



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 10:41 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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

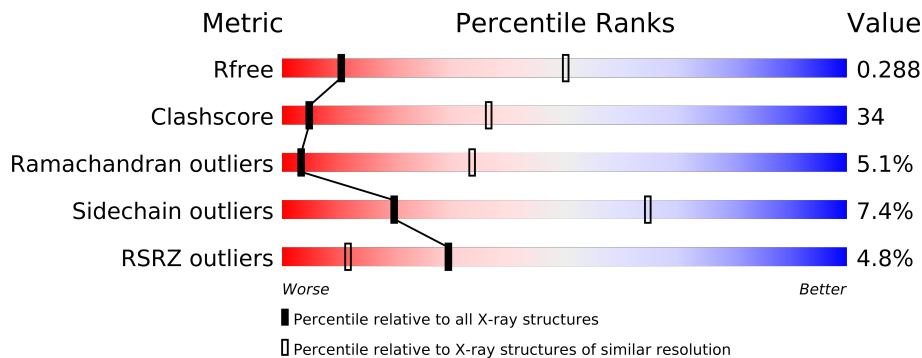
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 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}	66092	1017 (3.52-3.28)
Clashscore	79885	1214 (3.50-3.30)
Ramachandran outliers	78287	1177 (3.50-3.30)
Sidechain outliers	78261	1177 (3.50-3.30)
RSRZ outliers	66119	1017 (3.52-3.28)

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

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

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

Mol	Type	Chain	Res	Geometry	Electron density
2	NAG	A	801	-	X
3	52A	B	2001	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7823 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	518	Total	C	N	O	S	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:

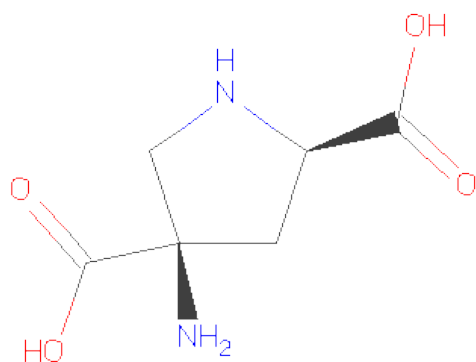
Chain	Residue	Modelled	Actual	Comment	Reference
A	414	GLN	ASN	ENGINEERED	UNP P31422
A	439	GLN	ASN	ENGINEERED	UNP P31422
A	576	LEU	-	CLONING ARTIFACT	UNP P31422
A	577	VAL	-	CLONING ARTIFACT	UNP P31422
A	578	PRO	-	CLONING ARTIFACT	UNP P31422
A	579	ARG	-	CLONING ARTIFACT	UNP P31422
B	414	GLN	ASN	ENGINEERED	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 SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 3 is (2R,4R)-4-AMINOPYRROLIDINE-2,4-DICARBOXYLICACID (three-letter code: 52A) (formula: C₆H₁₀N₂O₄).



