



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 10:48 pm GMT

PDB ID : 2E4Y  
Title : Crystal structure of the extracellular region of the group II metabotropic glutamate receptor complexed with 2R,4R-APDC  
Authors : Muto, T.; Tsuchiya, D.; Morikawa, K.; Jingami, H.  
Deposited on : 2006-12-17  
Resolution : 3.40 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.

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

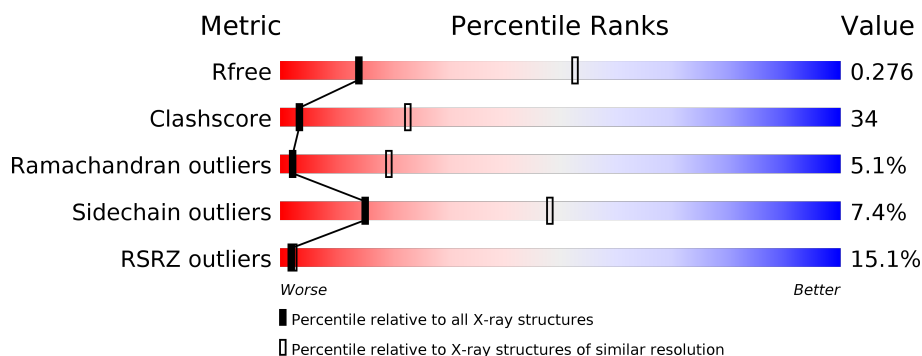
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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))
$R_{free}$	111664	1928 (3.50-3.30)
Clashscore	122126	2051 (3.50-3.30)
Ramachandran outliers	120053	2006 (3.50-3.30)
Sidechain outliers	120020	2006 (3.50-3.30)
RSRZ outliers	108989	1827 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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>5%</div> <div>41%</div> <div>45%</div> <div>7%</div> <div>7%</div> </div>
1	B	555	<div> <div>22%</div> <div>39%</div> <div>38%</div> <div>6%</div> <div>17%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

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

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7823 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	23	0	0
			4118	2606	709	776	27			
1	B	459	Total	C	N	O	S	23	0	0
			3667	2325	642	685	15			

There are 12 discrepancies between the modelled and reference sequences:

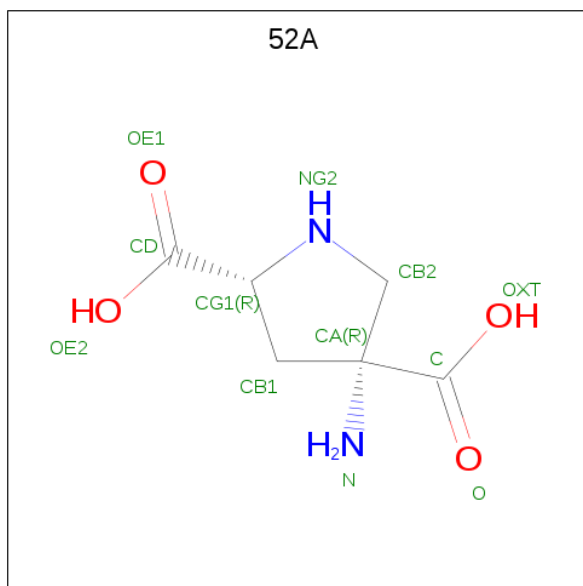
Chain	Residue	Modelled	Actual	Comment	Reference
A	414	GLN	ASN	ENGINEERED	UNP P31422
A	439	GLN	ASN	ENGINEERED	UNP P31422
A	576	LEU	-	CLONING ARTIFACT	UNP P31422
A	577	VAL	-	CLONING ARTIFACT	UNP P31422
A	578	PRO	-	CLONING ARTIFACT	UNP P31422
A	579	ARG	-	CLONING ARTIFACT	UNP P31422
B	414	GLN	ASN	ENGINEERED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

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

- Molecule 3 is (2R,4R)-4-aminopyrrolidine-2,4-dicarboxylic acid (three-letter code: 52A) (formula:  $C_6H_{10}N_2O_4$ ).

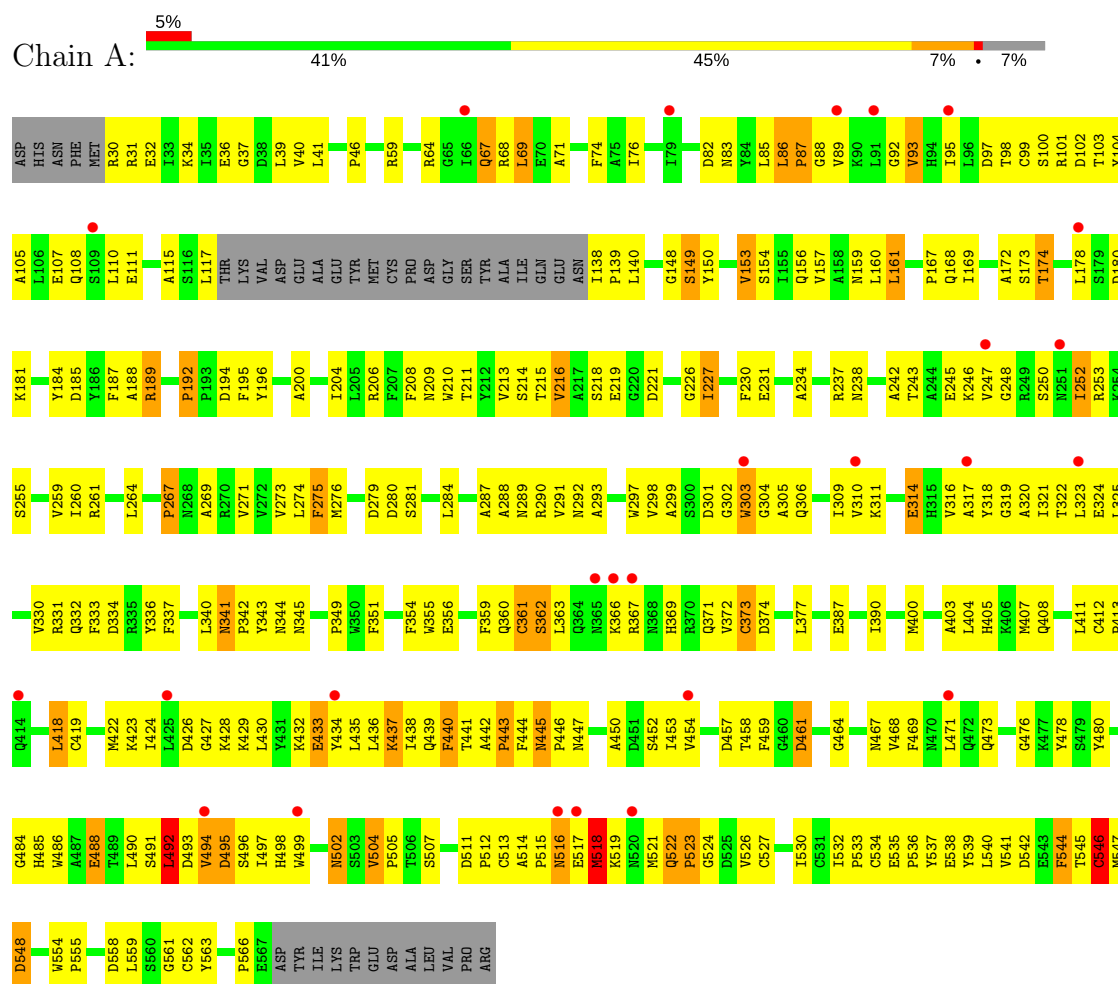


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	6	2	4		
3	B	1	Total	C	N	O	0	0
			12	6	2	4		

