



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:45 AM UTC

PDB ID : 2E4W / pdb_00002e4w
Title : Crystal structure of the extracellular region of the group II metabotropic glutamate receptor complexed with 1S,3S-ACPD
Authors : Muto, T.; Tsuchiya, D.; Morikawa, K.; Jingami, H.
Deposited on : 2006-12-17
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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

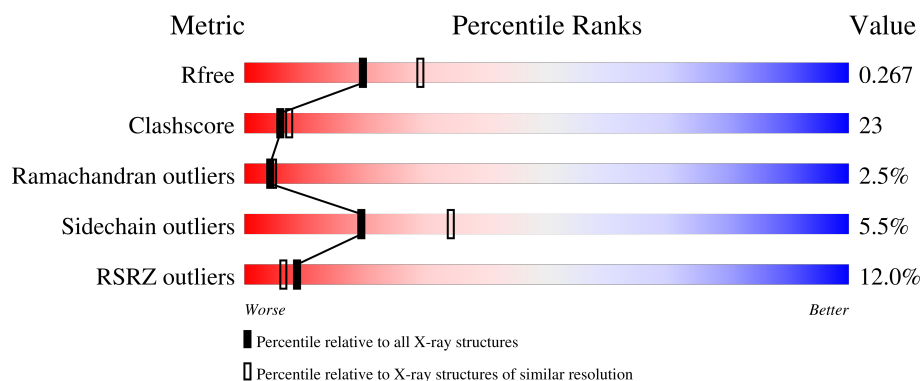
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	11% 59% 29% 5% 7%
1	B	555	11% 57% 31% 5% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8602 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:

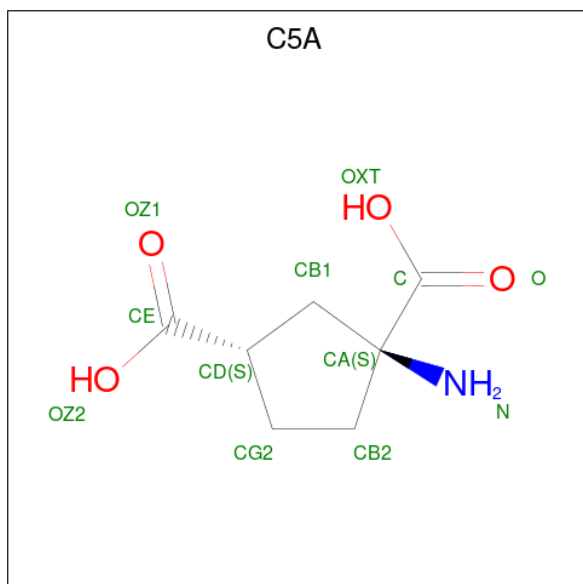
Chain	Residue	Modelled	Actual	Comment	Reference
A	414	GLN	ASN	engineered mutation	UNP P31422
A	439	GLN	ASN	engineered mutation	UNP P31422
A	576	LEU	-	cloning artifact	UNP P31422
A	577	VAL	-	cloning artifact	UNP P31422
A	578	PRO	-	cloning artifact	UNP P31422
A	579	ARG	-	cloning artifact	UNP P31422
B	414	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,3S)-1-aminocyclopentane-1,3-dicarboxylic acid (CCD ID: C5A) (formula: $C_7H_{11}NO_4$).



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		

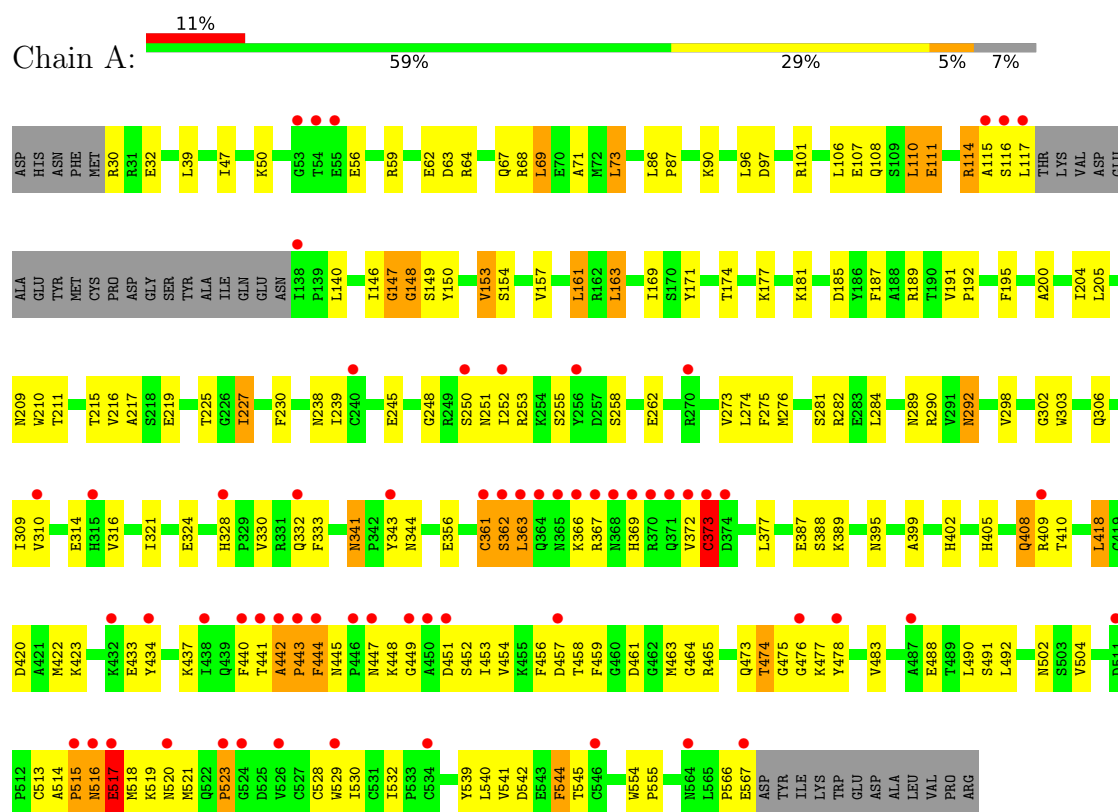
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	166	Total	O	0	0
			166	166		
4	B	129	Total	O	0	0
			129	129		