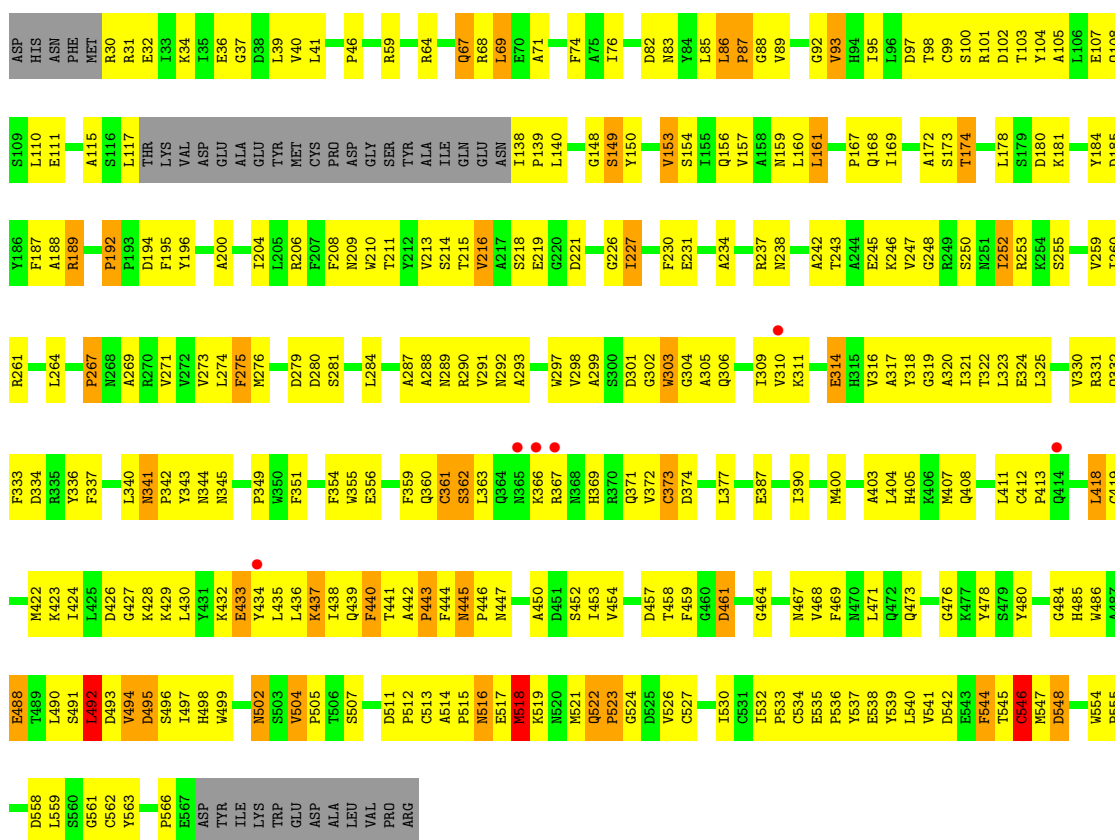
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	6	2	4		
3	B	1	Total	C	N	O	0	0
			12	6	2	4		

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

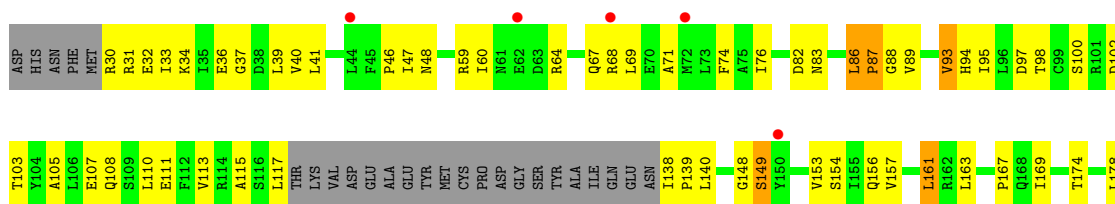
• Molecule 1: Metabotropic glutamate receptor 3

Chain A:



• Molecule 1: Metabotropic glutamate receptor 3

Chain B:





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 3.41Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.224 , 0.284 0.236 , 0.288	Depositor DCC
R_{free} test set	1632 reflections (7.35%)	DCC
Wilson B-factor (Å ²)	122.9	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 114.3	EDS
Estimated twinning fraction	0.043 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 23829 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7823	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4118	0	3994	302	0
1	B	3667	0	3605	227	0
2	A	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	12	0	8	2	0
3	B	12	0	8	1	0
All	All	7823	0	7628	526	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 34.

