



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:22 PM UTC

PDB ID : 2E4X / pdb_00002e4x
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

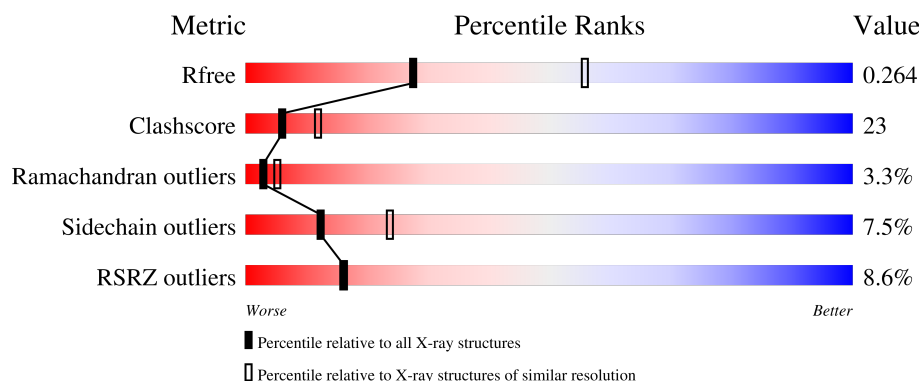
1 Overall quality at a glance

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}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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

2 Entry composition

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:

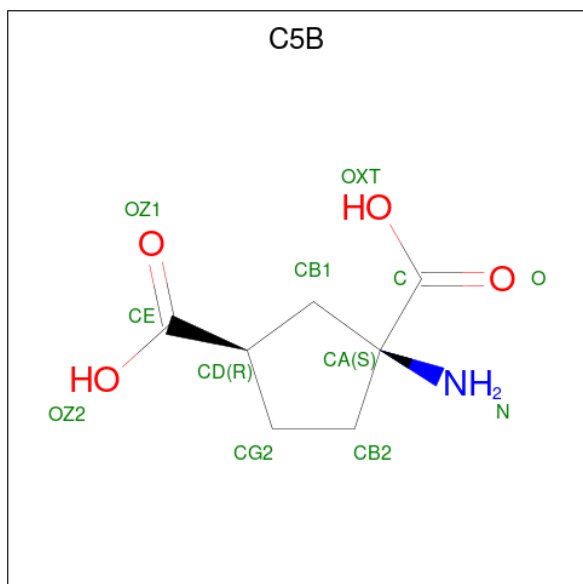
Chain	Residue	Modelled	Actual	Comment	Reference
A	414	GLN	ASN	engineered mutation	UNP P31422
A	439	GLN	ASN	engineered mutation	UNP P31422
A	576	LEU	-	cloning artifact	UNP P31422
A	577	VAL	-	cloning artifact	UNP P31422
A	578	PRO	-	cloning artifact	UNP P31422
A	579	ARG	-	cloning artifact	UNP P31422
B	414	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 (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 3 is (1S,3R)-1-AMINOCYCLOPENTANE-1,3-DICARBOXYLIC ACID (CCD ID: C5B) (formula: C₇H₁₁NO₄).