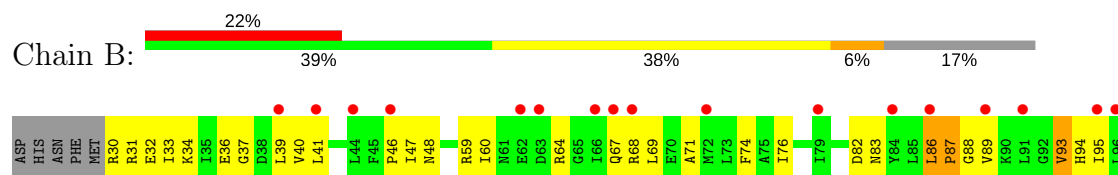
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.39Å 91.80Å 112.97Å 90.00° 92.28° 90.00°	Depositor
Resolution (Å)	12.00 – 3.40 84.33 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (12.00-3.40) 99.5 (84.33-3.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 3.41Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.224 , 0.284 0.220 , 0.276	Depositor DCC
$R_{free}$ test set	1632 reflections (6.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	122.9	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 137.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.043 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7823	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	132.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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: NAG, 52A

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	0.52	0/4212	0.71	2/5704 (0.0%)
1	B	0.37	0/3745	0.65	2/5062 (0.0%)
All	All	0.46	0/7957	0.68	4/10766 (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	419	CYS	CA-CB-SG	-7.22	101.01	114.00
1	A	419	CYS	CA-CB-SG	-7.08	101.25	114.00
1	A	546	CYS	CA-CB-SG	-7.05	101.30	114.00
1	B	412	CYS	CA-CB-SG	-5.14	104.75	114.00

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	3994	302	0
1	B	3667	0	3605	227	0
2	A	14	0	13	0	0
3	A	12	0	8	2	0
3	B	12	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7823	0	7628	526	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 34.