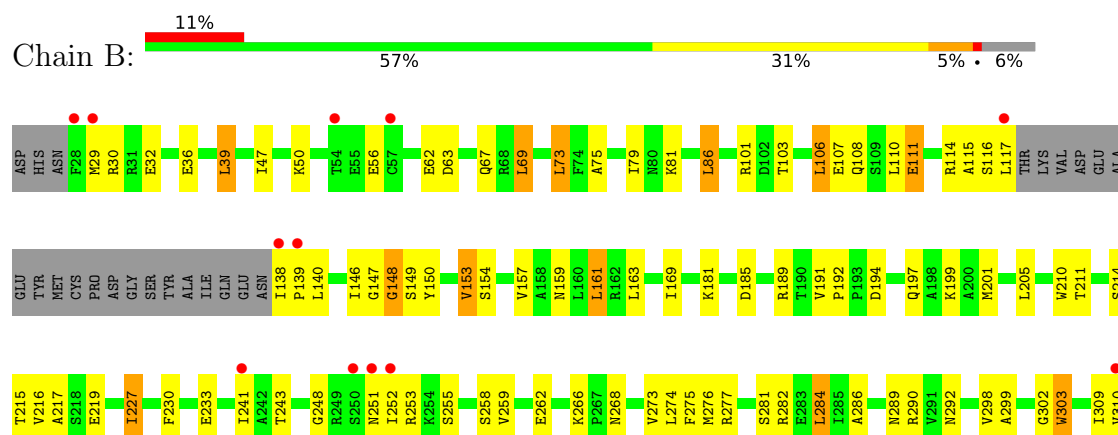
3 Residue-property plots

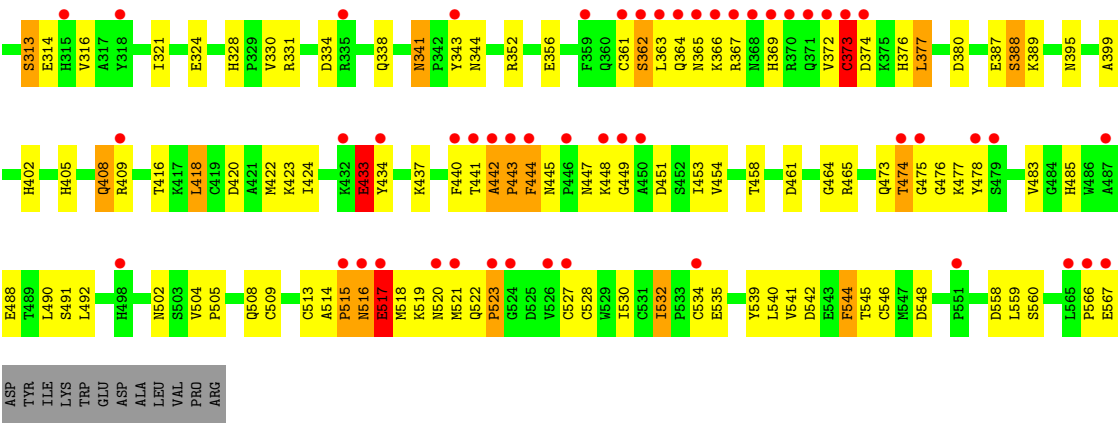
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Metabotropic glutamate receptor 3



• Molecule 1: Metabotropic glutamate receptor 3





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.74Å 97.31Å 107.81Å 90.00° 92.94° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.8 (20.00-2.40) 98.6 (20.00-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.236 , 0.267 0.237 , 0.267	Depositor DCC
R_{free} test set	4760 reflections (7.12%)	wwPDB-VP
Wilson B-factor (Å ²)	52.2	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8602	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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, C5A

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	0.46	0/4212	0.98	19/5704 (0.3%)
1	B	0.44	0/4232	0.98	23/5730 (0.4%)
All	All	0.45	0/8444	0.98	42/11434 (0.4%)

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	147	GLY	N-CA-C	10.09	124.29	110.56
1	A	147	GLY	N-CA-C	9.19	123.05	110.56
1	B	509	CYS	N-CA-C	8.65	120.33	111.07
1	A	149	SER	N-CA-C	-8.12	100.51	111.96
1	B	488	GLU	N-CA-C	-8.11	104.54	114.75
1	B	149	SER	N-CA-C	-7.75	99.25	111.02
1	A	488	GLU	N-CA-C	-7.41	105.42	114.75
1	A	114	ARG	N-CA-C	-7.13	103.54	111.82
1	A	195	PHE	N-CA-C	-6.87	103.79	111.28
1	B	458	THR	N-CA-C	-6.85	104.39	112.89
1	A	458	THR	N-CA-C	-6.76	103.97	111.82
1	B	62	GLU	N-CA-C	6.76	118.34	110.97
1	A	373	CYS	N-CA-C	6.58	120.13	109.40
1	B	373	CYS	N-CA-C	6.53	120.17	109.72
1	A	148	GLY	N-CA-C	-6.41	97.99	113.18
1	B	148	GLY	N-CA-C	-6.36	98.11	113.18
1	A	302	GLY	N-CA-C	-6.06	105.45	112.73
1	B	303	TRP	N-CA-C	-6.01	103.49	111.24
1	A	442	ALA	CA-C-N	5.95	127.28	119.84
1	A	442	ALA	C-N-CA	5.95	127.28	119.84
1	B	364	GLN	N-CA-C	-5.95	105.36	114.16
1	B	146	ILE	CA-C-N	-5.85	113.25	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	146	ILE	C-N-CA	-5.85	113.25	121.56
1	B	388	SER	N-CA-C	5.82	118.37	111.33
1	B	442	ALA	CA-C-N	5.71	126.98	119.84
1	B	442	ALA	C-N-CA	5.71	126.98	119.84
1	A	388	SER	N-CA-C	5.65	118.16	111.33
1	B	532	ILE	N-CA-C	5.55	113.05	107.55
1	B	302	GLY	N-CA-C	-5.50	106.13	112.73
1	B	331	ARG	N-CA-C	5.46	117.94	111.33
1	A	62	GLU	N-CA-C	5.46	116.92	110.97
1	A	87	PRO	N-CA-C	-5.32	102.83	111.19
1	B	266	LYS	CA-C-N	5.24	125.29	119.32
1	B	266	LYS	C-N-CA	5.24	125.29	119.32
1	B	416	THR	N-CA-C	-5.23	106.49	112.92
1	B	433	GLU	N-CA-C	-5.18	99.77	110.80
1	B	545	THR	N-CA-C	5.16	117.48	108.76
1	A	361	CYS	N-CA-C	5.12	121.71	110.80
1	A	146	ILE	CA-C-N	-5.11	114.31	121.56
1	A	146	ILE	C-N-CA	-5.11	114.31	121.56
1	A	545	THR	N-CA-C	5.08	116.69	108.26
1	A	410	THR	N-CA-C	5.01	116.83	111.36

There are no chirality outliers.

There are no planarity outliers.