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		

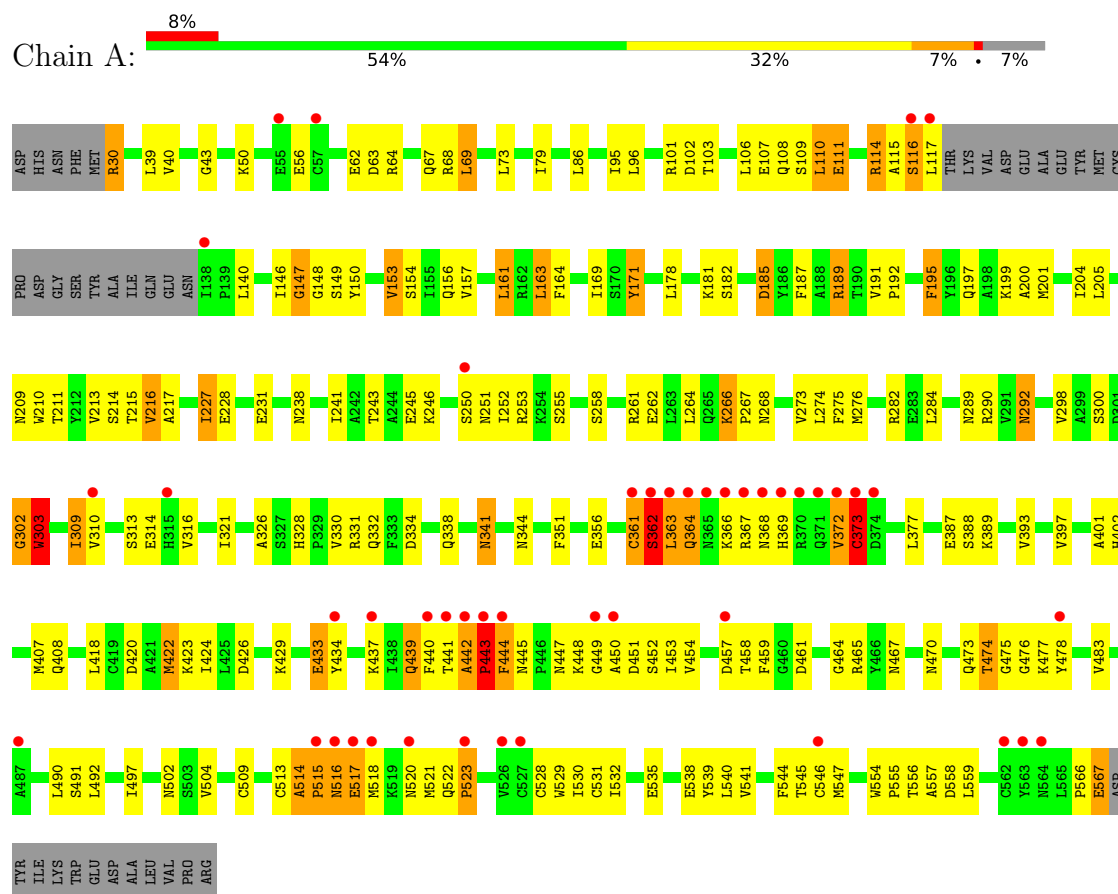
- Molecule 4 is water.

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

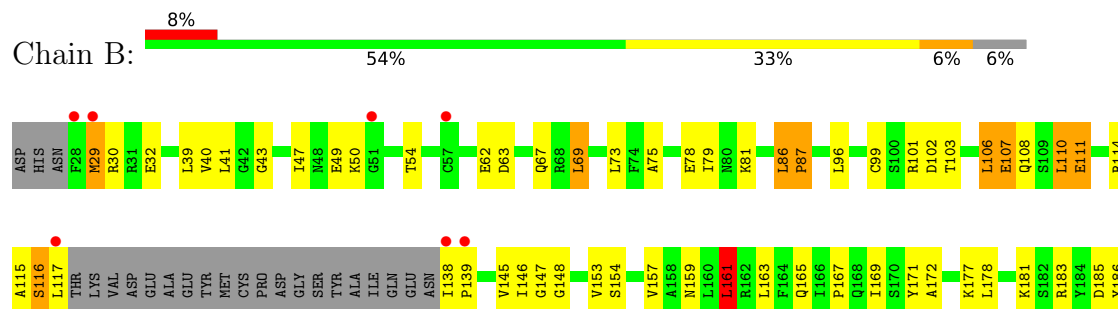
3 Residue-property plots [i](#)

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

• Molecule 1: Metabotropic glutamate receptor 3



• Molecule 1: Metabotropic glutamate receptor 3





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.62Å 97.14Å 108.16Å 90.00° 92.92° 90.00°	Depositor
Resolution (Å)	20.00 – 2.75 20.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.75) 99.6 (20.00-2.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.76Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.225 , 0.265 0.225 , 0.264	Depositor DCC
R_{free} test set	3201 reflections (7.11%)	wwPDB-VP
Wilson B-factor (Å ²)	65.4	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 66.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, C5B