All (526) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:LYS:HA	1:B:437:LYS:HE3	1.40	1.02
1:B:181:LYS:HE2	1:B:459:PHE:O	1.64	0.98
1:A:437:LYS:HA	1:A:437:LYS:HE3	1.44	0.97
1:A:519:LYS:HD2	1:A:546:CYS:HB2	1.45	0.96
1:A:181:LYS:HE2	1:A:459:PHE:O	1.67	0.95
1:A:514:ALA:HB3	1:A:518:MET:HG3	1.47	0.94
1:B:39:LEU:HD23	1:B:404:LEU:HD13	1.49	0.94
1:A:493:ASP:OD2	1:A:496:SER:HB3	1.69	0.93
1:A:39:LEU:HD23	1:A:404:LEU:HD13	1.51	0.93
1:A:538:GLU:HB3	1:A:548:ASP:HA	1.51	0.92
1:B:356:GLU:HA	1:B:361:CYS:HB2	1.50	0.92
1:A:341:ASN:HD22	1:A:343:TYR:H	1.16	0.90
1:A:442:ALA:O	1:A:444:PHE:N	2.08	0.87
1:A:213:VAL:HG12	1:A:271:VAL:HB	1.57	0.86
1:B:299:ALA:HB3	1:B:322:THR:HG22	1.56	0.86
1:B:276:MET:HE3	1:B:281:SER:HA	1.56	0.86
1:B:341:ASN:HD22	1:B:343:TYR:H	1.17	0.85
1:B:216:VAL:HG13	1:B:274:LEU:HD23	1.59	0.85
1:A:356:GLU:HA	1:A:361:CYS:HB2	1.59	0.84
1:B:252:ILE:HG22	1:B:253:ARG:H	1.42	0.84
1:B:213:VAL:HG12	1:B:271:VAL:HB	1.61	0.82
1:B:493:ASP:OD2	1:B:496:SER:HB3	1.80	0.82
1:A:252:ILE:HG22	1:A:253:ARG:H	1.43	0.81
1:A:366:LYS:HG2	1:A:367:ARG:H	1.45	0.80
1:A:216:VAL:HG13	1:A:274:LEU:HD23	1.65	0.79
1:B:442:ALA:O	1:B:444:PHE:N	2.16	0.79
1:A:148:GLY:HA3	1:A:154:SER:OG	1.85	0.77
1:A:310:VAL:HG13	1:A:317:ALA:HB3	1.66	0.77
1:B:366:LYS:HG2	1:B:367:ARG:H	1.46	0.77
1:A:494:VAL:C	1:A:496:SER:H	1.87	0.77
1:B:287:ALA:HA	1:B:290:ARG:NH1	1.99	0.76
1:A:515:PRO:HG2	1:A:516:ASN:H	1.49	0.76
1:B:216:VAL:HA	1:B:245:GLU:O	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:THR:HG23	1:B:452:SER:O	1.86	0.75
1:B:362:SER:O	1:B:363:LEU:HD22	1.87	0.74
1:A:310:VAL:HG12	1:A:314:GLU:HA	1.70	0.74
1:B:310:VAL:HG12	1:B:314:GLU:HA	1.70	0.74
1:A:540:LEU:N	1:A:540:LEU:HD12	2.02	0.73
1:A:442:ALA:C	1:A:444:PHE:H	1.90	0.73
1:A:287:ALA:HA	1:A:290:ARG:NH1	2.04	0.73
1:A:276:MET:HE3	1:A:281:SER:HA	1.70	0.72
1:B:148:GLY:HA3	1:B:154:SER:OG	1.90	0.72
1:A:216:VAL:HA	1:A:245:GLU:O	1.90	0.72
1:B:311:LYS:HA	1:B:314:GLU:OE2	1.89	0.71
1:A:299:ALA:HB3	1:A:322:THR:HG22	1.72	0.71
1:A:372:VAL:HG22	1:A:373:CYS:H	1.56	0.71
1:A:490:LEU:HG	1:A:492:LEU:HD22	1.72	0.71
1:A:538:GLU:CB	1:A:548:ASP:HA	2.21	0.70
1:A:74:PHE:HB2	1:A:336:TYR:CE2	2.26	0.70
1:A:362:SER:O	1:A:363:LEU:HD22	1.91	0.70
1:B:74:PHE:HB2	1:B:336:TYR:CE2	2.27	0.70
1:A:535:GLU:HA	1:A:535:GLU:OE2	1.91	0.69
1:A:187:PHE:HE2	1:A:189:ARG:HD2	1.57	0.69
1:A:408:GLN:HA	1:A:422:MET:HE2	1.74	0.68
1:A:438:ILE:HG23	1:A:453:ILE:HD12	1.75	0.68
1:A:521:MET:HB2	1:A:530:ILE:HG13	1.75	0.68
1:A:441:THR:HG23	1:A:452:SER:O	1.92	0.68
1:B:255:SER:O	1:B:259:VAL:HG23	1.93	0.68
1:B:310:VAL:HG13	1:B:317:ALA:HB3	1.74	0.68
1:A:213:VAL:CG1	1:A:271:VAL:HB	2.24	0.67
1:B:408:GLN:HA	1:B:422:MET:HE2	1.75	0.67
1:A:311:LYS:HA	1:A:314:GLU:OE2	1.94	0.67
1:A:342:PRO:HD3	1:A:355:TRP:CD2	2.31	0.66
1:A:518:MET:HA	1:A:532:ILE:O	1.96	0.66
1:A:342:PRO:HD3	1:A:355:TRP:CE3	2.31	0.66
1:B:115:ALA:HB1	1:B:140:LEU:O	1.96	0.66
1:B:342:PRO:HD3	1:B:355:TRP:CD2	2.31	0.66
1:A:115:ALA:HB1	1:A:140:LEU:O	1.95	0.65
1:B:442:ALA:C	1:B:444:PHE:H	1.96	0.65
1:A:255:SER:O	1:A:259:VAL:HG23	1.96	0.65
1:B:252:ILE:N	1:B:252:ILE:HD12	2.12	0.65
1:A:216:VAL:HG13	1:A:274:LEU:CD2	2.26	0.65
1:A:87:PRO:HG2	1:A:88:GLY:H	1.61	0.65
1:B:98:THR:HB	1:B:105:ALA:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:ASN:ND2	1:A:343:TYR:H	1.93	0.65
1:A:298:VAL:HA	1:A:321:ILE:O	1.98	0.64
1:B:372:VAL:HG22	1:B:373:CYS:H	1.63	0.64
1:A:274:LEU:HD11	1:A:297:TRP:CE3	2.32	0.64
1:A:518:MET:HA	1:A:533:PRO:HA	1.80	0.63
1:B:366:LYS:HE2	1:B:369:HIS:HD2	1.64	0.63
1:A:264:LEU:O	1:A:267:PRO:HD3	1.99	0.63
1:B:297:TRP:HB2	1:B:320:ALA:HB1	1.81	0.63
1:B:494:VAL:C	1:B:496:SER:H	1.98	0.63
1:A:64:ARG:HD3	3:A:1001:52A:OE1	1.99	0.62
1:B:264:LEU:O	1:B:267:PRO:HD3	1.98	0.62
1:B:260:ILE:CD1	1:B:288:ALA:HB2	2.29	0.62
1:A:490:LEU:HD12	1:A:491:SER:H	1.65	0.62
1:B:41:LEU:HD22	1:B:400:MET:HG2	1.82	0.62
1:A:366:LYS:HE2	1:A:369:HIS:HD2	1.63	0.62
1:B:86:LEU:CD1	1:B:405:HIS:HA	2.30	0.61
1:B:323:LEU:HD23	1:B:468:VAL:HA	1.82	0.61
1:B:169:ILE:HA	1:B:188:ALA:O	2.00	0.61
1:A:252:ILE:N	1:A:252:ILE:HD12	2.16	0.61
1:A:64:ARG:O	1:A:68:ARG:HD2	2.00	0.61
1:B:216:VAL:HB	1:B:245:GLU:HB2	1.83	0.61
1:B:32:GLU:OE2	1:B:34:LYS:HE3	2.01	0.60
1:B:473:GLN:NE2	1:B:476:GLY:H	1.99	0.60
1:B:64:ARG:HD3	3:B:2001:52A:OE1	2.01	0.60
1:A:260:ILE:CD1	1:A:288:ALA:HB2	2.30	0.60
1:A:340:LEU:HD22	1:A:345:ASN:ND2	2.16	0.60
1:A:467:ASN:HB3	1:A:469:PHE:HE1	1.66	0.60
1:A:246:LYS:O	1:A:246:LYS:HG3	2.00	0.60
1:B:340:LEU:HD22	1:B:345:ASN:ND2	2.17	0.60
1:B:490:LEU:HD12	1:B:491:SER:H	1.66	0.60
1:A:227:ILE:HD13	1:A:230:PHE:HB3	1.84	0.60
1:B:87:PRO:HG2	1:B:88:GLY:H	1.65	0.60
1:A:490:LEU:CD1	1:A:491:SER:H	2.15	0.60
1:B:298:VAL:HA	1:B:321:ILE:O	2.01	0.60
1:B:342:PRO:HD3	1:B:355:TRP:CE3	2.37	0.59
1:A:178:LEU:HA	1:A:184:TYR:CD1	2.38	0.59
1:A:110:LEU:HD21	1:B:113:VAL:HG23	1.83	0.59
1:B:341:ASN:ND2	1:B:343:TYR:H	1.96	0.59
1:A:424:ILE:HG13	1:A:424:ILE:O	2.01	0.59
1:A:169:ILE:HA	1:A:188:ALA:O	2.02	0.58
1:B:82:ASP:OD2	1:B:83:ASN:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ILE:N	1:A:139:PRO:HD2	2.18	0.58
1:B:298:VAL:O	1:B:298:VAL:HG12	2.04	0.58
1:A:535:GLU:O	1:A:537:TYR:N	2.36	0.58
1:A:341:ASN:HA	1:A:355:TRP:CZ3	2.38	0.58
1:B:64:ARG:O	1:B:68:ARG:HD2	2.02	0.58
1:A:323:LEU:HD23	1:A:468:VAL:HA	1.85	0.58
1:A:493:ASP:O	1:A:495:ASP:N	2.36	0.58
1:A:341:ASN:HD22	1:A:343:TYR:N	1.94	0.58
1:A:490:LEU:CG	1:A:491:SER:H	2.17	0.58
1:B:178:LEU:HA	1:B:184:TYR:CD1	2.38	0.58
1:A:41:LEU:HD22	1:A:400:MET:HG2	1.85	0.58
1:A:517:GLU:HG2	1:A:533:PRO:HB2	1.86	0.58
1:A:39:LEU:HD22	1:A:89:VAL:HG11	1.85	0.58
1:B:430:LEU:O	1:B:434:TYR:HB2	2.04	0.58
1:B:216:VAL:HG13	1:B:274:LEU:CD2	2.33	0.57
1:B:438:ILE:HG23	1:B:453:ILE:HD12	1.85	0.57
1:B:411:LEU:HD12	1:B:422:MET:HG2	1.86	0.57
1:B:362:SER:HA	1:B:366:LYS:HD2	1.87	0.57
1:A:108:GLN:O	1:A:111:GLU:HB2	2.05	0.57
1:A:86:LEU:CD1	1:A:405:HIS:HA	2.35	0.57
1:B:493:ASP:O	1:B:495:ASP:N	2.37	0.57
1:A:98:THR:HB	1:A:105:ALA:HB2	1.86	0.57
1:A:539:TYR:CD1	1:A:540:LEU:N	2.73	0.57
1:A:555:PRO:HA	1:A:561:GLY:O	2.05	0.57
1:B:227:ILE:HD13	1:B:230:PHE:HB3	1.87	0.57
1:B:138:ILE:N	1:B:139:PRO:HD2	2.20	0.56
1:B:213:VAL:CG1	1:B:271:VAL:HB	2.32	0.56
1:B:252:ILE:HD12	1:B:252:ILE:H	1.70	0.56
1:A:519:LYS:HE2	1:A:521:MET:SD	2.45	0.56
1:A:490:LEU:HG	1:A:491:SER:N	2.20	0.56
1:B:341:ASN:HD22	1:B:343:TYR:N	1.96	0.56
1:A:539:TYR:C	1:A:540:LEU:HD12	2.25	0.56
1:A:298:VAL:HG12	1:A:298:VAL:O	2.06	0.56
1:A:473:GLN:NE2	1:A:476:GLY:H	2.03	0.56
1:B:424:ILE:O	1:B:424:ILE:HG13	2.06	0.56
1:A:453:ILE:HG13	1:A:453:ILE:O	2.05	0.55
1:A:274:LEU:HD22	1:A:276:MET:HE1	1.88	0.55
1:B:279:ASP:OD1	1:B:280:ASP:N	2.39	0.55
1:B:437:LYS:HE2	1:B:438:ILE:H	1.71	0.55
1:A:216:VAL:HB	1:A:245:GLU:HB2	1.87	0.55
1:B:260:ILE:HD12	1:B:288:ALA:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:VAL:HG13	1:A:92:GLY:C	2.28	0.54
1:B:218:SER:N	1:B:276:MET:HG2	2.22	0.54
1:A:540:LEU:HG	1:A:546:CYS:SG	2.47	0.54
1:A:271:VAL:HG23	1:A:507:SER:HB2	1.89	0.54
1:A:260:ILE:HD12	1:A:288:ALA:HB2	1.88	0.54
1:A:430:LEU:O	1:A:434:TYR:HB2	2.07	0.54
1:B:31:ARG:HD2	1:B:349:PRO:HB2	1.88	0.54
1:B:437:LYS:HA	1:B:437:LYS:CE	2.25	0.54
1:A:153:VAL:O	1:A:157:VAL:HG23	2.07	0.54
1:B:400:MET:CE	1:B:400:MET:HA	2.37	0.54
1:B:437:LYS:CA	1:B:437:LYS:HE3	2.27	0.54
1:A:156:GLN:HA	1:A:156:GLN:OE1	2.06	0.54
1:A:192:PRO:HG3	1:A:464:GLY:HA2	1.90	0.54
1:A:211:THR:HG22	1:A:527:CYS:SG	2.48	0.54
1:B:214:SER:OG	1:B:243:THR:HG22	2.07	0.54
1:A:274:LEU:HD22	1:A:276:MET:CE	2.38	0.53
1:B:366:LYS:HE2	1:B:369:HIS:CD2	2.43	0.53
1:A:297:TRP:HB2	1:A:320:ALA:HB1	1.90	0.53
1:A:494:VAL:C	1:A:496:SER:N	2.58	0.53