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	177	0
1	B	4137	0	4012	201	0
2	A	14	0	13	1	0
2	B	14	0	13	0	0
3	A	12	0	9	0	0
3	B	12	0	9	0	0
4	A	166	0	0	10	0
4	B	129	0	0	13	0
All	All	8602	0	8049	374	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 (374) 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:402:HIS:HB3	1:B:437:LYS:HE2	1.31	1.11
1:B:30:ARG:HD2	1:B:108:GLN:HE22	1.28	0.98
1:A:356:GLU:HA	1:A:361:CYS:HB2	1.45	0.96
1:A:515:PRO:HG2	1:A:516:ASN:H	1.33	0.94
1:A:420:ASP:HA	1:A:423:LYS:HD3	1.50	0.93
1:B:356:GLU:HA	1:B:361:CYS:HB2	1.49	0.92
1:B:328:HIS:HB2	4:B:2026:HOH:O	1.70	0.91
1:B:216:VAL:HG12	1:B:274:LEU:HD22	1.53	0.90
1:B:216:VAL:CG1	1:B:274:LEU:HD22	2.03	0.89
1:A:402:HIS:HB3	1:A:437:LYS:HE2	1.56	0.87
1:B:47:ILE:HD12	1:B:69:LEU:HD12	1.57	0.86
1:A:30:ARG:HA	4:A:1133:HOH:O	1.74	0.86
1:B:274:LEU:HD13	1:B:276:MET:HE2	1.57	0.85
1:B:341:ASN:HD22	1:B:343:TYR:H	1.18	0.85
1:A:274:LEU:HD13	1:A:276:MET:HE2	1.60	0.84
1:B:515:PRO:HG2	1:B:516:ASN:H	1.43	0.82
1:A:181:LYS:HE2	1:A:459:PHE:O	1.82	0.80
1:A:289:ASN:HA	1:A:316:VAL:HG21	1.64	0.80
1:B:514:ALA:HB3	1:B:518:MET:HG3	1.61	0.80
1:B:289:ASN:HA	1:B:316:VAL:HG21	1.62	0.79
1:A:216:VAL:CG1	1:A:274:LEU:HD22	2.14	0.78
1:A:514:ALA:HB3	1:A:518:MET:HG3	1.66	0.77
1:A:107:GLU:HB3	4:A:1116:HOH:O	1.82	0.77
1:B:366:LYS:HG2	1:B:367:ARG:H	1.50	0.77
1:B:540:LEU:HD13	1:B:559:LEU:HD23	1.67	0.76
1:B:330:VAL:HG13	1:B:444:PHE:HB3	1.66	0.76
1:A:157:VAL:HG12	1:A:161:LEU:HD22	1.69	0.75
1:B:216:VAL:HG12	1:B:274:LEU:CD2	2.16	0.75
1:A:465:ARG:HH11	1:A:465:ARG:HG3	1.51	0.75
1:B:50:LYS:HG3	1:B:101:ARG:HD3	1.66	0.75
1:B:514:ALA:H	1:B:518:MET:CE	2.00	0.75
1:B:338:GLN:OE1	1:B:380:ASP:HA	1.88	0.74
1:A:101:ARG:HD3	4:A:1070:HOH:O	1.87	0.74
1:B:440:PHE:CE2	1:B:448:LYS:HB3	2.23	0.74
1:B:103:THR:O	1:B:107:GLU:HG2	1.88	0.73
1:A:366:LYS:HG2	1:A:367:ARG:H	1.54	0.72
1:B:362:SER:O	1:B:363:LEU:HD13	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:ARG:HD3	4:B:2033:HOH:O	1.88	0.72
1:A:330:VAL:HG13	1:A:444:PHE:HB3	1.71	0.71
1:A:258:SER:O	1:A:262:GLU:HG3	1.91	0.71
1:A:442:ALA:O	1:A:444:PHE:N	2.24	0.71
1:B:341:ASN:ND2	1:B:344:ASN:H	1.89	0.70
1:A:520:ASN:O	1:A:544:PHE:HB3	1.91	0.70
1:B:258:SER:O	1:B:262:GLU:HG3	1.91	0.69
1:B:442:ALA:O	1:B:444:PHE:N	2.25	0.69
1:B:424:ILE:HG12	4:B:2124:HOH:O	1.91	0.69
1:B:514:ALA:H	1:B:518:MET:HE2	1.57	0.69
1:A:341:ASN:ND2	1:A:344:ASN:H	1.92	0.68
1:A:515:PRO:CG	1:A:516:ASN:H	2.06	0.68
1:A:405:HIS:NE2	1:A:409:ARG:NE	2.42	0.68
1:A:440:PHE:CE2	1:A:448:LYS:HB3	2.31	0.66
1:B:341:ASN:ND2	1:B:343:TYR:H	1.93	0.66
1:B:352:ARG:HG3	4:B:2077:HOH:O	1.95	0.66
1:B:473:GLN:HE21	1:B:476:GLY:CA	2.09	0.66
1:A:276:MET:HE3	1:A:281:SER:HA	1.77	0.66
1:B:521:MET:HB2	1:B:530:ILE:HG13	1.76	0.66
1:B:253:ARG:HG2	1:B:290:ARG:HH22	1.60	0.66
1:B:420:ASP:HA	1:B:423:LYS:HD3	1.77	0.66
1:A:253:ARG:HG2	1:A:290:ARG:HH22	1.59	0.65
1:A:367:ARG:HB2	1:A:369:HIS:CD2	2.31	0.65
1:B:341:ASN:HD22	1:B:343:TYR:N	1.94	0.65
1:B:314:GLU:HG2	1:B:478:TYR:CD2	2.33	0.64
1:A:408:GLN:HB2	1:A:422:MET:HE1	1.79	0.64
1:B:253:ARG:HG2	1:B:290:ARG:NH2	2.12	0.64
1:B:282:ARG:HG2	1:B:282:ARG:HH11	1.61	0.64
1:A:514:ALA:H	1:A:518:MET:CE	2.10	0.64
1:A:253:ARG:HG2	1:A:290:ARG:NH2	2.12	0.64
1:A:328:HIS:HB2	4:A:1084:HOH:O	1.98	0.64
1:A:366:LYS:HG2	1:A:367:ARG:N	2.13	0.64
1:B:241:ILE:HG22	4:B:2071:HOH:O	1.97	0.64
1:B:366:LYS:HG2	1:B:367:ARG:N	2.12	0.63
1:A:452:SER:HA	4:A:1147:HOH:O	1.98	0.63
1:A:418:LEU:HD22	1:A:422:MET:HE3	1.81	0.63
1:B:310:VAL:CG1	1:B:314:GLU:HA	2.28	0.63
1:B:374:ASP:HB3	1:B:377:LEU:HD22	1.80	0.63
1:A:515:PRO:O	1:A:517:GLU:N	2.32	0.62
1:B:540:LEU:HD12	1:B:546:CYS:SG	2.38	0.62
1:A:465:ARG:HG3	1:A:465:ARG:NH1	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:ASN:OD1	1:B:441:THR:HG23	2.00	0.61
1:A:110:LEU:O	1:A:114:ARG:HG3	2.00	0.61
1:A:192:PRO:HG3	1:A:464:GLY:HA2	1.82	0.61
1:A:282:ARG:HG2	1:A:282:ARG:HH11	1.65	0.61
1:A:372:VAL:HG22	1:A:373:CYS:N	2.15	0.61
1:A:252:ILE:HG22	1:A:253:ARG:H	1.66	0.61
1:A:402:HIS:CB	1:A:437:LYS:HE2	2.30	0.60
1:B:520:ASN:O	1:B:544:PHE:HB3	2.00	0.60
1:B:215:THR:OG1	1:B:241:ILE:HD11	2.01	0.60
1:B:276:MET:HE1	1:B:284:LEU:HD12	1.83	0.60