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	0.50	0/4212	1.00	20/5704 (0.4%)
1	B	0.49	0/4232	1.01	23/5730 (0.4%)
All	All	0.50	0/8444	1.00	43/11434 (0.4%)

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 (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	458	THR	N-CA-C	-9.67	100.05	112.23
1	A	147	GLY	N-CA-C	9.49	122.25	110.96
1	B	147	GLY	N-CA-C	9.07	121.75	110.96
1	B	509	CYS	N-CA-C	8.46	120.12	111.07
1	B	458	THR	N-CA-C	-8.34	102.55	112.89
1	B	488	GLU	N-CA-C	-7.54	105.24	114.75
1	B	373	CYS	N-CA-C	7.37	121.45	109.59
1	B	433	GLU	N-CA-C	-7.06	95.77	110.80
1	A	373	CYS	N-CA-C	6.77	120.48	109.59
1	A	149	SER	N-CA-C	-6.63	102.62	111.96
1	B	388	SER	N-CA-C	6.41	119.08	111.33
1	A	433	GLU	N-CA-C	-6.34	97.29	110.80
1	A	114	ARG	N-CA-C	-6.22	104.56	111.71
1	B	183	ARG	N-CA-C	-6.15	106.42	114.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	266	LYS	CA-C-N	6.06	126.23	119.32
1	B	266	LYS	C-N-CA	6.06	126.23	119.32
1	A	62	GLU	N-CA-C	5.99	118.30	111.11
1	B	40	VAL	N-CA-C	5.98	116.48	108.11
1	B	545	THR	N-CA-C	5.91	119.04	109.40
1	A	195	PHE	N-CA-C	-5.90	104.92	111.71
1	B	161	LEU	N-CA-C	5.90	118.49	111.71
1	A	545	THR	N-CA-C	5.86	119.03	109.24
1	A	388	SER	N-CA-C	5.84	118.39	111.33
1	B	442	ALA	CA-C-N	5.83	127.12	119.84
1	B	442	ALA	C-N-CA	5.83	127.12	119.84
1	B	62	GLU	N-CA-C	5.71	117.99	111.02
1	B	81	LYS	N-CA-C	-5.52	106.54	113.72
1	B	303	TRP	N-CA-C	-5.43	104.77	111.40
1	A	442	ALA	CA-C-N	5.42	126.62	119.84
1	A	442	ALA	C-N-CA	5.42	126.62	119.84
1	A	40	VAL	N-CA-C	5.42	115.70	108.11
1	B	276	MET	N-CA-C	5.32	117.77	109.52
1	B	87	PRO	N-CA-C	-5.18	102.46	111.32
1	A	302	GLY	N-CA-C	-5.17	106.53	112.73
1	B	145	VAL	N-CA-C	5.16	115.34	108.11
1	B	360	GLN	N-CA-C	-5.10	104.39	111.52
1	B	389	LYS	N-CA-C	5.05	119.53	113.17
1	A	182	SER	N-CA-C	-5.04	106.97	113.23
1	A	351	PHE	N-CA-C	5.04	116.77	111.28
1	A	303	TRP	N-CA-C	-5.04	104.79	112.04
1	A	514	ALA	N-CA-C	-5.03	103.14	110.08
1	A	266	LYS	CA-C-N	5.02	126.11	119.84
1	A	266	LYS	C-N-CA	5.02	126.11	119.84

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	186	0
1	B	4137	0	4012	192	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	6	0
4	B	78	0	0	9	0
All	All	8478	0	8049	371	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 23.

