:GLN:HB3	1.98	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:HG22	1:B:211:THR:O	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:A:209:ASN:ND2	2:A:801:NAG:H82	2.32	0.44
1:B:352:ARG:HG2	1:B:352:ARG:HH11	1.83	0.44
1:A:164:PHE:N	1:A:164:PHE:CD1	2.85	0.44
1:A:216:VAL:CG1	1:A:274:LEU:HD22	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:PHE:HD2	1:B:208:PHE:CD1	2.36	0.43
1:A:213:VAL:O	1:A:241:ILE:HA	2.18	0.43
1:B:514:ALA:CB	1:B:518:MET:HG3	2.35	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:208:PHE:CE2	1:B:499:TRP:HZ2	2.37	0.43
1:B:473:GLN:HE21	1:B:476:GLY:HA2	1.80	0.43
1:A:147:GLY:HA2	1:A:171:TYR:CE2	2.53	0.43
1:B:107:GLU:O	1:B:110:LEU:HB2	2.18	0.43
1:B:157:VAL:CG1	1:B:161:LEU:HD22	2.47	0.43
1:A:69:LEU:HD22	1:A:69:LEU:C	2.37	0.43
1:A:268:ASN:ND2	1:A:509:CYS:O	2.51	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:B:102:ASP:OD2	1:B:103:THR:N	2.50	0.43
1:B:205:LEU:HD22	1:B:210:TRP:CE3	2.49	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:A:102:ASP:HB2	1:A:156:GLN:HG3	2.01	0.43
1:A:146:ILE:HG13	1:A:397:VAL:HG22	2.01	0.43
1:B:352:ARG:HG2	1:B:352:ARG:NH1	2.34	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:41:LEU:CD2	1:B:400:MET:HG2	2.49	0.42
1:B:437:LYS:HD2	1:B:437:LYS:HA	1.68	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:A:69:LEU:HD23	1:A:95:ILE:HG21	2.01	0.42
1:B:440:PHE:CD2	1:B:448:LYS:HD3	2.54	0.42
1:A:266:LYS:N	1:A:267:PRO:CD	2.82	0.42
1:A:341:ASN:ND2	1:A:341:ASN:C	2.70	0.42
1:A:451:ASP:OD1	1:A:453:ILE:HG12	2.20	0.42
1:B:211:THR:HG23	1:B:239:ILE:HA	2.02	0.42
1:B:212:TYR:HB2	1:B:509:CYS:N	2.35	0.42
1:B:377:LEU:HD13	1:B:377:LEU:HA	1.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:523:PRO:HD3	1:A:529:TRP:HA	2.02	0.41
1:B:310:VAL:HG12	1:B:310:VAL:O	2.20	0.41
1:A:530:ILE:HD12	1:A:532:ILE:HD11	2.02	0.41
1:B:216:VAL:HG22	1:B:276:MET:SD	2.60	0.41
1:A:181:LYS:HA	1:A:181:LYS:HD3	1.83	0.41
1:A:444:PHE:N	1:A:444:PHE:CD2	2.85	0.41
1:A:282:ARG:HG2	1:A:282:ARG:HH11	1.85	0.41
1:A:261:ARG:O	1:A:264:LEU:N	2.53	0.41
1:B:341:ASN:HD21	1:B:343:TYR:HB2	1.86	0.41
1:B:353:ASP:OD1	1:B:353:ASP:N	2.50	0.41
1:B:520:ASN:HB3	1:B:544:PHE:CD2	2.54	0.41
1:A:289:ASN:CA	1:A:316:VAL:HG21	2.51	0.41
1:B:470:ASN:HB2	1:B:483:VAL:HG11	2.02	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:A:470:ASN:OD1	1:A:497:ILE:HG23	2.21	0.41
1:B:86:LEU:HD12	1:B:86:LEU:HA	1.91	0.41
1:B:365:ASN:OD1	1:B:365:ASN:O	2.39	0.41
1:B:418:LEU:HD13	1:B:422:MET:CB	2.51	0.41
1:A:116:SER:C	1:A:117:LEU:HD12	2.42	0.41
1:A:252:ILE:O	1:A:253:ARG:C	2.59	0.41
1:A:558:ASP:OD2	1:A:558:ASP:C	2.57	0.41
1:B:492:LEU:N	1:B:492:LEU:HD23	2.35	0.41
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:B:363:LEU:N	1:B:363:LEU:HD22	2.36	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: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:A:475:GLY:C	1:A:477:LYS:H	2.25	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:169:ILE:HD13	1:B:434:TYR:OH	2.22	0.40
1:B:216:VAL:HA	1:B:245:GLU:O	2.22	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%)	4	5
1	B	516/555 (93%)	443 (86%)	56 (11%)	17 (3%)	4	5
All	All	1030/1110 (93%)	889 (86%)	107 (10%)	34 (3%)	4	5

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

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Mol	Chain	Res	Type
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%)	14	25
1	B	449/481 (93%)	411 (92%)	38 (8%)	10	19
All	All	896/962 (93%)	826 (92%)	70 (8%)	12	22

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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

Sometimes 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 molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides 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	$\# Z  > 2$
2	NAG	B	802	1	14,14,15	0.59	0	17,19,21	0.65	0
3	C5B	B	2001	-	6,12,12	0.87	0	4,18,18	2.15	1 (25%)
3	C5B	A	1001	-	6,12,12	0.89	0	4,18,18	2.16	1 (25%)
2	NAG	A	801	1	14,14,15	0.70	0	17,19,21	0.61	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
2	NAG	B	802	1	-	2/6/23/26	0/1/1/1
3	C5B	B	2001	-	-	0/0/21/21	0/1/1/1
3	C5B	A	1001	-	-	0/0/21/21	0/1/1/1
2	NAG	A	801	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	C5B	CB2-CA-CB1	3.44	108.45	102.70
3	B	2001	C5B	CB2-CA-CB1	3.37	108.34	102.70

There are no chirality outliers.