1:B:490:LEU:HD12	1:B:491:SER:H	1.67	0.60
1:B:441:THR:O	1:B:442:ALA:C	2.43	0.60
1:A:362:SER:C	1:A:363:LEU:HD22	2.27	0.59
1:B:252:ILE:HG22	1:B:253:ARG:H	1.65	0.59
1:B:483:VAL:O	1:B:492:LEU:HB2	2.02	0.59
1:B:217:ALA:HB2	1:B:227:ILE:HG13	1.84	0.59
1:A:521:MET:HB2	1:A:530:ILE:HG13	1.85	0.59
1:B:367:ARG:HB2	1:B:369:HIS:CD2	2.38	0.59
1:A:216:VAL:HA	1:A:245:GLU:O	2.02	0.58
1:B:47:ILE:CD1	1:B:69:LEU:HD12	2.31	0.58
1:A:169:ILE:HG12	1:A:434:TYR:OH	2.04	0.58
1:B:201:MET:HE2	1:B:273:VAL:HG13	1.85	0.58
1:A:523:PRO:HD2	1:A:528:CYS:O	2.04	0.58
1:B:310:VAL:HG12	1:B:314:GLU:HA	1.86	0.58
1:A:150:TYR:HB2	1:A:153:VAL:HG13	1.86	0.58
1:B:330:VAL:HG13	1:B:444:PHE:CB	2.35	0.57
1:A:441:THR:O	1:A:442:ALA:C	2.46	0.57
1:A:211:THR:HG23	1:A:238:ASN:O	2.04	0.57
1:A:372:VAL:HG22	1:A:373:CYS:H	1.67	0.57
1:B:199:LYS:HD3	4:B:2063:HOH:O	2.04	0.57
1:B:523:PRO:HD2	1:B:528:CYS:O	2.04	0.57
1:B:418:LEU:HD22	1:B:422:MET:HE3	1.86	0.57
1:A:473:GLN:NE2	1:A:476:GLY:HA2	2.20	0.57
1:B:341:ASN:HD22	1:B:341:ASN:C	2.13	0.57
1:B:515:PRO:O	1:B:517:GLU:N	2.38	0.56
1:A:282:ARG:HD2	1:A:309:ILE:O	2.05	0.56
1:A:303:TRP:HA	1:A:309:ILE:CD1	2.35	0.56
1:A:310:VAL:CG1	1:A:314:GLU:HA	2.36	0.56
1:B:374:ASP:HB3	1:B:377:LEU:CD2	2.34	0.56
1:A:189:ARG:HD3	1:A:461:ASP:OD1	2.06	0.56
1:A:514:ALA:CB	1:A:518:MET:HE2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:VAL:HG13	1:A:444:PHE:CB	2.36	0.56
1:B:86:LEU:H	1:B:405:HIS:HD1	1.53	0.55
1:B:473:GLN:HE21	1:B:476:GLY:HA2	1.70	0.55
1:A:314:GLU:HG2	1:A:478:TYR:CD2	2.41	0.55
1:A:514:ALA:HB2	1:A:518:MET:HE2	1.87	0.55
1:B:303:TRP:HA	1:B:309:ILE:CD1	2.37	0.55
1:B:408:GLN:HB2	1:B:422:MET:HE1	1.88	0.55
1:B:251:ASN:HD22	1:B:255:SER:HB3	1.72	0.55
1:B:81:LYS:HG3	4:B:2098:HOH:O	2.06	0.55
1:A:56:GLU:HG2	1:A:101:ARG:HH22	1.72	0.54
1:A:169:ILE:CD1	1:A:434:TYR:OH	2.55	0.54
1:B:473:GLN:NE2	1:B:476:GLY:HA2	2.21	0.54
1:A:216:VAL:HG13	1:A:274:LEU:HD22	1.89	0.54
1:B:362:SER:C	1:B:363:LEU:HD22	2.32	0.54
1:B:219:GLU:OE2	1:B:248:GLY:HA3	2.08	0.54
1:A:483:VAL:O	1:A:492:LEU:HB2	2.08	0.54
1:A:367:ARG:HB2	1:A:369:HIS:NE2	2.22	0.54
1:A:399:ALA:HB1	1:A:434:TYR:HE1	1.73	0.54
1:B:181:LYS:HE2	1:B:181:LYS:HA	1.90	0.54
1:B:465:ARG:HG3	1:B:465:ARG:HH11	1.73	0.54
1:A:363:LEU:HD22	1:A:363:LEU:N	2.23	0.54
1:A:115:ALA:HB1	1:A:140:LEU:O	2.08	0.53
1:B:86:LEU:HD13	1:B:405:HIS:HB2	1.89	0.53
1:A:209:ASN:ND2	2:A:801:NAG:H82	2.23	0.53
1:B:157:VAL:HG12	1:B:161:LEU:HD22	1.90	0.53
1:A:405:HIS:NE2	1:A:409:ARG:CZ	2.72	0.53
1:B:169:ILE:HG12	1:B:434:TYR:OH	2.09	0.53
1:B:150:TYR:HB2	1:B:153:VAL:HG13	1.89	0.53
1:B:189:ARG:HG3	1:B:191:VAL:O	2.09	0.53
1:B:514:ALA:H	1:B:518:MET:HE3	1.72	0.53
1:A:473:GLN:HE21	1:A:476:GLY:CA	2.22	0.53
1:B:252:ILE:HG22	1:B:253:ARG:N	2.23	0.53
1:A:90:LYS:NZ	4:A:1106:HOH:O	2.40	0.53
1:B:63:ASP:O	1:B:67:GLN:HB2	2.09	0.53
1:B:108:GLN:O	1:B:111:GLU:HB2	2.09	0.53
1:B:214:SER:OG	1:B:243:THR:HG22	2.08	0.53
1:B:56:GLU:HG2	1:B:101:ARG:NH2	2.24	0.52
1:A:341:ASN:C	1:A:341:ASN:HD22	2.18	0.52
1:A:252:ILE:HG22	1:A:253:ARG:N	2.24	0.52
1:A:554:TRP:CG	1:A:555:PRO:HD2	2.44	0.52
1:B:30:ARG:HD2	1:B:108:GLN:NE2	2.11	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:GLU:HG2	1:B:388:SER:OG	2.10	0.52
1:A:341:ASN:HD22	1:A:343:TYR:H	1.56	0.52
1:A:451:ASP:OD1	1:A:453:ILE:HG12	2.10	0.52
1:A:515:PRO:HG2	1:A:516:ASN:N	2.14	0.52
1:B:211:THR:HG22	1:B:211:THR:O	2.10	0.52
1:A:189:ARG:HG3	1:A:191:VAL:O	2.10	0.52
1:A:514:ALA:H	1:A:518:MET:HE3	1.74	0.52
1:B:169:ILE:CD1	1:B:434:TYR:OH	2.58	0.51
1:B:282:ARG:HD2	1:B:309:ILE:O	2.09	0.51
1:B:539:TYR:CZ	1:B:541:VAL:HG22	2.46	0.51
1:A:457:ASP:HB2	1:A:461:ASP:H	1.75	0.51
1:A:449:GLY:C	1:A:451:ASP:H	2.18	0.51
1:A:504:VAL:O	1:A:504:VAL:HG13	2.10	0.51
1:A:362:SER:O	1:A:363:LEU:HD13	2.11	0.51
1:A:443:PRO:C	1:A:445:ASN:H	2.18	0.51
1:B:334:ASP:O	1:B:338:GLN:HG3	2.10	0.51
1:A:216:VAL:CG1	1:A:274:LEU:CD2	2.88	0.51
1:A:514:ALA:H	1:A:518:MET:HE2	1.75	0.51
1:A:298:VAL:HA	1:A:321:ILE:O	2.11	0.51
1:A:64:ARG:O	1:A:68:ARG:HD2	2.10	0.51
1:B:169:ILE:CD1	1:B:434:TYR:CZ	2.94	0.51
1:A:169:ILE:HD13	1:A:434:TYR:OH	2.10	0.50
1:A:215:THR:HG22	1:A:273:VAL:HB	1.93	0.50
1:A:332:GLN:HB2	4:A:1125:HOH:O	2.11	0.50
1:B:115:ALA:HB1	1:B:140:LEU:O	2.11	0.50