All (371) 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: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
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:341:ASN:C	1:B:341:ASN:HD22	1.96	0.73
1:B:50:LYS:HG3	1:B:101:ARG:HD3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:514:ALA:HB2	1:A:518:MET:HE2	1.71	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:A:341:ASN:C	1:A:341:ASN:HD22	1.99	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:514:ALA:H	1:B:518:MET:CE	2.04	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:A:217:ALA:HB2	1:A:227:ILE:HG13	1.76	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: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: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:29:MET:HE3	1:B:29:MET:O	1.97	0.65
1:B:440:PHE:HE2	1:B:448:LYS:HB3	1.62	0.65
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:ILE:HG12	1:B:434:TYR:OH	1.98	0.63
1:A:541:VAL:HG21	1:A:547:MET:HE3	1.80	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: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:A:441:THR:O	1:A:442:ALA:C	2.43	0.61
1:B:535:GLU:OE2	1:B:535:GLU:HA	2.00	0.61
1:B:558:ASP:O	1:B:559:LEU:HB2	2.01	0.61
1:B:441:THR:O	1:B:442:ALA:C	2.43	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:514:ALA:CB	1:A:518:MET:HE2	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:B:514:ALA:H	1:B:518:MET:HE3	1.67	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: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: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:449:GLY:C	1:B:451:ASP:H	2.14	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:A:514:ALA:H	1:A:518:MET:HE3	1.72	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:516:ASN:C	1:A:517:GLU:HG3	2.34	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:C	1:A:445:ASN:H	2.19	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:514:ALA:H	1:B:518:MET:HE2	1.74	0.50
1:A:274:LEU:HD13	1:A:276:MET:HE2	1.93	0.50
1:B:310:VAL:HG12	1:B:314:GLU:HA	1.94	0.50
1:A:201:MET:HE2	1:A:273:VAL:HG13	1.92	0.50
1:A:473:GLN:HE21	1:A:476:GLY:C	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:115:ALA:C	1:B:117:LEU:H	2.21	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:B:284:LEU:C	1:B:284:LEU:HD13	2.37	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:69:LEU:HD22	1:A:69:LEU:C	2.37	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:A:108:GLN:O	1:A:111:GLU:HB2	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:VAL:CG2	1:A:373:CYS:N	2.78	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
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: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:116:SER:C	1:A:117:LEU:HD12	2.42	0.45
1:A:310:VAL:CG1	1:A:314:GLU:HA	2.46	0.45
1:A:558:ASP:C	1:A:558:ASP:OD2	2.57	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:366:LYS:CG	1:B:367:ARG:H	2.25	0.45
1:A:475:GLY:C	1:A:477:LYS:H	2.25	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:B:513:CYS:HA	1:B:518:MET:HE3	1.98	0.45
1:A:169:ILE:CG1	1:A:434:TYR:OH	2.65	0.45
1:A:252:ILE:O	1:A:253:ARG:C	2.59	0.45
1:A:473:GLN:O	1:A:474:THR:C	2.60	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:A:387:GLU:CD	1:A:389:LYS:H	2.24	0.44
1:B:96:LEU:HD13	1:B:108:GLN:HB3	1.98	0.44
1:B:514:ALA:HB2	1:B:518:MET:HE2	1.98	0.44
1:B:359:PHE:HE2	1:B:383:ASN:HD22	1.65	0.44
1:B:473:GLN:O	1:B:474:THR:C	2.60	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:165:GLN:CD	4:B:2031:HOH:O	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:PHE:O	1:B:441:THR:C	2.61	0.44
1:A:209:ASN:ND2	2:A:801:NAG:H82	2.32	0.44
1:B:264:LEU:C	1:B:266:LYS:H	2.26	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:303:TRP:CD1	1:A:303:TRP:C	2.95	0.43
1:A:490:LEU:HG	1:A:492:LEU:HD22	2.00	0.43
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:A:449:GLY:C	1:A:451:ASP:H	2.26	0.43
1:B:493:ASP:O	1:B:493:ASP:CG	2.61	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:109:SER:C	1:A:111:GLU:N	2.73	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:A:558:ASP:O	1:A:559:LEU:HB2	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:171:TYR:CD1	1:B:171:TYR:C	2.95	0.43
1:B:257:ASP:OD2	1:B:290:ARG:NH1	2.52	0.43
1:A:195:PHE:CZ	1:A:199:LYS:NZ	2.86	0.43
1:A:341:ASN:ND2	1:A:341:ASN:C	2.70	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:B:268:ASN:HD22	1:B:509:CYS:C	2.26	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:442:ALA:C	1:B:444:PHE:N	2.77	0.43
1:B:356:GLU:CD	1:B:366:LYS:HB2	2.43	0.42
1:B:374:ASP:HB3	1:B:377:LEU:HD22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:408:GLN:CD	1:B:408:GLN:C	2.87	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:451:ASP:OD1	1:A:453:ILE:HG12	2.20	0.42
1:A:556:THR:O	1:A:557:ALA:C	2.63	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
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:B:449:GLY:C	1:B:451:ASP:N	2.78	0.41
1:A:300:SER:C	1:A:302:GLY:N	2.79	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:B:290:ARG:C	1:B:292:ASN:H	2.28	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:A:426:ASP:CG	1:A:429:LYS:HB2	2.46	0.41
1:A:442:ALA:O	1:A:443:PRO:C	2.63	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:A:450:ALA:O	1:A:451:ASP:C	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:290:ARG:C	1:A:292:ASN:H	2.28	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:B:276:MET:HE1	1:B:284:LEU:HB2	2.04	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%)	3	5
1	B	516/555 (93%)	443 (86%)	56 (11%)	17 (3%)	3	5
All	All	1030/1110 (93%)	889 (86%)	107 (10%)	34 (3%)	3	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
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%)	412 (92%)	35 (8%)	11	21
1	B	449/481 (93%)	417 (93%)	32 (7%)	13	25
All	All	896/962 (93%)	829 (92%)	67 (8%)	12	24