1:A:168:GLN:C	1:A:169:ILE:HG13	2.29	0.53
1:A:200:ALA:O	1:A:204:ILE:HG13	2.09	0.53
1:A:226:GLY:HA3	1:A:275:PHE:CE2	2.44	0.53
1:A:169:ILE:HD11	1:A:400:MET:SD	2.48	0.53
1:B:102:ASP:OD2	1:B:103:THR:N	2.37	0.53
1:B:74:PHE:HB2	1:B:336:TYR:CD2	2.43	0.53
1:B:461:ASP:N	1:B:461:ASP:OD2	2.38	0.53
1:A:362:SER:HA	1:A:366:LYS:HD2	1.90	0.53
1:A:491:SER:C	1:A:492:LEU:HD22	2.29	0.53
1:A:519:LYS:HE3	1:A:544:PHE:O	2.08	0.53
1:A:82:ASP:OD2	1:A:83:ASN:N	2.41	0.53
1:B:453:ILE:HG13	1:B:453:ILE:O	2.08	0.53
1:A:490:LEU:CG	1:A:491:SER:N	2.73	0.52
1:B:214:SER:OG	1:B:242:ALA:HB3	2.10	0.52
1:A:160:LEU:HB2	1:B:163:LEU:HD23	1.92	0.52
1:A:442:ALA:C	1:A:444:PHE:N	2.59	0.52
1:B:76:ILE:HG13	1:B:93:VAL:HG11	1.91	0.52
1:A:515:PRO:CG	1:A:516:ASN:H	2.21	0.52
1:B:185:ASP:N	1:B:185:ASP:OD2	2.42	0.52
1:A:366:LYS:HE2	1:A:369:HIS:CD2	2.42	0.52
1:A:490:LEU:HG	1:A:491:SER:H	1.73	0.52
1:A:86:LEU:HD13	1:A:405:HIS:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ILE:H	1:A:252:ILE:HD12	1.73	0.52
1:A:31:ARG:HD2	1:A:349:PRO:HB2	1.92	0.52
1:A:74:PHE:HB2	1:A:336:TYR:CD2	2.45	0.52
1:A:341:ASN:HB2	1:A:342:PRO:HD2	1.91	0.52
1:B:260:ILE:HD11	1:B:288:ALA:HB2	1.92	0.52
1:B:191:VAL:HG12	1:B:392:PHE:CD2	2.45	0.52
1:A:32:GLU:OE2	1:A:34:LYS:HE3	2.10	0.52
1:A:542:ASP:OD2	1:A:545:THR:N	2.40	0.52
1:B:252:ILE:HG22	1:B:253:ARG:N	2.21	0.52
1:B:314:GLU:CD	1:B:314:GLU:H	2.13	0.51
1:B:297:TRP:HB2	1:B:320:ALA:CB	2.39	0.51
1:A:46:PRO:HD3	1:A:149:SER:HB2	1.92	0.51
1:A:554:TRP:CG	1:A:555:PRO:HD2	2.45	0.51
1:B:117:LEU:HD12	1:B:117:LEU:N	2.24	0.51
1:B:418:LEU:HD22	1:B:422:MET:HE3	1.93	0.51
1:A:435:LEU:C	1:A:437:LYS:H	2.13	0.51
1:A:76:ILE:HG13	1:A:93:VAL:HG11	1.91	0.51
1:A:411:LEU:HD12	1:A:422:MET:HG2	1.93	0.51
1:A:428:LYS:O	1:A:432:LYS:HG2	2.10	0.51
1:B:169:ILE:HD11	1:B:400:MET:SD	2.50	0.51
1:A:86:LEU:HG	1:A:89:VAL:HB	1.93	0.51
1:A:521:MET:HB2	1:A:530:ILE:CG1	2.41	0.51
1:B:204:ILE:HG22	1:B:205:LEU:HD23	1.92	0.51
1:B:301:ASP:HA	1:B:323:LEU:O	2.11	0.51
1:B:411:LEU:C	1:B:412:CYS:SG	2.89	0.51
1:B:291:VAL:O	1:B:293:ALA:N	2.44	0.51
1:A:372:VAL:HG22	1:A:373:CYS:N	2.23	0.51
1:B:108:GLN:O	1:B:111:GLU:HB2	2.10	0.51
1:B:205:LEU:HD22	1:B:210:TRP:CE3	2.46	0.51
1:B:435:LEU:C	1:B:437:LYS:H	2.14	0.51
1:B:490:LEU:HG	1:B:492:LEU:HD22	1.92	0.51
1:A:305:ALA:HA	1:A:480:TYR:CE2	2.47	0.50
1:B:442:ALA:C	1:B:444:PHE:N	2.64	0.50
1:A:332:GLN:OE1	1:A:332:GLN:N	2.40	0.50
1:A:494:VAL:O	1:A:496:SER:N	2.44	0.50
1:B:246:LYS:HG3	1:B:246:LYS:O	2.12	0.50
1:B:486:TRP:CH2	1:B:488:GLU:HA	2.47	0.50
1:A:341:ASN:C	1:A:341:ASN:HD22	2.14	0.50
1:A:411:LEU:C	1:A:412:CYS:SG	2.90	0.50
1:A:558:ASP:O	1:A:559:LEU:HB2	2.11	0.50
1:B:274:LEU:HD22	1:B:276:MET:CE	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ILE:O	1:B:94:HIS:HA	2.12	0.50
1:A:157:VAL:HG12	1:A:161:LEU:HD22	1.93	0.50
1:A:185:ASP:OD2	1:A:185:ASP:N	2.44	0.50
1:A:461:ASP:N	1:A:461:ASP:OD2	2.39	0.50
1:A:59:ARG:HB2	1:A:59:ARG:HH11	1.76	0.50
1:A:359:PHE:O	1:A:360:GLN:HB2	2.12	0.50
1:B:195:PHE:HD2	1:B:196:TYR:CE1	2.30	0.50
1:B:314:GLU:HG3	1:B:478:TYR:CD2	2.47	0.50
1:B:76:ILE:HG13	1:B:93:VAL:CG1	2.42	0.50
1:A:261:ARG:O	1:A:264:LEU:HB2	2.11	0.49
1:A:322:THR:O	1:A:469:PHE:HB2	2.12	0.49
1:B:362:SER:C	1:B:363:LEU:HD22	2.32	0.49
1:B:341:ASN:HA	1:B:355:TRP:CZ3	2.46	0.49
1:B:156:GLN:OE1	1:B:156:GLN:HA	2.12	0.49
1:A:41:LEU:CD2	1:A:400:MET:HG2	2.42	0.49
1:A:301:ASP:HA	1:A:323:LEU:O	2.12	0.49
1:A:301:ASP:O	1:A:304:GLY:N	2.46	0.49
1:A:457:ASP:HB2	1:A:461:ASP:OD2	2.13	0.49
1:A:515:PRO:O	1:A:517:GLU:N	2.46	0.49
1:A:522:GLN:HE21	1:A:522:GLN:HA	1.77	0.49
1:A:64:ARG:HG2	1:A:68:ARG:CZ	2.42	0.49
1:A:117:LEU:N	1:A:117:LEU:HD12	2.26	0.49
1:A:260:ILE:HD11	1:A:288:ALA:HB2	1.94	0.49
1:A:437:LYS:CA	1:A:437:LYS:HE3	2.30	0.49
1:B:437:LYS:CE	1:B:438:ILE:H	2.25	0.49
1:A:434:TYR:O	1:A:437:LYS:HB2	2.13	0.49
1:B:205:LEU:HD22	1:B:210:TRP:HE3	1.78	0.49
1:B:387:GLU:HB3	1:B:390:ILE:HG12	1.95	0.49
1:A:314:GLU:CD	1:A:314:GLU:H	2.15	0.48
1:A:341:ASN:ND2	1:A:341:ASN:C	2.66	0.48
1:A:544:PHE:N	1:A:544:PHE:CD1	2.81	0.48
1:B:192:PRO:HG3	1:B:464:GLY:HA2	1.95	0.48
1:A:159:ASN:HB3	1:B:163:LEU:HD11	1.95	0.48
1:A:306:GLN:HB2	1:A:309:ILE:HD12	1.94	0.48
1:A:289:ASN:CB	1:A:316:VAL:HG21	2.44	0.48
1:B:219:GLU:HB2	1:B:248:GLY:HA2	1.94	0.48
1:B:372:VAL:HG22	1:B:373:CYS:N	2.27	0.48
1:A:355:TRP:CE2	1:A:359:PHE:CE1	3.01	0.48
1:B:187:PHE:HE2	1:B:189:ARG:HD2	1.78	0.48
1:B:30:ARG:HG2	1:B:30:ARG:HH11	1.78	0.48
1:B:46:PRO:HD3	1:B:149:SER:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ASP:OD1	1:A:280:ASP:N	2.46	0.48
1:A:40:VAL:HG12	1:A:41:LEU:N	2.29	0.48
1:A:433:GLU:O	1:A:433:GLU:HG3	2.14	0.48
1:A:445:ASN:ND2	1:A:447:ASN:O	2.47	0.48
1:A:563:TYR:O	1:A:563:TYR:CD1	2.66	0.48
1:B:330:VAL:HG13	1:B:444:PHE:HB3	1.94	0.48
1:A:36:GLU:HG2	1:A:37:GLY:N	2.28	0.48
1:A:426:ASP:O	1:A:427:GLY:C	2.52	0.48
1:A:554:TRP:O	1:A:562:CYS:HA	2.14	0.48
1:A:173:SER:HA	3:A:1001:52A:OXT	2.13	0.48
1:B:36:GLU:HG2	1:B:37:GLY:N	2.28	0.48
1:A:493:ASP:CG	1:A:496:SER:HB3	2.33	0.48
1:B:64:ARG:CZ	1:B:306:GLN:NE2	2.77	0.48
1:B:289:ASN:HA	1:B:316:VAL:HG21	1.96	0.48
1:B:440:PHE:CD2	1:B:453:ILE:HG22	2.49	0.48
1:A:486:TRP:CH2	1:A:488:GLU:HA	2.49	0.48
1:B:331:ARG:O	1:B:334:ASP:HB2	2.13	0.48
1:B:322:THR:O	1:B:469:PHE:HB2	2.14	0.48
1:B:200:ALA:HA	1:B:486:TRP:CD1	2.49	0.48
1:A:284:LEU:HD13	1:A:284:LEU:C	2.34	0.47
1:A:306:GLN:HB2	1:A:309:ILE:CD1	2.45	0.47
1:A:59:ARG:NH1	1:A:59:ARG:CB	2.76	0.47
1:A:276:MET:HB2	1:A:281:SER:OG	2.14	0.47
1:A:535:GLU:C	1:A:537:TYR:H	2.18	0.47
1:B:284:LEU:C	1:B:284:LEU:HD13	2.34	0.47
1:A:101:ARG:HD3	1:A:103:THR:OG1	2.14	0.47
1:A:99:CYS:HB2	1:A:104:TYR:CD2	2.50	0.47
1:A:99:CYS:SG	1:A:104:TYR:CE2	3.07	0.47
1:A:138:ILE:N	1:A:139:PRO:CD	2.78	0.47
1:A:324:GLU:HG3	1:A:325:LEU:N	2.29	0.47
1:A:492:LEU:HD23	1:A:492:LEU:N	2.30	0.47
1:B:324:GLU:HG3	1:B:325:LEU:N	2.29	0.47
1:A:187:PHE:CE2	1:A:189:ARG:HB3	2.49	0.47
1:A:71:ALA:HA	1:A:333:PHE:CE1	2.49	0.47
1:A:403:ALA:HB2	1:A:434:TYR:CD1	2.50	0.47
1:A:484:GLY:HA3	1:A:492:LEU:HA	1.97	0.47
1:A:514:ALA:CB	1:A:518:MET:HG3	2.32	0.47
1:B:227:ILE:O	1:B:231:GLU:HG3	2.15	0.47
1:B:337:PHE:CD1	1:B:340:LEU:HD12	2.48	0.47
1:B:445:ASN:ND2	1:B:447:ASN:O	2.47	0.47
1:B:59:ARG:HH11	1:B:59:ARG:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:GLU:HB2	1:A:248:GLY:HA2	1.97	0.47
1:A:539:TYR:HE1	1:A:541:VAL:HA	1.80	0.47
1:B:359:PHE:HB3	1:B:377:LEU:HD21	1.97	0.47
1:A:303:TRP:CD1	1:A:303:TRP:C	2.87	0.47
1:A:330:VAL:HG13	1:A:444:PHE:HB3	1.97	0.47
1:A:68:ARG:NH1	1:A:149:SER:OG	2.48	0.47
1:B:456:PHE:HB3	1:B:460:GLY:HA2	1.97	0.47
1:A:76:ILE:HG13	1:A:93:VAL:CG1	2.44	0.47
1:A:499:TRP:CD2	1:A:505:PRO:HD3	2.50	0.47
1:A:102:ASP:OD2	1:A:103:THR:N	2.41	0.47
1:A:40:VAL:HG13	1:A:92:GLY:O	2.15	0.47
1:B:490:LEU:CD1	1:B:491:SER:H	2.27	0.47
1:B:494:VAL:C	1:B:496:SER:N	2.68	0.47
1:A:227:ILE:O	1:A:231:GLU:HG3	2.16	0.46
1:A:540:LEU:HB3	1:A:542:ASP:O	2.15	0.46
1:B:69:LEU:HD23	1:B:69:LEU:C	2.35	0.46
1:A:441:THR:O	1:A:442:ALA:C	2.54	0.46
1:A:497:ILE:HG21	1:A:499:TRP:CZ2	2.50	0.46
1:B:467:ASN:HB3	1:B:469:PHE:HE1	1.79	0.46
1:A:519:LYS:HG2	1:A:532:ILE:O	2.16	0.46
1:A:535:GLU:C	1:A:537:TYR:N	2.69	0.46
1:B:274:LEU:HD22	1:B:276:MET:HE1	1.97	0.46
1:B:341:ASN:HD22	1:B:341:ASN:C	2.19	0.46
1:B:441:THR:O	1:B:442:ALA:C	2.54	0.46
1:A:540:LEU:CD1	1:A:540:LEU:N	2.76	0.46
1:B:157:VAL:HG12	1:B:161:LEU:HD22	1.96	0.46
1:A:310:VAL:HG21	1:A:471:LEU:HD22	1.97	0.46
1:B:341:ASN:HB2	1:B:342:PRO:HD2	1.98	0.46
1:A:211:THR:HG23	1:A:238:ASN:O	2.16	0.46
1:A:86:LEU:HD13	1:A:405:HIS:CA	2.46	0.46
1:A:491:SER:C	1:A:492:LEU:CD2	2.84	0.46
1:B:107:GLU:O	1:B:110:LEU:HB2	2.16	0.46
1:B:195:PHE:HD2	1:B:196:TYR:HE1	1.64	0.46