1:A:303:TRP:HA	1:A:309:ILE:HD13	1.93	0.50
1:A:310:VAL:HG12	1:A:314:GLU:HA	1.92	0.50
1:B:116:SER:O	1:B:117:LEU:HD12	2.10	0.50
1:B:276:MET:HE3	1:B:281:SER:HA	1.92	0.50
1:B:362:SER:OG	1:B:366:LYS:HD3	2.11	0.50
1:A:50:LYS:NZ	1:A:250:SER:H	2.10	0.50
1:A:362:SER:OG	1:A:366:LYS:HD3	2.12	0.50
1:A:516:ASN:C	1:A:517:GLU:HG3	2.36	0.50
1:A:306:GLN:NE2	1:A:309:ILE:HD11	2.27	0.50
1:B:402:HIS:CB	1:B:437:LYS:HE2	2.23	0.50
1:A:513:CYS:HB3	1:A:518:MET:HB2	1.94	0.50
1:B:255:SER:O	1:B:259:VAL:HG23	2.12	0.49
1:B:408:GLN:HB2	1:B:422:MET:CE	2.42	0.49
1:A:114:ARG:HG2	1:B:114:ARG:HH21	1.76	0.49
1:B:372:VAL:HG22	1:B:373:CYS:H	1.76	0.49
1:A:174:THR:C	1:A:189:ARG:NH2	2.71	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:GLN:O	1:A:111:GLU:HB2	2.12	0.49
1:A:289:ASN:CA	1:A:316:VAL:HG21	2.40	0.49
1:B:485:HIS:HB2	4:B:2054:HOH:O	2.11	0.49
1:B:216:VAL:HG13	1:B:276:MET:SD	2.53	0.49
1:B:268:ASN:HB3	1:B:508:GLN:O	2.13	0.49
1:B:366:LYS:HE2	1:B:369:HIS:CD2	2.48	0.49
1:A:56:GLU:HG2	1:A:101:ARG:NH2	2.28	0.48
1:A:169:ILE:CG1	1:A:434:TYR:OH	2.61	0.48
1:A:219:GLU:HB2	1:A:248:GLY:HA2	1.94	0.48
1:B:75:ALA:O	1:B:79:ILE:HG13	2.13	0.48
1:A:163:LEU:HD11	1:B:159:ASN:HB3	1.95	0.48
1:B:443:PRO:C	1:B:445:ASN:H	2.21	0.48
1:A:492:LEU:HD23	1:A:492:LEU:N	2.28	0.48
1:B:328:HIS:CD2	4:B:2128:HOH:O	2.66	0.48
1:B:344:ASN:C	4:B:2119:HOH:O	2.56	0.48
1:B:519:LYS:HG2	1:B:532:ILE:HB	1.95	0.48
1:B:189:ARG:HD3	1:B:461:ASP:OD1	2.14	0.48
1:A:252:ILE:HD12	1:A:252:ILE:N	2.29	0.47
1:B:515:PRO:CG	1:B:516:ASN:H	2.16	0.47
1:B:516:ASN:HB2	1:B:517:GLU:OE2	2.14	0.47
1:B:539:TYR:OH	1:B:541:VAL:HG22	2.14	0.47
1:A:395:ASN:OD1	1:A:441:THR:HG23	2.14	0.47
1:B:217:ALA:HB2	1:B:227:ILE:CG1	2.44	0.47
1:A:116:SER:C	1:A:117:LEU:HD12	2.39	0.47
1:A:177:LYS:HE3	1:A:225:THR:HG21	1.97	0.47
1:A:211:THR:HG23	1:A:239:ILE:HA	1.97	0.47
1:B:282:ARG:HG2	1:B:282:ARG:NH1	2.29	0.47
1:B:138:ILE:N	1:B:139:PRO:HD2	2.30	0.47
1:A:181:LYS:HE3	1:A:187:PHE:O	2.15	0.47
1:B:169:ILE:HD13	1:B:434:TYR:OH	2.14	0.46
1:A:116:SER:O	1:A:117:LEU:HD12	2.14	0.46
1:B:30:ARG:NH2	1:B:32:GLU:OE1	2.48	0.46
1:A:169:ILE:CD1	1:A:434:TYR:CZ	2.98	0.46
1:B:341:ASN:HD21	1:B:343:TYR:HB2	1.81	0.46
1:B:449:GLY:C	1:B:451:ASP:H	2.24	0.46
1:A:276:MET:CE	1:A:281:SER:HA	2.44	0.46
1:A:473:GLN:HE21	1:A:476:GLY:HA2	1.78	0.46
1:A:441:THR:HG22	4:A:1045:HOH:O	2.15	0.46
1:B:39:LEU:HD12	1:B:39:LEU:HA	1.82	0.46
1:B:341:ASN:ND2	1:B:341:ASN:C	2.74	0.46
1:B:341:ASN:HD21	1:B:344:ASN:H	1.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:558:ASP:O	1:B:559:LEU:HB2	2.15	0.46
1:A:211:THR:HG22	1:A:211:THR:O	2.16	0.46
1:B:504:VAL:O	1:B:504:VAL:HG13	2.16	0.46
1:A:147:GLY:HA2	1:A:171:TYR:CE2	2.51	0.46
1:A:418:LEU:HD22	1:A:422:MET:CE	2.45	0.45
1:A:473:GLN:NE2	1:A:476:GLY:CA	2.79	0.45
1:A:282:ARG:HG2	1:A:282:ARG:NH1	2.31	0.45
1:B:69:LEU:C	1:B:69:LEU:HD23	2.41	0.45
1:B:363:LEU:HD22	1:B:363:LEU:N	2.32	0.45
1:A:310:VAL:HG12	1:A:310:VAL:O	2.16	0.45
1:A:523:PRO:HD3	1:A:529:TRP:HA	1.98	0.45
1:B:286:ALA:O	1:B:290:ARG:HG3	2.16	0.45
1:B:442:ALA:C	1:B:444:PHE:H	2.24	0.45
1:A:442:ALA:C	1:A:444:PHE:N	2.74	0.45
1:B:274:LEU:HD13	1:B:276:MET:CE	2.37	0.45
1:B:205:LEU:CD2	1:B:210:TRP:HE3	2.29	0.45
1:A:217:ALA:HB2	1:A:227:ILE:HG13	1.98	0.45
1:A:230:PHE:CZ	1:A:273:VAL:HG21	2.52	0.45
1:A:341:ASN:HD22	1:A:343:TYR:N	2.15	0.45
1:A:473:GLN:O	1:A:474:THR:C	2.60	0.45
1:B:69:LEU:CD2	1:B:73:LEU:HD22	2.46	0.45
1:B:473:GLN:O	1:B:474:THR:C	2.59	0.45
1:B:399:ALA:HB1	1:B:434:TYR:HE1	1.81	0.44
1:B:558:ASP:OD2	1:B:560:SER:HB3	2.17	0.44
1:A:444:PHE:N	1:A:444:PHE:CD2	2.84	0.44
1:A:539:TYR:CZ	1:A:541:VAL:HG22	2.53	0.44
1:A:542:ASP:OD2	1:A:542:ASP:C	2.61	0.44
1:B:387:GLU:CD	1:B:389:LYS:H	2.25	0.44
1:B:473:GLN:HA	1:B:477:LYS:O	2.17	0.44
1:B:475:GLY:C	1:B:477:LYS:H	2.26	0.44
1:A:96:LEU:HD13	1:A:108:GLN:HB3	1.98	0.44
1:A:463:MET:HG2	4:A:1079:HOH:O	2.17	0.44
1:A:475:GLY:C	1:A:477:LYS:H	2.25	0.44
1:A:519:LYS:HG2	1:A:532:ILE:HB	1.99	0.44
1:B:517:GLU:N	1:B:517:GLU:CD	2.74	0.44
1:B:148:GLY:HA3	1:B:154:SER:OG	2.18	0.44
1:B:192:PRO:HG3	1:B:464:GLY:HA2	2.00	0.44
1:B:465:ARG:HG3	1:B:465:ARG:NH1	2.30	0.44
1:B:492:LEU:N	1:B:492:LEU:HD23	2.32	0.44
1:B:241:ILE:HG23	1:B:241:ILE:O	2.18	0.44