All (526) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:B:356:GLU:HA	1:B:361:CYS:HB2	1.50	0.92
1:A:538:GLU:HB3	1:A:548:ASP:HA	1.51	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:B:442:ALA:O	1:B:444:PHE:N	2.16	0.79
1:A:216:VAL:HG13	1:A:274:LEU:HD23	1.65	0.79
1:B:366:LYS:HG2	1:B:367:ARG:H	1.46	0.77
1:A:310:VAL:HG13	1:A:317:ALA:HB3	1.66	0.77
1:A:148:GLY:HA3	1:A:154:SER:OG	1.85	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	Distance(Å)	Clash(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:490:LEU:HG	1:A:492:LEU:HD22	1.72	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: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:310:VAL:HG13	1:B:317:ALA:HB3	1.74	0.68
1:B:255:SER:O	1:B:259:VAL:HG23	1.93	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:B:115:ALA:HB1	1:B:140:LEU:O	1.96	0.66
1:A:342:PRO:HD3	1:A:355:TRP:CE3	2.31	0.66
1:B:342:PRO:HD3	1:B:355:TRP:CD2	2.31	0.66
1:B:442:ALA:C	1:B:444:PHE:H	1.96	0.65
1:A:115:ALA:HB1	1:A:140:LEU:O	1.95	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
1:A:341:ASN:ND2	1:A:343:TYR:H	1.93	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:297:TRP:HB2	1:B:320:ALA:HB1	1.81	0.63
1:A:264:LEU:O	1:A:267:PRO:HD3	1.99	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:B:41:LEU:HD22	1:B:400:MET:HG2	1.82	0.62
1:A:490:LEU:HD12	1:A:491:SER:H	1.65	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:B:216:VAL:HB	1:B:245:GLU:HB2	1.83	0.61
1:A:64:ARG:O	1:A:68:ARG:HD2	2.00	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:490:LEU:HD12	1:B:491:SER:H	1.66	0.60
1:B:340:LEU:HD22	1:B:345:ASN:ND2	2.17	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
1:B:298:VAL:O	1:B:298:VAL:HG12	2.04	0.58
1:A:138:ILE:N	1:A:139:PRO:HD2	2.18	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:493:ASP:O	1:A:495:ASP:N	2.36	0.58
1:A:323:LEU:HD23	1:A:468:VAL:HA	1.85	0.58
1:B:178:LEU:HA	1:B:184:TYR:CD1	2.38	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:430:LEU:O	1:B:434:TYR:HB2	2.04	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:A:41:LEU:HD22	1:A:400:MET:HG2	1.85	0.58
1:B:438:ILE:HG23	1:B:453:ILE:HD12	1.85	0.57
1:B:216:VAL:HG13	1:B:274:LEU:CD2	2.33	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: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:108:GLN:O	1:A:111:GLU:HB2	2.05	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:B:227:ILE:HD13	1:B:230:PHE:HB3	1.87	0.57
1:A:555:PRO:HA	1:A:561:GLY:O	2.05	0.57
1:B:252:ILE:HD12	1:B:252:ILE:H	1.70	0.56
1:B:213:VAL:CG1	1:B:271:VAL:HB	2.32	0.56
1:B:138:ILE:N	1:B:139:PRO:HD2	2.20	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:HG13	1:B:424:ILE:O	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
1:B:218:SER:N	1:B:276:MET:HG2	2.22	0.54
1:A:40:VAL:HG13	1:A:92:GLY:C	2.28	0.54
1:A:540:LEU:HG	1:A:546:CYS:SG	2.47	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:271:VAL:HG23	1:A:507:SER:HB2	1.89	0.54
1:A:430:LEU:O	1:A:434:TYR:HB2	2.07	0.54