1:A:174:THR:HB	1:A:194:ASP:OD1	2.15	0.46
1:A:206:ARG:HD2	1:A:237:ARG:HB3	1.97	0.46
1:A:492:LEU:N	1:A:492:LEU:CD2	2.79	0.46
1:A:400:MET:HA	1:A:400:MET:CE	2.45	0.46
1:B:196:TYR:N	1:B:196:TYR:CD1	2.84	0.46
1:B:287:ALA:HA	1:B:290:ARG:CZ	2.44	0.46
1:B:69:LEU:CD2	1:B:69:LEU:C	2.85	0.46
1:A:230:PHE:CZ	1:A:273:VAL:HG21	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:GLU:O	1:B:433:GLU:HG3	2.15	0.45
1:B:491:SER:O	1:B:492:LEU:HB3	2.16	0.45
1:A:231:GLU:O	1:A:234:ALA:HB3	2.15	0.45
1:A:412:CYS:HA	1:A:413:PRO:HD2	1.73	0.45
1:A:539:TYR:HD1	1:A:540:LEU:N	2.15	0.45
1:B:196:TYR:HD1	1:B:196:TYR:N	2.14	0.45
1:B:403:ALA:HB2	1:B:434:TYR:CD1	2.51	0.45
1:B:374:ASP:O	1:B:377:LEU:HB2	2.17	0.45
1:B:167:PRO:HG3	1:B:430:LEU:HD23	1.98	0.45
1:B:86:LEU:HD13	1:B:405:HIS:CA	2.46	0.45
1:A:361:CYS:HB3	1:A:362:SER:H	1.39	0.45
1:A:435:LEU:O	1:A:437:LYS:N	2.49	0.45
1:B:110:LEU:HA	1:B:110:LEU:HD12	1.77	0.45
1:B:86:LEU:HD13	1:B:405:HIS:HA	1.99	0.45
1:A:437:LYS:CE	1:A:438:ILE:H	2.30	0.45
1:A:437:LYS:HE2	1:A:438:ILE:H	1.80	0.45
1:B:303:TRP:C	1:B:303:TRP:CD1	2.91	0.45
1:B:86:LEU:HG	1:B:89:VAL:HB	1.98	0.45
1:A:535:GLU:O	1:A:538:GLU:HG2	2.17	0.45
1:A:64:ARG:CZ	1:A:306:GLN:NE2	2.80	0.45
1:A:314:GLU:HG3	1:A:478:TYR:CD2	2.53	0.44
1:B:426:ASP:HB3	1:B:429:LYS:HB2	1.99	0.44
1:A:387:GLU:HB3	1:A:390:ILE:HG12	1.99	0.44
1:B:138:ILE:N	1:B:139:PRO:CD	2.79	0.44
1:B:341:ASN:C	1:B:341:ASN:ND2	2.71	0.44
1:A:30:ARG:HH11	1:A:30:ARG:HG2	1.81	0.44
1:A:517:GLU:HB3	1:A:518:MET:H	1.61	0.44
1:A:87:PRO:HG2	1:A:88:GLY:N	2.30	0.44
1:A:442:ALA:HA	1:A:443:PRO:HD2	1.63	0.44
1:A:59:ARG:CB	1:A:59:ARG:HH11	2.30	0.44
1:A:355:TRP:CE2	1:A:359:PHE:HE1	2.36	0.44
1:A:323:LEU:HD21	1:A:468:VAL:HG22	1.99	0.44
1:B:178:LEU:O	1:B:181:LYS:NZ	2.48	0.44
1:B:97:ASP:OD1	1:B:98:THR:N	2.50	0.44
1:A:359:PHE:HB3	1:A:377:LEU:HD21	1.99	0.44
1:B:218:SER:OG	1:B:280:ASP:HB2	2.18	0.44
1:B:422:MET:O	1:B:423:LYS:C	2.55	0.44
1:B:48:ASN:OD1	1:B:60:ILE:HD13	2.17	0.44
1:A:490:LEU:HG	1:A:492:LEU:CD2	2.45	0.44
1:B:442:ALA:HA	1:B:443:PRO:HD2	1.71	0.44
1:B:86:LEU:HD13	1:B:405:HIS:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ALA:HA	1:A:290:ARG:CZ	2.47	0.44
1:A:374:ASP:O	1:A:377:LEU:HB2	2.18	0.44
1:A:473:GLN:NE2	1:A:476:GLY:N	2.66	0.44
1:B:332:GLN:OE1	1:B:332:GLN:N	2.40	0.44
1:B:457:ASP:HB2	1:B:461:ASP:OD2	2.17	0.44
1:A:291:VAL:O	1:A:293:ALA:N	2.51	0.43
1:B:446:PRO:HG2	1:B:447:ASN:H	1.81	0.43
1:A:440:PHE:CD2	1:A:453:ILE:HG22	2.53	0.43
1:A:499:TRP:CG	1:A:505:PRO:HD3	2.53	0.43
1:A:515:PRO:HG2	1:A:516:ASN:N	2.24	0.43
1:B:220:GLY:O	1:B:222:TYR:N	2.50	0.43
1:B:289:ASN:CB	1:B:316:VAL:HG21	2.48	0.43
1:B:366:LYS:HG2	1:B:367:ARG:N	2.24	0.43
1:A:150:TYR:HB2	1:A:153:VAL:HG12	2.00	0.43
1:A:310:VAL:HG11	1:A:471:LEU:HD21	2.01	0.43
1:A:310:VAL:HG21	1:A:471:LEU:CD2	2.48	0.43
1:A:310:VAL:CG1	1:A:317:ALA:HB3	2.44	0.43
1:A:459:PHE:HB2	1:A:461:ASP:OD2	2.18	0.43
1:B:187:PHE:CE2	1:B:189:ARG:HB3	2.54	0.43
1:A:208:PHE:O	1:A:210:TRP:N	2.51	0.43
1:A:269:ALA:HA	1:A:507:SER:OG	2.18	0.43
1:B:499:TRP:CG	1:B:505:PRO:HD3	2.53	0.43
1:A:178:LEU:O	1:A:181:LYS:NZ	2.51	0.43
1:B:47:ILE:HB	1:B:97:ASP:CG	2.39	0.43
1:B:174:THR:O	1:B:193:PRO:HA	2.19	0.43
1:B:434:TYR:O	1:B:437:LYS:HB2	2.19	0.43
1:B:473:GLN:HE21	1:B:476:GLY:N	2.17	0.43
1:A:301:ASP:O	1:A:302:GLY:C	2.57	0.43
1:A:362:SER:C	1:A:363:LEU:HD22	2.39	0.43
1:A:511:ASP:HB3	1:A:512:PRO:HD2	2.00	0.43
1:A:540:LEU:CD1	1:A:559:LEU:HB3	2.49	0.43
1:A:554:TRP:CD2	1:A:555:PRO:HD2	2.54	0.43
1:A:69:LEU:C	1:A:69:LEU:CD2	2.87	0.43
1:B:47:ILE:HD13	1:B:350:TRP:CE3	2.54	0.43
1:B:208:PHE:O	1:B:210:TRP:N	2.52	0.43
1:B:261:ARG:O	1:B:264:LEU:HB2	2.19	0.43
1:A:196:TYR:CD1	1:A:196:TYR:N	2.86	0.43
1:B:41:LEU:CD2	1:B:400:MET:HG2	2.47	0.43
1:B:469:PHE:HD2	1:B:480:TYR:HB3	1.84	0.43
1:A:337:PHE:CD1	1:A:340:LEU:HD12	2.54	0.42
1:A:418:LEU:HD22	1:A:422:MET:HE3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:PHE:O	1:B:360:GLN:HB2	2.19	0.42
1:A:157:VAL:HG12	1:A:161:LEU:CD2	2.49	0.42
1:A:443:PRO:C	1:A:445:ASN:H	2.21	0.42
1:A:93:VAL:HG23	1:A:95:ILE:HG13	2.00	0.42
1:B:389:LYS:O	1:B:392:PHE:N	2.52	0.42
1:B:400:MET:O	1:B:403:ALA:HB3	2.19	0.42
1:B:59:ARG:NH1	1:B:59:ARG:CB	2.82	0.42
1:A:195:PHE:HD2	1:A:196:TYR:CE1	2.36	0.42
1:A:517:GLU:HG3	1:A:534:CYS:H	1.84	0.42
1:A:97:ASP:OD1	1:A:98:THR:N	2.52	0.42
1:B:484:GLY:HA3	1:B:492:LEU:HA	2.00	0.42
1:B:71:ALA:HA	1:B:333:PHE:CE1	2.55	0.42
1:B:317:ALA:O	1:B:471:LEU:HD23	2.20	0.42
1:B:93:VAL:HG23	1:B:95:ILE:HG13	2.00	0.42
1:A:196:TYR:HD1	1:A:196:TYR:N	2.18	0.42
1:B:473:GLN:NE2	1:B:476:GLY:N	2.64	0.42
1:A:167:PRO:HG3	1:A:430:LEU:HD23	2.01	0.42
1:A:252:ILE:HG22	1:A:253:ARG:N	2.22	0.42
1:A:467:ASN:CB	1:A:469:PHE:HE1	2.33	0.42
1:A:513:CYS:HB3	1:A:518:MET:HB2	2.00	0.42
1:B:187:PHE:CD2	1:B:188:ALA:N	2.88	0.42
1:B:219:GLU:HB2	1:B:247:VAL:O	2.19	0.42
1:A:107:GLU:O	1:A:110:LEU:HB2	2.19	0.42
1:A:227:ILE:HD13	1:A:227:ILE:HA	1.82	0.42
1:B:303:TRP:CD1	1:B:322:THR:HG21	2.54	0.42
1:A:215:THR:HG22	1:A:273:VAL:HB	2.02	0.42
1:A:426:ASP:HB3	1:A:429:LYS:HB2	2.02	0.42
1:B:400:MET:HA	1:B:400:MET:HE3	2.02	0.42
1:B:412:CYS:HA	1:B:413:PRO:HD2	1.66	0.42
1:B:341:ASN:OD1	1:B:344:ASN:ND2	2.53	0.42
1:B:399:ALA:O	1:B:400:MET:C	2.58	0.42
1:B:440:PHE:O	1:B:441:THR:C	2.56	0.42
1:B:443:PRO:C	1:B:445:ASN:H	2.22	0.42
1:A:218:SER:N	1:A:276:MET:HG2	2.35	0.41
1:A:407:MET:HG2	1:A:422:MET:SD	2.60	0.41
1:A:523:PRO:HG2	1:A:524:GLY:H	1.84	0.41
1:A:541:VAL:HG23	1:A:547:MET:CB	2.50	0.41
1:A:468:VAL:HG23	1:A:485:HIS:HA	2.02	0.41
1:A:41:LEU:HD12	1:A:76:ILE:HD11	2.02	0.41
1:B:215:THR:O	1:B:245:GLU:N	2.41	0.41
1:B:40:VAL:HG12	1:B:41:LEU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:ALA:HA	1:B:480:TYR:CE2	2.55	0.41
1:A:219:GLU:HB2	1:A:247:VAL:O	2.20	0.41
1:B:205:LEU:HA	1:B:210:TRP:HE3	1.86	0.41
1:B:356:GLU:OE1	1:B:363:LEU:HB2	2.21	0.41
1:A:67:GLN:HB3	1:A:390:ILE:HD11	2.02	0.41
1:A:486:TRP:O	1:A:486:TRP:HE3	2.03	0.41
1:B:251:ASN:HD22	1:B:255:SER:HB3	1.85	0.41
1:B:355:TRP:CE2	1:B:359:PHE:CE1	3.08	0.41
1:A:331:ARG:O	1:A:334:ASP:HB2	2.21	0.41
1:A:305:ALA:HA	1:A:480:TYR:CD2	2.56	0.41
1:B:40:VAL:HG21	1:B:140:LEU:HD22	2.02	0.41
1:B:328:HIS:HA	1:B:329:PRO:HD2	1.87	0.41
1:B:459:PHE:HB2	1:B:461:ASP:OD2	2.21	0.41
1:A:213:VAL:HB	1:A:271:VAL:O	2.20	0.41
1:A:289:ASN:OD1	1:A:316:VAL:HG21	2.21	0.41
1:A:422:MET:O	1:A:423:LYS:C	2.57	0.41
1:B:426:ASP:O	1:B:427:GLY:C	2.57	0.41
1:A:208:PHE:HB2	1:A:210:TRP:CE3	2.56	0.41
1:B:435:LEU:O	1:B:437:LYS:N	2.51	0.41
1:B:68:ARG:NH1	1:B:149:SER:OG	2.54	0.41
1:A:310:VAL:HG13	1:A:317:ALA:CB	2.45	0.41
1:A:289:ASN:HA	1:A:316:VAL:HG21	2.03	0.41
1:A:318:TYR:CG	1:A:319:GLY:N	2.89	0.41
1:A:515:PRO:CG	1:A:516:ASN:N	2.84	0.41
1:A:215:THR:O	1:A:245:GLU:N	2.46	0.40
1:A:214:SER:OG	1:A:243:THR:HG22	2.21	0.40
1:A:356:GLU:OE1	1:A:363:LEU:HB2	2.20	0.40
1:A:40:VAL:HA	1:A:92:GLY:O	2.21	0.40
1:A:351:PHE:O	1:A:354:PHE:HB3	2.21	0.40
1:A:504:VAL:HA	1:A:505:PRO:HD3	1.76	0.40
1:A:519:LYS:N	1:A:532:ILE:O	2.53	0.40
1:A:541:VAL:HG23	1:A:547:MET:HB2	2.02	0.40
1:A:85:LEU:O	1:A:86:LEU:C	2.59	0.40
1:B:301:ASP:O	1:B:304:GLY:N	2.54	0.40
1:A:341:ASN:ND2	1:A:341:ASN:O	2.54	0.40
1:B:169:ILE:HG12	1:B:434:TYR:OH	2.22	0.40
1:A:341:ASN:OD1	1:A:344:ASN:ND2	2.54	0.40
1:B:215:THR:HG22	1:B:273:VAL:HB	2.03	0.40
1:B:399:ALA:HB1	1:B:434:TYR:HE1	1.85	0.40
1:B:428:LYS:O	1:B:432:LYS:HG2	2.21	0.40
1:B:426:ASP:CG	1:B:429:LYS:HB2	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:LYS:CE	1:B:459:PHE:O	2.53	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%)	415 (81%)	71 (14%)	28 (5%)	2	18
1	B	455/555 (82%)	368 (81%)	66 (14%)	21 (5%)	2	21
All	All	969/1110 (87%)	783 (81%)	137 (14%)	49 (5%)	2	19