1:A:387:GLU:CD	1:A:389:LYS:H	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:LEU:HD12	1:A:491:SER:H	1.82	0.44
1:B:451:ASP:OD1	1:B:453:ILE:HG12	2.17	0.44
1:A:63:ASP:O	1:A:67:GLN:HB2	2.18	0.43
1:B:513:CYS:HB3	1:B:518:MET:HB2	2.00	0.43
1:B:548:ASP:HB2	4:B:2083:HOH:O	2.18	0.43
1:A:366:LYS:CG	1:A:367:ARG:H	2.26	0.43
1:A:434:TYR:CZ	1:A:456:PHE:CZ	3.07	0.43
1:A:251:ASN:HD22	1:A:255:SER:HB3	1.84	0.43
1:A:290:ARG:C	1:A:292:ASN:H	2.25	0.43
1:B:289:ASN:CA	1:B:316:VAL:HG21	2.41	0.43
1:A:434:TYR:OH	1:A:456:PHE:CZ	2.70	0.43
1:A:473:GLN:HA	1:A:477:LYS:O	2.18	0.43
1:B:377:LEU:HD13	1:B:377:LEU:HA	1.79	0.43
1:B:405:HIS:NE2	1:B:409:ARG:NE	2.67	0.43
1:B:437:LYS:HD2	1:B:437:LYS:HA	1.75	0.43
1:A:185:ASP:OD2	1:A:185:ASP:N	2.42	0.43
1:A:473:GLN:HE21	1:A:476:GLY:C	2.25	0.43
1:B:514:ALA:CB	1:B:518:MET:HE2	2.49	0.43
1:A:71:ALA:HA	1:A:333:PHE:CE1	2.54	0.43
1:B:169:ILE:HD11	1:B:434:TYR:CZ	2.54	0.43
1:B:442:ALA:C	1:B:444:PHE:N	2.74	0.43
1:A:30:ARG:HG3	1:A:30:ARG:O	2.18	0.43
1:A:148:GLY:HA3	1:A:154:SER:OG	2.18	0.43
1:B:230:PHE:CZ	1:B:273:VAL:HG21	2.54	0.43
1:B:453:ILE:HG13	1:B:453:ILE:O	2.18	0.43
1:A:252:ILE:O	1:A:253:ARG:C	2.62	0.42
1:B:116:SER:C	1:B:117:LEU:HD12	2.43	0.42
1:B:366:LYS:CG	1:B:367:ARG:H	2.26	0.42
1:A:114:ARG:NH2	1:B:114:ARG:HG2	2.34	0.42
1:B:522:GLN:HA	1:B:522:GLN:NE2	2.35	0.42
1:A:252:ILE:HD12	1:A:252:ILE:H	1.83	0.42
1:A:408:GLN:HE21	1:A:409:ARG:HA	1.84	0.42
1:B:219:GLU:HB2	1:B:248:GLY:HA2	2.01	0.42
1:B:366:LYS:HE2	1:B:369:HIS:HD2	1.84	0.42
1:A:324:GLU:HG3	4:A:1146:HOH:O	2.20	0.42
1:A:402:HIS:HB3	1:A:437:LYS:CE	2.37	0.42
1:B:290:ARG:C	1:B:292:ASN:H	2.27	0.42
1:B:185:ASP:OD2	1:B:185:ASP:N	2.53	0.42
1:B:227:ILE:HD13	1:B:227:ILE:HA	1.85	0.42
1:A:420:ASP:O	1:A:423:LYS:HB2	2.20	0.42
1:B:169:ILE:HG12	1:B:434:TYR:CZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:LEU:HD22	1:A:210:TRP:HE3	1.84	0.42
1:B:205:LEU:HD22	1:B:210:TRP:HE3	1.85	0.42
1:B:372:VAL:HG22	1:B:373:CYS:N	2.35	0.42
1:B:408:GLN:CB	1:B:422:MET:HE1	2.50	0.42
1:B:440:PHE:HE2	1:B:448:LYS:HB3	1.77	0.42
1:A:47:ILE:HB	1:A:97:ASP:CG	2.45	0.42
1:A:163:LEU:HB3	1:B:106:LEU:HD11	2.01	0.42
1:B:150:TYR:HE2	1:B:277:ARG:HB3	1.85	0.42
1:B:215:THR:HG22	1:B:273:VAL:HB	2.00	0.42
1:B:367:ARG:HB2	1:B:369:HIS:NE2	2.34	0.42
1:B:542:ASP:OD2	1:B:542:ASP:C	2.63	0.41
1:B:56:GLU:HG2	1:B:101:ARG:HH22	1.85	0.41
1:B:517:GLU:O	1:B:534:CYS:N	2.48	0.41
1:A:59:ARG:HH11	1:A:59:ARG:HB2	1.85	0.41
1:B:73:LEU:HD12	1:B:73:LEU:HA	1.94	0.41
1:A:30:ARG:NH2	1:A:32:GLU:OE1	2.53	0.41
1:A:200:ALA:O	1:A:204:ILE:HG13	2.20	0.41
1:A:205:LEU:CD2	1:A:210:TRP:HE3	2.33	0.41
1:A:440:PHE:O	1:A:441:THR:C	2.64	0.41
1:A:440:PHE:HE2	1:A:448:LYS:HB3	1.82	0.41
1:A:443:PRO:O	1:A:445:ASN:N	2.54	0.41
1:B:199:LYS:HG2	1:B:233:GLU:CD	2.46	0.41
1:B:356:GLU:OE1	1:B:366:LYS:HB2	2.21	0.41
1:A:69:LEU:HD22	1:A:73:LEU:HD22	2.02	0.41
1:A:366:LYS:CG	1:A:367:ARG:N	2.81	0.41
1:B:36:GLU:HB3	4:B:2037:HOH:O	2.20	0.41
1:B:169:ILE:CG1	1:B:434:TYR:OH	2.67	0.41
1:B:405:HIS:NE2	1:B:409:ARG:CZ	2.83	0.41
1:B:516:ASN:C	1:B:517:GLU:HG3	2.46	0.41
1:A:361:CYS:HB3	1:A:362:SER:H	1.31	0.41
1:A:408:GLN:HB2	1:A:422:MET:CE	2.48	0.41
1:B:211:THR:HG22	1:B:527:CYS:SG	2.61	0.41
1:B:540:LEU:CD1	1:B:546:CYS:SG	3.08	0.41
1:A:437:LYS:HA	1:A:437:LYS:HD2	1.88	0.41
1:B:298:VAL:HA	1:B:321:ILE:O	2.21	0.41
1:B:418:LEU:HD22	1:B:422:MET:CE	2.51	0.41
1:A:372:VAL:CG2	1:A:373:CYS:N	2.83	0.40
1:B:374:ASP:C	1:B:376:HIS:H	2.30	0.40
1:B:515:PRO:CG	1:B:516:ASN:N	2.82	0.40
1:B:535:GLU:OE2	1:B:535:GLU:HA	2.21	0.40
1:B:276:MET:CE	1:B:284:LEU:HD12	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:SER:N	1:B:314:GLU:OE1	2.54	0.40
1:B:365:ASN:OD1	1:B:365:ASN:O	2.38	0.40
1:A:169:ILE:HG12	1:A:434:TYR:CZ	2.56	0.40
1:B:194:ASP:OD1	1:B:197:GLN:NE2	2.53	0.40
1:B:299:ALA:HB2	1:B:303:TRP:CE3	2.56	0.40
1:B:409:ARG:NH1	4:B:2115:HOH:O	2.53	0.40
1:A:69:LEU:CD2	1:A:69:LEU:C	2.95	0.40
1:A:442:ALA:C	1:A:444:PHE:H	2.30	0.40
1:B:181:LYS:HE2	1:B:181:LYS:CA	2.51	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%)	456 (89%)	46 (9%)	12 (2%)	5	6
1	B	516/555 (93%)	453 (88%)	49 (10%)	14 (3%)	4	4
All	All	1030/1110 (93%)	909 (88%)	95 (9%)	26 (2%)	4	5