1:A:260:ILE:HD12	1:A:288:ALA:HB2	1.88	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: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:153:VAL:O	1:A:157:VAL:HG23	2.07	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:B:214:SER:OG	1:B:243:THR:HG22	2.07	0.54
1:A:211:THR:HG22	1:A:527:CYS:SG	2.48	0.54
1:B:366:LYS:HE2	1:B:369:HIS:CD2	2.43	0.53
1:A:274:LEU:HD22	1:A:276:MET:CE	2.38	0.53
1:A:494:VAL:C	1:A:496:SER:N	2.58	0.53
1:A:297:TRP:HB2	1:A:320:ALA:HB1	1.90	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:461:ASP:N	1:B:461:ASP:OD2	2.38	0.53
1:B:74:PHE:HB2	1:B:336:TYR:CD2	2.43	0.53
1:A:519:LYS:HE3	1:A:544:PHE:O	2.08	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:B:453:ILE:HG13	1:B:453:ILE:O	2.08	0.53
1:A:82:ASP:OD2	1:A:83:ASN:N	2.41	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: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:160:LEU:HB2	1:B:163:LEU:HD23	1.92	0.52
1:A:515:PRO:CG	1:A:516:ASN:H	2.21	0.52
1:B:185:ASP:OD2	1:B:185:ASP:N	2.42	0.52
1:A:366:LYS:HE2	1:A:369:HIS:CD2	2.42	0.52
1:A:86:LEU:HD13	1:A:405:HIS:HA	1.91	0.52
1:A:490:LEU:HG	1:A:491:SER:H	1.73	0.52
1:A:341:ASN:HB2	1:A:342:PRO:HD2	1.91	0.52
1:A:252:ILE:HD12	1:A:252:ILE:H	1.73	0.52
1:A:74:PHE:HB2	1:A:336:TYR:CD2	2.45	0.52
1:B:260:ILE:HD11	1:B:288:ALA:HB2	1.92	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:191:VAL:HG12	1:B:392:PHE:CD2	2.45	0.52
1:A:31:ARG:HD2	1:A:349:PRO:HB2	1.92	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:A:32:GLU:OE2	1:A:34:LYS:HE3	2.10	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:B:418:LEU:HD22	1:B:422:MET:HE3	1.93	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: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:B:169:ILE:HD11	1:B:400:MET:SD	2.50	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: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:411:LEU:C	1:B:412:CYS:SG	2.89	0.51
1:B:301:ASP:HA	1:B:323:LEU:O	2.11	0.51
1:B:204:ILE:HG22	1:B:205:LEU:HD23	1.92	0.51
1:B:291:VAL:O	1:B:293:ALA:N	2.44	0.51
1:B:435:LEU:C	1:B:437:LYS:H	2.14	0.51
1:A:372:VAL:HG22	1:A:373:CYS:N	2.23	0.51
1:B:490:LEU:HG	1:B:492:LEU:HD22	1.92	0.51
1:B:205:LEU:HD22	1:B:210:TRP:CE3	2.46	0.51
1:B:108:GLN:O	1:B:111:GLU:HB2	2.10	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:558:ASP:O	1:A:559:LEU:HB2	2.11	0.50
1:A:341:ASN:C	1:A:341:ASN:HD22	2.14	0.50
1:B:274:LEU:HD22	1:B:276:MET:CE	2.42	0.50
1:A:411:LEU:C	1:A:412:CYS:SG	2.90	0.50
1:B:33:ILE:O	1:B:94:HIS:HA	2.12	0.50
1:A:461:ASP:N	1:A:461:ASP:OD2	2.39	0.50
1:A:157:VAL:HG12	1:A:161:LEU:HD22	1.93	0.50
1:A:185:ASP:N	1:A:185:ASP:OD2	2.44	0.50
1:A:59:ARG:HB2	1:A:59:ARG:HH11	1.76	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:359:PHE:O	1:A:360:GLN:HB2	2.12	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:B:195:PHE:HD2	1:B:196:TYR:CE1	2.30	0.50
1:B:362:SER:C	1:B:363:LEU:HD22	2.32	0.49
1:A:322:THR:O	1:A:469:PHE:HB2	2.12	0.49
1:A:261:ARG:O	1:A:264:LEU:HB2	2.11	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:515:PRO:O	1:A:517:GLU:N	2.46	0.49
1:A:457:ASP:HB2	1:A:461:ASP:OD2	2.13	0.49
1:A:64:ARG:HG2	1:A:68:ARG:CZ	2.42	0.49
1:A:301:ASP:O	1:A:304:GLY:N	2.46	0.49
1:A:522:GLN:HE21	1:A:522:GLN:HA	1.77	0.49