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	242	ALA
1	A	292	ASN
1	A	361	CYS
1	A	443	PRO
1	A	494	VAL
1	A	518	MET
1	B	242	ALA
1	B	292	ASN
1	B	361	CYS
1	B	443	PRO
1	B	494	VAL
1	A	87	PRO
1	A	209	ASN
1	A	221	ASP
1	A	371	GLN
1	A	436	LEU
1	A	488	GLU

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Mol	Chain	Res	Type
1	A	495	ASP
1	A	516	ASN
1	A	523	PRO
1	A	566	PRO
1	B	87	PRO
1	B	100	SER
1	B	209	ASN
1	B	221	ASP
1	B	314	GLU
1	B	371	GLN
1	B	436	LEU
1	B	488	GLU
1	B	495	ASP
1	B	502	ASN
1	A	100	SER
1	A	314	GLU
1	A	450	ALA
1	A	502	ASN
1	B	441	THR
1	A	172	ALA
1	A	180	ASP
1	A	362	SER
1	A	492	LEU
1	A	536	PRO
1	B	180	ASP
1	B	362	SER
1	B	450	ALA
1	B	492	LEU
1	A	250	SER
1	A	446	PRO
1	B	446	PRO
1	A	267	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%)	411 (92%)	36 (8%)	13	44
1	B	394/481 (82%)	368 (93%)	26 (7%)	18	54
All	All	841/962 (87%)	779 (93%)	62 (7%)	15	48