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	39	LEU
1	A	69	LEU
1	A	73	LEU
1	A	86	LEU
1	A	106	LEU
1	A	110	LEU
1	A	111	GLU
1	A	153	VAL
1	A	161	LEU
1	A	163	LEU
1	A	185	ASP
1	A	189	ARG
1	A	216	VAL
1	A	227	ILE
1	A	275	PHE
1	A	284	LEU
1	A	292	ASN
1	A	303	TRP
1	A	309	ILE
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	443	PRO
1	A	454	VAL
1	A	491	SER
1	A	517	GLU
1	A	567	GLU

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Mol	Chain	Res	Type
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	279	ASP
1	B	309	ILE
1	B	341	ASN
1	B	373	CYS
1	B	377	LEU
1	B	381	SER
1	B	408	GLN
1	B	418	LEU
1	B	422	MET
1	B	439	GLN
1	B	443	PRO
1	B	454	VAL
1	B	491	SER
1	B	517	GLU
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 (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	108	GLN
1	A	251	ASN
1	A	292	ASN
1	A	341	ASN
1	A	365	ASN

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Mol	Chain	Res	Type
1	A	473	GLN
1	A	485	HIS
1	A	520	ASN
1	A	522	GLN
1	B	108	GLN
1	B	251	ASN
1	B	292	ASN
1	B	306	GLN
1	B	341	ASN
1	B	365	ASN
1	B	369	HIS
1	B	473	GLN
1	B	485	HIS
1	B	522	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	C5B	B	2001	-	10,12,12	1.05	0	14,18,18	1.56	3 (21%)
3	C5B	A	1001	-	10,12,12	1.00	0	14,18,18	1.53	3 (21%)
2	NAG	A	801	1	14,14,15	0.73	0	17,19,21	0.64	0
2	NAG	B	802	1	14,14,15	0.61	0	17,19,21	0.68	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	C5B	B	2001	-	-	0/10/21/21	0/1/1/1
3	C5B	A	1001	-	-	1/10/21/21	0/1/1/1
2	NAG	A	801	1	-	2/6/23/26	0/1/1/1
2	NAG	B	802	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	C5B	CB2-CA-CB1	3.50	108.45	102.73
3	B	2001	C5B	CB2-CA-CB1	3.42	108.34	102.73
3	B	2001	C5B	OZ2-CE-CD	2.21	119.90	114.16
3	B	2001	C5B	OXT-C-CA	2.15	119.44	113.69
3	A	1001	C5B	OXT-C-CA	2.14	119.39	113.69
3	A	1001	C5B	OZ2-CE-CD	2.06	119.50	114.16