1:B:437:LYS:CE	1:B:438:ILE:H	2.25	0.49
1:A:437:LYS:CA	1:A:437:LYS:HE3	2.30	0.49
1:A:260:ILE:HD11	1:A:288:ALA:HB2	1.94	0.49
1:A:117:LEU:N	1:A:117:LEU:HD12	2.26	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:544:PHE:N	1:A:544:PHE:CD1	2.81	0.48
1:A:341:ASN:ND2	1:A:341:ASN:C	2.66	0.48
1:A:314:GLU:CD	1:A:314:GLU:H	2.15	0.48
1:B:192:PRO:HG3	1:B:464:GLY:HA2	1.95	0.48
1:B:372:VAL:HG22	1:B:373:CYS:N	2.27	0.48
1:A:306:GLN:HB2	1:A:309:ILE:HD12	1.94	0.48
1:A:159:ASN:HB3	1:B:163:LEU:HD11	1.95	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:187:PHE:HE2	1:B:189:ARG:HD2	1.78	0.48
1:A:355:TRP:CE2	1:A:359:PHE:CE1	3.01	0.48
1:B:46:PRO:HD3	1:B:149:SER:HB2	1.95	0.48
1:B:30:ARG:HG2	1:B:30:ARG:HH11	1.78	0.48
1:B:330:VAL:HG13	1:B:444:PHE:HB3	1.94	0.48
1:A:445:ASN:ND2	1:A:447:ASN:O	2.47	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:563:TYR:CD1	1:A:563:TYR:O	2.66	0.48
1:A:279:ASP:OD1	1:A:280:ASP:N	2.46	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:554:TRP:O	1:A:562:CYS:HA	2.14	0.48
1:A:426:ASP:O	1:A:427:GLY:C	2.52	0.48
1:A:36:GLU:HG2	1:A:37:GLY:N	2.28	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:440:PHE:CD2	1:B:453:ILE:HG22	2.49	0.48
1:B:289:ASN:HA	1:B:316:VAL:HG21	1.96	0.48
1:A:486:TRP:CH2	1:A:488:GLU:HA	2.49	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:B:331:ARG:O	1:B:334:ASP:HB2	2.13	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:535:GLU:C	1:A:537:TYR:H	2.18	0.47
1:A:276:MET:HB2	1:A:281:SER:OG	2.14	0.47
1:B:284:LEU:C	1:B:284:LEU:HD13	2.34	0.47
1:A:492:LEU:HD23	1:A:492:LEU:N	2.30	0.47
1:A:138:ILE:N	1:A:139:PRO:CD	2.78	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:324:GLU:HG3	1:A:325:LEU:N	2.29	0.47
1:B:324:GLU:HG3	1:B:325:LEU:N	2.29	0.47
1:B:445:ASN:ND2	1:B:447:ASN:O	2.47	0.47
1:A:403:ALA:HB2	1:A:434:TYR:CD1	2.50	0.47
1:A:514:ALA:CB	1:A:518:MET:HG3	2.32	0.47
1:A:484:GLY:HA3	1:A:492:LEU:HA	1.97	0.47
1:A:187:PHE:CE2	1:A:189:ARG:HB3	2.49	0.47
1:B:337:PHE:CD1	1:B:340:LEU:HD12	2.48	0.47
1:B:227:ILE:O	1:B:231:GLU:HG3	2.15	0.47
1:B:59:ARG:HH11	1:B:59:ARG:HB2	1.79	0.47
1:A:71:ALA:HA	1:A:333:PHE:CE1	2.49	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:219:GLU:HB2	1:A:248:GLY:HA2	1.97	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:A:303:TRP:C	1:A:303:TRP:CD1	2.87	0.47
1:B:456:PHE:HB3	1:B:460:GLY:HA2	1.97	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:494:VAL:C	1:B:496:SER:N	2.68	0.47
1:B:490:LEU:CD1	1:B:491:SER:H	2.27	0.47
1:A:40:VAL:HG13	1:A:92:GLY:O	2.15	0.47
1:A:102:ASP:OD2	1:A:103:THR:N	2.41	0.47
1:A:540:LEU:HB3	1:A:542:ASP:O	2.15	0.46
1:A:227:ILE:O	1:A:231:GLU:HG3	2.16	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:B:467:ASN:HB3	1:B:469:PHE:HE1	1.79	0.46
1:A:497:ILE:HG21	1:A:499:TRP:CZ2	2.50	0.46
1:A:519:LYS:HG2	1:A:532:ILE:O	2.16	0.46
1:B:441:THR:O	1:B:442:ALA:C	2.54	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: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:B:341:ASN:HB2	1:B:342:PRO:HD2	1.98	0.46
1:A:310:VAL:HG21	1:A:471:LEU:HD22	1.97	0.46
1:A:86:LEU:HD13	1:A:405:HIS:CA	2.46	0.46
1:A:211:THR:HG23	1:A:238:ASN:O	2.16	0.46