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	69	LEU
1	A	86	LEU
1	A	93	VAL
1	A	149	SER
1	A	153	VAL
1	A	161	LEU
1	A	174	THR
1	A	189	ARG
1	A	192	PRO
1	A	216	VAL
1	A	227	ILE
1	A	252	ILE
1	A	275	PHE
1	A	303	TRP
1	A	341	ASN
1	A	373	CYS
1	A	418	LEU
1	A	433	GLU
1	A	437	LYS
1	A	439	GLN
1	A	440	PHE
1	A	445	ASN
1	A	454	VAL
1	A	458	THR
1	A	461	ASP
1	A	492	LEU
1	A	498	HIS
1	A	502	ASN
1	A	504	VAL
1	A	518	MET
1	A	522	GLN
1	A	526	VAL
1	A	544	PHE
1	A	546	CYS

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Mol	Chain	Res	Type
1	A	548	ASP
1	B	67	GLN
1	B	86	LEU
1	B	93	VAL
1	B	149	SER
1	B	153	VAL
1	B	161	LEU
1	B	189	ARG
1	B	216	VAL
1	B	227	ILE
1	B	252	ILE
1	B	275	PHE
1	B	298	VAL
1	B	303	TRP
1	B	341	ASN
1	B	373	CYS
1	B	418	LEU
1	B	433	GLU
1	B	437	LYS
1	B	439	GLN
1	B	440	PHE
1	B	445	ASN
1	B	454	VAL
1	B	461	ASP
1	B	492	LEU
1	B	498	HIS
1	B	502	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	292	ASN
1	A	306	GLN
1	A	328	HIS
1	A	341	ASN
1	A	365	ASN
1	A	369	HIS
1	A	473	GLN
1	A	522	GLN
1	B	251	ASN
1	B	292	ASN
1	B	306	GLN