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	443	PRO
1	A	474	THR
1	A	502	ASN
1	A	516	ASN
1	A	523	PRO
1	B	443	PRO
1	B	502	ASN
1	B	516	ASN
1	A	362	SER

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Mol	Chain	Res	Type
1	A	444	PHE
1	A	517	GLU
1	B	362	SER
1	B	474	THR
1	B	523	PRO
1	A	515	PRO
1	B	444	PHE
1	B	447	ASN
1	B	505	PRO
1	B	515	PRO
1	B	517	GLU
1	A	433	GLU
1	A	447	ASN
1	B	313	SER
1	B	433	GLU
1	B	566	PRO
1	A	566	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%)	422 (94%)	25 (6%)	19	33
1	B	449/481 (93%)	425 (95%)	24 (5%)	20	36
All	All	896/962 (93%)	847 (94%)	49 (6%)	19	34

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	69	LEU
1	A	73	LEU
1	A	86	LEU
1	A	106	LEU
1	A	110	LEU

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Mol	Chain	Res	Type
1	A	111	GLU
1	A	153	VAL
1	A	161	LEU
1	A	163	LEU
1	A	227	ILE
1	A	275	PHE
1	A	284	LEU
1	A	292	ASN
1	A	341	ASN
1	A	363	LEU
1	A	373	CYS
1	A	377	LEU
1	A	408	GLN
1	A	418	LEU
1	A	454	VAL
1	A	517	GLU
1	A	540	LEU
1	A	544	PHE
1	A	567	GLU
1	B	29	MET
1	B	39	LEU
1	B	69	LEU
1	B	73	LEU
1	B	86	LEU
1	B	106	LEU
1	B	110	LEU
1	B	111	GLU
1	B	153	VAL
1	B	161	LEU
1	B	163	LEU
1	B	227	ILE
1	B	275	PHE
1	B	284	LEU
1	B	341	ASN
1	B	373	CYS
1	B	377	LEU
1	B	408	GLN
1	B	418	LEU
1	B	433	GLU
1	B	454	VAL
1	B	517	GLU
1	B	544	PHE