1:A:491:SER:C	1:A:492:LEU:CD2	2.84	0.46
1:B:195:PHE:HD2	1:B:196:TYR:HE1	1.64	0.46
1:B:107:GLU:O	1:B:110:LEU:HB2	2.16	0.46
1:A:492:LEU:N	1:A:492:LEU:CD2	2.79	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:B:287:ALA:HA	1:B:290:ARG:CZ	2.44	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: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
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:539:TYR:HD1	1:A:540:LEU:N	2.15	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: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:167:PRO:HG3	1:B:430:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:374:ASP:O	1:B:377:LEU:HB2	2.17	0.45
1:B:86:LEU:HD13	1:B:405:HIS:CA	2.46	0.45
1:A:435:LEU:O	1:A:437:LYS:N	2.49	0.45
1:A:361:CYS:HB3	1:A:362:SER:H	1.39	0.45
1:B:86:LEU:HD13	1:B:405:HIS:HA	1.99	0.45
1:B:110:LEU:HA	1:B:110:LEU:HD12	1.77	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:B:341:ASN:C	1:B:341:ASN:ND2	2.71	0.44
1:B:138:ILE:N	1:B:139:PRO:CD	2.79	0.44
1:A:387:GLU:HB3	1:A:390:ILE:HG12	1.99	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:30:ARG:HH11	1:A:30:ARG:HG2	1.81	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:B:178:LEU:O	1:B:181:LYS:NZ	2.48	0.44
1:A:355:TRP:CE2	1:A:359:PHE:HE1	2.36	0.44
1:B:97:ASP:OD1	1:B:98:THR:N	2.50	0.44
1:A:323:LEU:HD21	1:A:468:VAL:HG22	1.99	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:B:442:ALA:HA	1:B:443:PRO:HD2	1.71	0.44
1:A:490:LEU:HG	1:A:492:LEU:CD2	2.45	0.44
1:B:86:LEU:HD13	1:B:405:HIS:HB2	2.00	0.44
1:B:457:ASP:HB2	1:B:461:ASP:OD2	2.17	0.44
1:A:374:ASP:O	1:A:377:LEU:HB2	2.18	0.44
1:A:287:ALA:HA	1:A:290:ARG:CZ	2.47	0.44
1:A:473:GLN:NE2	1:A:476:GLY:N	2.66	0.44
1:B:332:GLN:N	1:B:332:GLN:OE1	2.40	0.44
1:B:446:PRO:HG2	1:B:447:ASN:H	1.81	0.43
1:A:291:VAL:O	1:A:293:ALA:N	2.51	0.43
1:A:440:PHE:CD2	1:A:453:ILE:HG22	2.53	0.43
1:A:515:PRO:HG2	1:A:516:ASN:N	2.24	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:366:LYS:HG2	1:B:367:ARG:N	2.24	0.43
1:B:289:ASN:CB	1:B:316:VAL:HG21	2.48	0.43
1:A:499:TRP:CG	1:A:505:PRO:HD3	2.53	0.43
1:B:220:GLY:O	1:B:222:TYR:N	2.50	0.43
1:B:187:PHE:CE2	1:B:189:ARG:HB3	2.54	0.43
1:A:459:PHE:HB2	1:A:461:ASP:OD2	2.18	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:150:TYR:HB2	1:A:153:VAL:HG12	2.00	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: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:B:174:THR:O	1:B:193:PRO:HA	2.19	0.43
1:A:540:LEU:CD1	1:A:559:LEU:HB3	2.49	0.43
1:A:362:SER:C	1:A:363:LEU:HD22	2.39	0.43
1:B:47:ILE:HD13	1:B:350:TRP:CE3	2.54	0.43
1:A:301:ASP:O	1:A:302:GLY:C	2.57	0.43
1:A:554:TRP:CD2	1:A:555:PRO:HD2	2.54	0.43
1:A:69:LEU:CD2	1:A:69:LEU:C	2.87	0.43
1:A:511:ASP:HB3	1:A:512:PRO:HD2	2.00	0.43
1:B:261:ARG:O	1:B:264:LEU:HB2	2.19	0.43
1:B:208:PHE:O	1:B:210:TRP:N	2.52	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:196:TYR:CD1	1:A:196:TYR:N	2.86	0.43
1:B:359:PHE:O	1:B:360:GLN:HB2	2.19	0.42
1:A:418:LEU:HD22	1:A:422:MET:HE3	2.00	0.42
1:A:337:PHE:CD1	1:A:340:LEU:HD12	2.54	0.42
1:B:400:MET:O	1:B:403:ALA:HB3	2.19	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:A:157:VAL:HG12	1:A:161:LEU:CD2	2.49	0.42