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Mol	Chain	Res	Type
1	B	328	HIS
1	B	341	ASN
1	B	344	ASN
1	B	365	ASN
1	B	369	HIS
1	B	473	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

3 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	52A	A	1001	-	4,12,12	0.81	0	3,18,18	0.77	0
2	NAG	A	801	1	14,14,15	0.78	1 (7%)	17,19,21	0.55	0
3	52A	B	2001	-	4,12,12	0.63	0	3,18,18	0.77	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	52A	A	1001	-	-	0/0/21/21	0/1/1/1
2	NAG	A	801	1	-	0/6/23/26	0/1/1/1
3	52A	B	2001	-	-	0/0/21/21	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	NAG	C1-C2	2.21	1.55	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	52A	2	0
3	B	2001	52A	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%)	0.57	26 (5%)	29 28	38, 98, 201, 397	5 (0%)
1	B	459/555 (82%)	1.26	122 (26%)	0 0	52, 151, 269, 371	5 (1%)
All	All	977/1110 (88%)	0.90	148 (15%)	2 2	38, 117, 249, 397	10 (1%)

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	367	ARG	14.9
1	B	365	ASN	10.9
1	B	369	HIS	9.7
1	B	310	VAL	9.2
1	B	370	ARG	8.8
1	B	250	SER	7.8
1	B	321	ILE	7.5
1	B	323	LEU	6.9
1	A	365	ASN	6.6
1	B	364	GLN	6.5
1	A	366	LYS	5.8
1	B	298	VAL	5.7
1	B	274	LEU	5.7
1	B	210	TRP	5.6
1	B	254	LYS	5.6
1	B	284	LEU	5.4
1	B	443	PRO	5.2
1	B	272	VAL	5.1
1	B	303	TRP	5.1
1	B	297	TRP	4.9
1	B	322	THR	4.7
1	B	204	ILE	4.6
1	B	471	LEU	4.6
1	B	271	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	201	MET	4.5
1	B	273	VAL	4.5
1	B	200	ALA	4.5
1	B	492	LEU	4.4
1	B	371	GLN	4.4
1	B	62	GLU	4.4
1	B	379	ILE	4.4
1	B	483	VAL	4.2
1	B	198	ALA	4.0
1	B	299	ALA	4.0
1	B	469	PHE	3.9
1	B	213	VAL	3.9
1	B	434	TYR	3.9
1	A	310	VAL	3.9
1	B	233	GLU	3.9
1	B	368	ASN	3.8
1	B	72	MET	3.8
1	B	247	VAL	3.8
1	B	418	LEU	3.8
1	B	307	GLU	3.8
1	B	44	LEU	3.7
1	B	497	ILE	3.7
1	B	149	SER	3.7
1	B	478	TYR	3.6
1	B	251	ASN	3.6
1	B	486	TRP	3.6
1	A	414	GLN	3.6
1	B	171	TYR	3.5
1	B	494	VAL	3.5
1	B	390	ILE	3.5
1	B	389	LYS	3.5
1	B	320	ALA	3.4
1	B	480	TYR	3.3
1	A	66	ILE	3.3
1	B	350	TRP	3.3
1	B	67	GLN	3.3
1	B	355	TRP	3.2
1	B	172	ALA	3.2
1	B	173	SER	3.2
1	B	63	ASP	3.2
1	B	465	ARG	3.2
1	B	275	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	395	ASN	3.2
1	A	303	TRP	3.2
1	A	434	TYR	3.2
1	B	296	THR	3.1
1	B	354	PHE	3.1
1	A	425	LEU	3.1
1	B	150	TYR	3.0
1	A	247	VAL	3.0
1	B	456	PHE	3.0
1	A	516	ASN	3.0
1	A	520	ASN	2.9
1	B	340	LEU	2.9
1	B	317	ALA	2.9
1	A	109	SER	2.8
1	B	351	PHE	2.8
1	B	507	SER	2.8
1	B	490	LEU	2.8
1	B	46	PRO	2.8
1	B	214	SER	2.8
1	A	494	VAL	2.8
1	B	366	LYS	2.8
1	B	109	SER	2.8
1	B	205	LEU	2.7
1	B	68	ARG	2.7
1	B	202	ALA	2.7
1	B	398	TYR	2.7
1	B	216	VAL	2.7
1	B	263	LEU	2.7
1	B	248	GLY	2.7
1	B	95	ILE	2.7
1	B	96	LEU	2.6
1	B	253	ARG	2.6
1	B	66	ILE	2.6
1	A	471	LEU	2.6
1	B	396	ALA	2.6
1	B	363	LEU	2.6
1	B	337	PHE	2.6
1	B	241	ILE	2.6
1	B	199	LYS	2.6
1	B	89	VAL	2.6
1	A	95	ILE	2.6
1	B	333	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	86	LEU	2.6
1	B	285	ILE	2.6
1	B	470	ASN	2.5
1	B	156	GLN	2.5
1	A	91	LEU	2.5
1	B	237	ARG	2.5
1	B	190	THR	2.5
1	B	336	TYR	2.5
1	B	325	LEU	2.4
1	B	468	VAL	2.4
1	B	359	PHE	2.4
1	B	499	TRP	2.4
1	B	384	TYR	2.3
1	A	323	LEU	2.3
1	B	39	LEU	2.3
1	A	178	LEU	2.3
1	A	454	VAL	2.3
1	B	249	ARG	2.3
1	A	499	TRP	2.2
1	B	264	LEU	2.2
1	B	309	ILE	2.2
1	B	372	VAL	2.2
1	B	281	SER	2.2
1	B	197	GLN	2.2
1	B	300	SER	2.2
1	A	317	ALA	2.2
1	B	222	TYR	2.1
1	A	251	ASN	2.1
1	B	84	TYR	2.1
1	B	79	ILE	2.1
1	B	444	PHE	2.1
1	B	446	PRO	2.1
1	A	89	VAL	2.1
1	B	208	PHE	2.0
1	A	79	ILE	2.0
1	A	517	GLU	2.0
1	B	212	TYR	2.0
1	B	41	LEU	2.0
1	B	91	LEU	2.0
1	B	311	LYS	2.0



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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	A	801	14/15	0.64	0.43	210,210,210,210	0
3	52A	B	2001	12/12	0.93	0.59	94,94,94,94	0
3	52A	A	1001	12/12	0.97	0.33	64,64,64,64	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.