All (4) 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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	C5B	1	0
2	A	801	NAG	1	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%)	0.66	50 (9%) <b>7</b> <b>8</b>	33, 66, 105, 141	0
1	B	520/555 (93%)	0.68	64 (12%) <b>4</b> <b>4</b>	35, 68, 107, 141	0
All	All	1038/1110 (93%)	0.67	114 (10%) <b>5</b> <b>6</b>	33, 67, 106, 141	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	368	ASN	11.1
1	B	516	ASN	8.3
1	A	516	ASN	8.3
1	A	368	ASN	7.8
1	B	369	HIS	7.6
1	B	567	GLU	7.3
1	B	367	ARG	7.2
1	B	365	ASN	6.9
1	B	366	LYS	6.8
1	A	369	HIS	6.3
1	B	28	PHE	6.1
1	A	449	GLY	5.9
1	A	367	ARG	5.8
1	A	366	LYS	5.8
1	A	443	PRO	5.7
1	B	474	THR	5.6
1	A	365	ASN	5.6
1	A	250	SER	5.4
1	A	450	ALA	5.4
1	B	449	GLY	5.1
1	B	250	SER	5.0
1	B	52	THR	4.8
1	B	450	ALA	4.8
1	B	343	TYR	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	54	THR	4.5
1	A	370	ARG	4.4
1	B	251	ASN	4.4
1	A	446	PRO	4.2
1	A	55	GLU	4.2
1	B	29	MET	4.1
1	A	478	TYR	4.1
1	A	474	THR	4.0
1	B	566	PRO	4.0
1	B	477	LYS	3.9
1	B	298	VAL	3.9
1	B	475	GLY	3.8
1	A	524	GLY	3.8
1	B	440	PHE	3.8
1	B	443	PRO	3.7
1	B	331	ARG	3.7
1	B	478	TYR	3.6
1	A	361	CYS	3.6
1	A	299	ALA	3.5
1	B	315	HIS	3.4
1	A	254	LYS	3.4
1	B	299	ALA	3.3
1	B	249	ARG	3.3
1	A	53	GLY	3.3
1	B	273	VAL	3.3
1	B	252	ILE	3.3
1	B	373	CYS	3.2
1	B	254	LYS	3.2
1	A	54	THR	3.1
1	A	253	ARG	3.0
1	B	374	ASP	3.0
1	A	298	VAL	3.0
1	B	476	GLY	3.0
1	B	139	PRO	3.0
1	A	147	GLY	2.9
1	A	274	LEU	2.9
1	A	448	LYS	2.9
1	A	567	GLU	2.9
1	B	551	PRO	2.8
1	A	441	THR	2.8
1	B	51	GLY	2.7
1	A	527	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	451	ASP	2.7
1	A	297	TRP	2.7
1	A	564	ASN	2.7
1	B	364	GLN	2.7
1	B	272	VAL	2.7
1	A	138	ILE	2.6
1	B	147	GLY	2.6
1	B	360	GLN	2.6
1	B	473	GLN	2.6
1	A	434	TYR	2.6
1	A	520	ASN	2.5
1	A	272	VAL	2.5
1	B	359	PHE	2.5
1	B	53	GLY	2.5
1	B	296	THR	2.5
1	A	116	SER	2.5
1	B	376	HIS	2.5
1	B	235	ARG	2.4
1	B	521	MET	2.4
1	B	434	TYR	2.4
1	B	297	TRP	2.4
1	B	274	LEU	2.3
1	B	43	GLY	2.3
1	B	335	ARG	2.3
1	B	523	PRO	2.3
1	A	447	ASN	2.2
1	A	146	ILE	2.2
1	A	321	ILE	2.2
1	A	318	TYR	2.2
1	B	502	ASN	2.2
1	A	517	GLU	2.2
1	B	371	GLN	2.2
1	B	375	LYS	2.1
1	A	144	GLY	2.1
1	A	273	VAL	2.1
1	A	526	VAL	2.1
1	B	524	GLY	2.1
1	B	498	HIS	2.1
1	B	361	CYS	2.1
1	A	528	CYS	2.1
1	A	300	SER	2.1
1	B	529	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	458	THR	2.0
1	A	440	PHE	2.0
1	A	529	TRP	2.0
1	A	204	ILE	2.0
1	B	55	GLU	2.0
1	B	481	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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(Å <sup>2</sup> )	Q<0.9
2	NAG	A	801	14/15	0.81	0.24	95,97,100,100	0
2	NAG	B	802	14/15	0.81	0.23	88,95,96,98	0
3	C5B	B	2001	12/12	0.96	0.24	48,50,51,52	0
3	C5B	A	1001	12/12	0.97	0.25	45,46,51,53	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.