1:B:389:LYS:O	1:B:392:PHE:N	2.52	0.42
1:B:59:ARG:NH1	1:B:59:ARG:CB	2.82	0.42
1:A:517:GLU:HG3	1:A:534:CYS:H	1.84	0.42
1:B:484:GLY:HA3	1:B:492:LEU:HA	2.00	0.42
1:A:97:ASP:OD1	1:A:98:THR:N	2.52	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:195:PHE:HD2	1:A:196:TYR:CE1	2.36	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:B:71:ALA:HA	1:B:333:PHE:CE1	2.55	0.42
1:B:473:GLN:NE2	1:B:476:GLY:N	2.64	0.42
1:A:196:TYR:HD1	1:A:196:TYR:N	2.18	0.42
1:B:187:PHE:CD2	1:B:188:ALA:N	2.88	0.42
1:A:167:PRO:HG3	1:A:430:LEU:HD23	2.01	0.42
1:A:513:CYS:HB3	1:A:518:MET:HB2	2.00	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:B:219:GLU:HB2	1:B:247:VAL:O	2.19	0.42
1:B:303:TRP:CD1	1:B:322:THR:HG21	2.54	0.42
1:A:227:ILE:HD13	1:A:227:ILE:HA	1.82	0.42
1:A:107:GLU:O	1:A:110:LEU:HB2	2.19	0.42
1:B:400:MET:HA	1:B:400:MET:HE3	2.02	0.42
1:A:215:THR:HG22	1:A:273:VAL:HB	2.02	0.42
1:B:412:CYS:HA	1:B:413:PRO:HD2	1.66	0.42
1:A:426:ASP:HB3	1:A:429:LYS:HB2	2.02	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:B:341:ASN:OD1	1:B:344:ASN:ND2	2.53	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:541:VAL:HG23	1:A:547:MET:CB	2.50	0.41
1:A:523:PRO:HG2	1:A:524:GLY:H	1.84	0.41
1:B:40:VAL:HG12	1:B:41:LEU:N	2.35	0.41
1:B:305:ALA:HA	1:B:480:TYR:CE2	2.55	0.41
1:B:215:THR:O	1:B:245:GLU:N	2.41	0.41
1:A:41:LEU:HD12	1:A:76:ILE:HD11	2.02	0.41
1:A:468:VAL:HG23	1:A:485:HIS:HA	2.02	0.41
1:B:356:GLU:OE1	1:B:363:LEU:HB2	2.21	0.41
1:B:205:LEU:HA	1:B:210:TRP:HE3	1.86	0.41
1:A:219:GLU:HB2	1:A:247:VAL:O	2.20	0.41
1:B:355:TRP:CE2	1:B:359:PHE:CE1	3.08	0.41
1:B:251:ASN:HD22	1:B:255:SER:HB3	1.85	0.41
1:A:486:TRP:O	1:A:486:TRP:HE3	2.03	0.41
1:A:67:GLN:HB3	1:A:390:ILE:HD11	2.02	0.41
1:B:40:VAL:HG21	1:B:140:LEU:HD22	2.02	0.41
1:B:459:PHE:HB2	1:B:461:ASP:OD2	2.21	0.41
1:A:305:ALA:HA	1:A:480:TYR:CD2	2.56	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:331:ARG:O	1:A:334:ASP:HB2	2.21	0.41
1:B:328:HIS:HA	1:B:329:PRO:HD2	1.87	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:B:435:LEU:O	1:B:437:LYS:N	2.51	0.41
1:A:310:VAL:HG13	1:A:317:ALA:CB	2.45	0.41
1:B:68:ARG:NH1	1:B:149:SER:OG	2.54	0.41
1:A:208:PHE:HB2	1:A:210:TRP:CE3	2.56	0.41
1:A:515:PRO:CG	1:A:516:ASN:N	2.84	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:356:GLU:OE1	1:A:363:LEU:HB2	2.20	0.40
1:A:215:THR:O	1:A:245:GLU:N	2.46	0.40
1:A:40:VAL:HA	1:A:92:GLY:O	2.21	0.40
1:A:214:SER:OG	1:A:243:THR:HG22	2.21	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:504:VAL:HA	1:A:505:PRO:HD3	1.76	0.40
1:A:351:PHE:O	1:A:354:PHE:HB3	2.21	0.40
1:B:169:ILE:HG12	1:B:434:TYR:OH	2.22	0.40
1:A:341:ASN:ND2	1:A:341:ASN:O	2.54	0.40
1:B:399:ALA:HB1	1:B:434:TYR:HE1	1.85	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:181:LYS:CE	1:B:459:PHE:O	2.53	0.40
1:B:426:ASP:CG	1:B:429:LYS:HB2	2.42	0.40
1:B:428:LYS:O	1:B:432:LYS:HG2	2.21	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%)	415 (81%)	71 (14%)	28 (5%)	3	31
1	B	455/555 (82%)	368 (81%)	66 (14%)	21 (5%)	4	37
All	All	969/1110 (87%)	783 (81%)	137 (14%)	49 (5%)	3	33