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	NAG	C8-C7-N2-C2
2	A	801	NAG	O7-C7-N2-C2
2	B	802	NAG	C8-C7-N2-C2
2	B	802	NAG	O7-C7-N2-C2
3	A	1001	C5B	CG2-CD-CE-OZ1

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, 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%)	0.37	46 (8%)	15 15	33, 66, 105, 141	0
1	B	520/555 (93%)	0.37	43 (8%)	17 18	35, 68, 107, 141	0
All	All	1038/1110 (93%)	0.37	89 (8%)	16 16	33, 67, 106, 141	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	516	ASN	9.0
1	B	516	ASN	7.3
1	A	361	CYS	5.9
1	A	443	PRO	5.6
1	A	138	ILE	5.3
1	B	443	PRO	4.7
1	A	478	TYR	4.4
1	B	361	CYS	4.3
1	A	366	LYS	4.2
1	A	441	THR	4.1
1	A	450	ALA	4.1
1	B	440	PHE	4.0
1	A	369	HIS	4.0
1	B	138	ILE	3.9
1	A	434	TYR	3.8
1	B	567	GLU	3.7
1	B	450	ALA	3.7
1	A	250	SER	3.6
1	A	373	CYS	3.5
1	B	57	CYS	3.5
1	A	368	ASN	3.4
1	A	370	ARG	3.4
1	A	116	SER	3.4
1	B	449	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	478	TYR	3.3
1	A	365	ASN	3.3
1	B	373	CYS	3.2
1	A	363	LEU	3.2
1	A	449	GLY	3.1
1	B	434	TYR	3.1
1	A	487	ALA	3.1
1	A	520	ASN	3.1
1	A	517	GLU	3.1
1	A	371	GLN	3.1
1	B	441	THR	3.1
1	A	457	ASP	3.0
1	A	523	PRO	3.0
1	B	372	VAL	3.0
1	B	370	ARG	3.0
1	B	363	LEU	2.9
1	A	374	ASP	2.8
1	A	57	CYS	2.8
1	A	55	GLU	2.8
1	B	369	HIS	2.7
1	B	343	TYR	2.7
1	B	251	ASN	2.7
1	B	318	TYR	2.7
1	B	517	GLU	2.7
1	A	515	PRO	2.7
1	A	362	SER	2.7
1	B	366	LYS	2.6
1	B	515	PRO	2.6
1	A	562	CYS	2.6
1	A	310	VAL	2.6
1	B	566	PRO	2.6
1	B	310	VAL	2.5
1	A	440	PHE	2.5
1	B	371	GLN	2.5
1	B	527	CYS	2.5
1	A	117	LEU	2.5
1	B	526	VAL	2.5
1	B	29	MET	2.4
1	B	551	PRO	2.4
1	A	546	CYS	2.4
1	A	564	ASN	2.4
1	A	367	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	28	PHE	2.4
1	B	444	PHE	2.4
1	B	368	ASN	2.3
1	B	51	GLY	2.3
1	A	444	PHE	2.3
1	A	372	VAL	2.3
1	A	315	HIS	2.2
1	A	364	GLN	2.2
1	B	250	SER	2.2
1	A	563	TYR	2.2
1	B	252	ILE	2.2
1	B	442	ALA	2.1
1	B	487	ALA	2.1
1	B	139	PRO	2.1
1	A	526	VAL	2.1
1	A	437	LYS	2.1
1	B	117	LEU	2.1
1	A	527	CYS	2.1
1	A	518	MET	2.0
1	B	534	CYS	2.0
1	A	442	ALA	2.0
1	B	524	GLY	2.0
1	B	367	ARG	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 oligosaccharides 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, 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	A	801	14/15	0.65	0.14	95,97,100,100	0
2	NAG	B	802	14/15	0.69	0.12	88,95,96,98	0
3	C5B	B	2001	12/12	0.95	0.09	48,50,51,52	0
3	C5B	A	1001	12/12	0.97	0.07	45,46,51,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.