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Mol	Chain	Res	Type
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	251	ASN
1	A	292	ASN
1	A	306	GLN
1	A	341	ASN
1	A	365	ASN
1	A	369	HIS
1	A	408	GLN
1	A	473	GLN
1	A	522	GLN
1	B	108	GLN
1	B	251	ASN
1	B	292	ASN
1	B	341	ASN
1	B	365	ASN
1	B	369	HIS
1	B	408	GLN
1	B	473	GLN
1	B	485	HIS
1	B	520	ASN
1	B	522	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	A	801	1	14,14,15	0.63	0	17,19,21	0.69	0
3	C5A	B	2001	-	10,12,12	1.11	0	14,18,18	1.48	3 (21%)
3	C5A	A	1001	-	10,12,12	1.09	0	14,18,18	1.48	3 (21%)
2	NAG	B	802	1	14,14,15	0.56	0	17,19,21	0.61	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	801	1	-	4/6/23/26	0/1/1/1
3	C5A	B	2001	-	-	1/10/21/21	0/1/1/1
3	C5A	A	1001	-	-	2/10/21/21	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	B	2001	C5A	CB2-CA-CB1	2.84	107.38	102.73
3	A	1001	C5A	CB2-CA-CB1	2.70	107.15	102.73
3	B	2001	C5A	OXT-C-CA	2.30	119.84	113.69
3	A	1001	C5A	OZ2-CE-CD	2.30	120.12	114.16
3	A	1001	C5A	OXT-C-CA	2.28	119.79	113.69
3	B	2001	C5A	OZ2-CE-CD	2.16	119.75	114.16

There are no chirality outliers.

All (9) 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
2	A	801	NAG	C4-C5-C6-O6
2	A	801	NAG	O5-C5-C6-O6
3	A	1001	C5A	O-C-CA-CB2
3	A	1001	C5A	CB1-CD-CE-OZ2
3	B	2001	C5A	CB1-CD-CE-OZ2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
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%)	0.57	62 (11%) 9 6	28, 58, 98, 133	0
1	B	520/555 (93%)	0.61	63 (12%) 8 6	27, 59, 100, 133	0
All	All	1038/1110 (93%)	0.59	125 (12%) 9 6	27, 58, 99, 133	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	516	ASN	10.0
1	A	516	ASN	8.8
1	A	361	CYS	6.8
1	A	450	ALA	6.8
1	A	443	PRO	6.4
1	A	138	ILE	6.0
1	A	116	SER	5.8
1	B	443	PRO	5.7
1	A	478	TYR	5.5
1	B	361	CYS	5.0
1	B	440	PHE	4.7
1	A	250	SER	4.7
1	A	370	ARG	4.6
1	A	363	LEU	4.6
1	A	365	ASN	4.6
1	A	366	LYS	4.6
1	A	449	GLY	4.4
1	A	441	THR	4.4
1	B	138	ILE	4.4
1	A	373	CYS	4.3
1	B	478	TYR	4.3
1	A	368	ASN	4.3
1	B	310	VAL	4.2
1	B	28	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	362	SER	4.1
1	A	369	HIS	4.0
1	A	409	ARG	4.0
1	B	567	GLU	4.0
1	B	450	ALA	3.8
1	A	446	PRO	3.8
1	B	434	TYR	3.8
1	B	372	VAL	3.6
1	A	54	THR	3.6
1	B	373	CYS	3.6
1	A	434	TYR	3.6
1	A	367	ARG	3.6
1	B	370	ARG	3.6
1	A	371	GLN	3.5
1	A	372	VAL	3.5
1	B	343	TYR	3.4
1	B	371	GLN	3.4
1	B	117	LEU	3.3
1	B	474	THR	3.3
1	B	366	LYS	3.3
1	A	487	ALA	3.3
1	A	457	ASP	3.3
1	B	526	VAL	3.3
1	B	29	MET	3.3
1	B	368	ASN	3.2
1	B	449	GLY	3.2
1	A	55	GLU	3.2
1	A	440	PHE	3.1
1	B	487	ALA	3.1
1	B	362	SER	3.1
1	B	363	LEU	3.1
1	A	315	HIS	3.1
1	B	515	PRO	3.1
1	A	515	PRO	3.0
1	B	250	SER	3.0
1	A	310	VAL	3.0
1	B	441	THR	3.0
1	A	523	PRO	2.9
1	A	444	PHE	2.9
1	B	369	HIS	2.9
1	B	444	PHE	2.9
1	B	315	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	566	PRO	2.9
1	B	57	CYS	2.8
1	A	517	GLU	2.8
1	A	117	LEU	2.8
1	B	524	GLY	2.8
1	B	517	GLU	2.8
1	A	564	ASN	2.8
1	A	526	VAL	2.7
1	A	451	ASP	2.7
1	A	534	CYS	2.7
1	A	520	ASN	2.7
1	B	251	ASN	2.6
1	B	365	ASN	2.6
1	A	438	ILE	2.5
1	B	252	ILE	2.5
1	B	442	ALA	2.5
1	B	523	PRO	2.5
1	A	524	GLY	2.5
1	B	565	LEU	2.5
1	B	139	PRO	2.4
1	A	432	LYS	2.4
1	B	54	THR	2.4
1	A	476	GLY	2.4
1	A	240	CYS	2.4
1	B	521	MET	2.4
1	B	551	PRO	2.4
1	B	241	ILE	2.4
1	B	367	ARG	2.3
1	A	511	ASP	2.3
1	B	374	ASP	2.3
1	B	409	ARG	2.3
1	A	252	ILE	2.3
1	B	448	LYS	2.2
1	A	442	ALA	2.2
1	B	520	ASN	2.2
1	B	364	GLN	2.2
1	B	432	LYS	2.2
1	A	256	TYR	2.2
1	B	318	TYR	2.2
1	B	534	CYS	2.2
1	B	479	SER	2.2
1	B	446	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	343	TYR	2.1
1	A	332	GLN	2.1
1	A	529	TRP	2.1
1	B	475	GLY	2.1
1	A	546	CYS	2.1
1	B	359	PHE	2.1
1	A	270	ARG	2.1
1	A	567	GLU	2.1
1	B	527	CYS	2.1
1	B	335	ARG	2.0
1	A	447	ASN	2.0
1	A	53	GLY	2.0
1	A	364	GLN	2.0
1	A	115	ALA	2.0
1	A	374	ASP	2.0
1	A	328	HIS	2.0
1	B	498	HIS	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 oligosaccharides 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. 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	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	A	801	14/15	0.66	0.14	87,89,93,94	0
2	NAG	B	802	14/15	0.76	0.11	86,90,92,93	0
3	C5A	B	2001	12/12	0.94	0.09	36,39,40,41	0
3	C5A	A	1001	12/12	0.97	0.07	35,37,38,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.