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
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

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Mol	Chain	Res	Type
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%)	17	60
1	B	394/481 (82%)	368 (93%)	26 (7%)	24	70
All	All	841/962 (87%)	779 (93%)	62 (7%)	20	65

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 chains in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	-	12,12,12	0.85	0	18,18,18	1.38	2 (11%)
2	NAG	A	801	1	12,14,15	0.52	0	15,19,21	0.58	0
3	52A	B	2001	-	12,12,12	0.84	0	18,18,18	1.37	2 (11%)

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	-	-	0/10/21/21	0/1/1/1
2	NAG	A	801	1	-	0/6/23/26	0/1/1/1
3	52A	B	2001	-	-	0/10/21/21	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2001	52A	CA-CB1-CG1	-3.63	101.73	104.89
3	A	1001	52A	CA-CB1-CG1	-3.62	101.73	104.89
3	A	1001	52A	OXT-C-CA	2.59	119.79	113.70
3	B	2001	52A	OXT-C-CA	2.45	119.45	113.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	518/555 (93%)	0.24	6 (1%) 75 39	38, 98, 201, 397	5 (0%)
1	B	459/555 (82%)	0.62	41 (8%) 10 5	52, 151, 269, 371	5 (1%)
All	All	977/1110 (88%)	0.42	47 (4%) 29 12	38, 117, 249, 397	10 (1%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	367	ARG	10.9
1	B	365	ASN	5.8
1	B	369	HIS	5.0
1	B	310	VAL	4.7
1	B	370	ARG	4.6
1	B	321	ILE	4.5
1	B	323	LEU	4.1
1	B	364	GLN	4.1
1	B	274	LEU	3.7
1	B	254	LYS	3.5
1	A	365	ASN	3.3
1	B	443	PRO	3.3
1	A	366	LYS	3.3
1	B	284	LEU	3.1
1	B	298	VAL	3.1
1	B	492	LEU	3.0
1	B	201	MET	3.0
1	B	62	GLU	2.9
1	B	250	SER	2.8
1	B	210	TRP	2.7
1	B	272	VAL	2.7
1	B	303	TRP	2.6
1	B	434	TYR	2.6
1	B	271	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	478	TYR	2.6
1	B	273	VAL	2.5
1	B	389	LYS	2.5
1	B	465	ARG	2.5
1	B	44	LEU	2.4
1	B	72	MET	2.4
1	B	307	GLU	2.4
1	B	379	ILE	2.4
1	A	414	GLN	2.4
1	B	322	THR	2.4
1	B	204	ILE	2.3
1	B	471	LEU	2.3
1	B	297	TRP	2.3
1	B	497	ILE	2.2
1	B	299	ALA	2.2
1	B	200	ALA	2.2
1	B	150	TYR	2.1
1	B	68	ARG	2.1
1	B	483	VAL	2.1
1	B	418	LEU	2.1
1	A	310	VAL	2.0
1	B	480	TYR	2.0
1	A	434	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	A	801	14/15	0.41	3.72	210,210,210,210	0
3	52A	B	2001	12/12	0.54	0.76	94,94,94,94	0
3	52A	A	1001	12/12	0.30	0.47	64,64,64,64	0

6.5 Other polymers ⓘ

There are no such residues in this entry.