



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:50 AM UTC

PDB ID : 1R4L / pdb_00001r4l
Title : Inhibitor Bound Human Angiotensin Converting Enzyme-Related Carboxypeptidase (ACE2)
Authors : Towler, P.; Staker, B.; Prasad, S.G.; Menon, S.; Ryan, D.; Tang, J.; Parsons, T.; Fisher, M.; Williams, D.; Dales, N.A.; Patane, M.A.; Pantoliano, M.W.
Deposited on : 2003-10-07
Resolution : 3.00 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

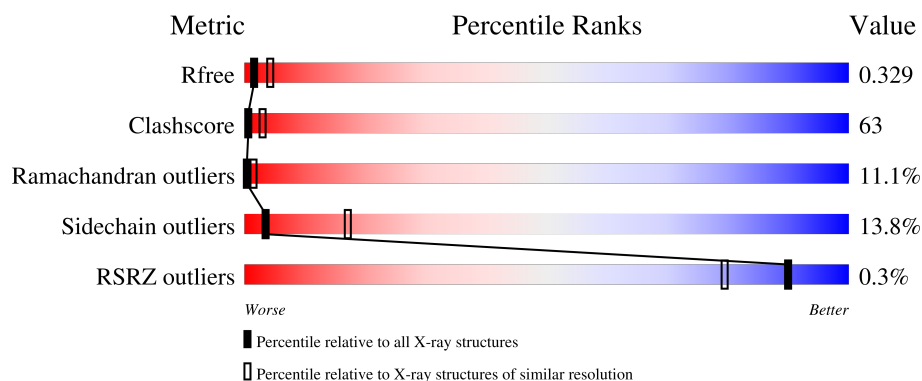
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	615	
2	B	6	
3	C	20	
4	D	18	

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Mol	Chain	Length	Quality of chain
5	E	14	 64%36%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	A	800	X	-	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 5218 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 angiotensin I converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	597	Total	C	N	O	S	0	0	0
			4853	3103	805	916	29			

- Molecule 2 is a protein called disordered segment of collectrin homology domain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	6	Total	C	N	O	0	0	0
			31	18	6	7			

- Molecule 3 is a protein called disordered segment of collectrin homology domain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	20	Total	C	N	O	0	0	0
			101	60	20	21			

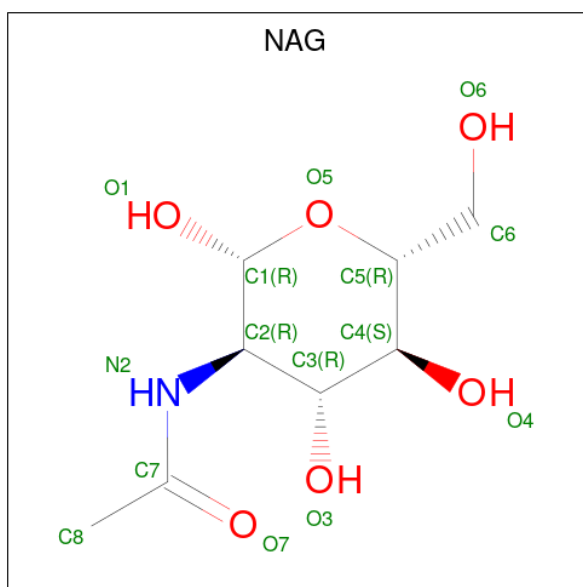
- Molecule 4 is a protein called disordered segment of collectrin homology domain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	18	Total	C	N	O	0	0	0
			91	54	18	19			

- Molecule 5 is a protein called disordered segment of collectrin homology domain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	14	Total	C	N	O	0	0	0
			71	42	14	15			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

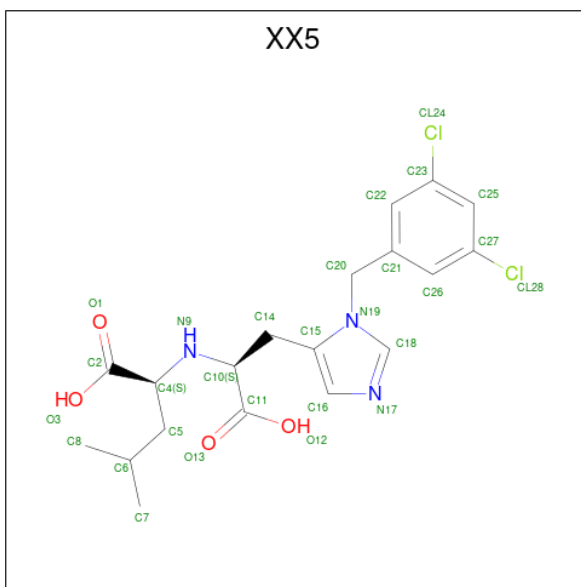
- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Zn	0	0
			1	1		

- Molecule 9 is (S,S)-2-{1-CARBOXY-2-[3-(3,5-DICHLORO-BENZYL)-3H-IMIDAZO L-4-YL]-ETHYLAMINO}-4-METHYL-PENTANOIC ACID (CCD ID: XX5) (formula: C₁₉H₂₃Cl₂N₃O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	Cl	N	O	0	0
			28	19	2	3	4		

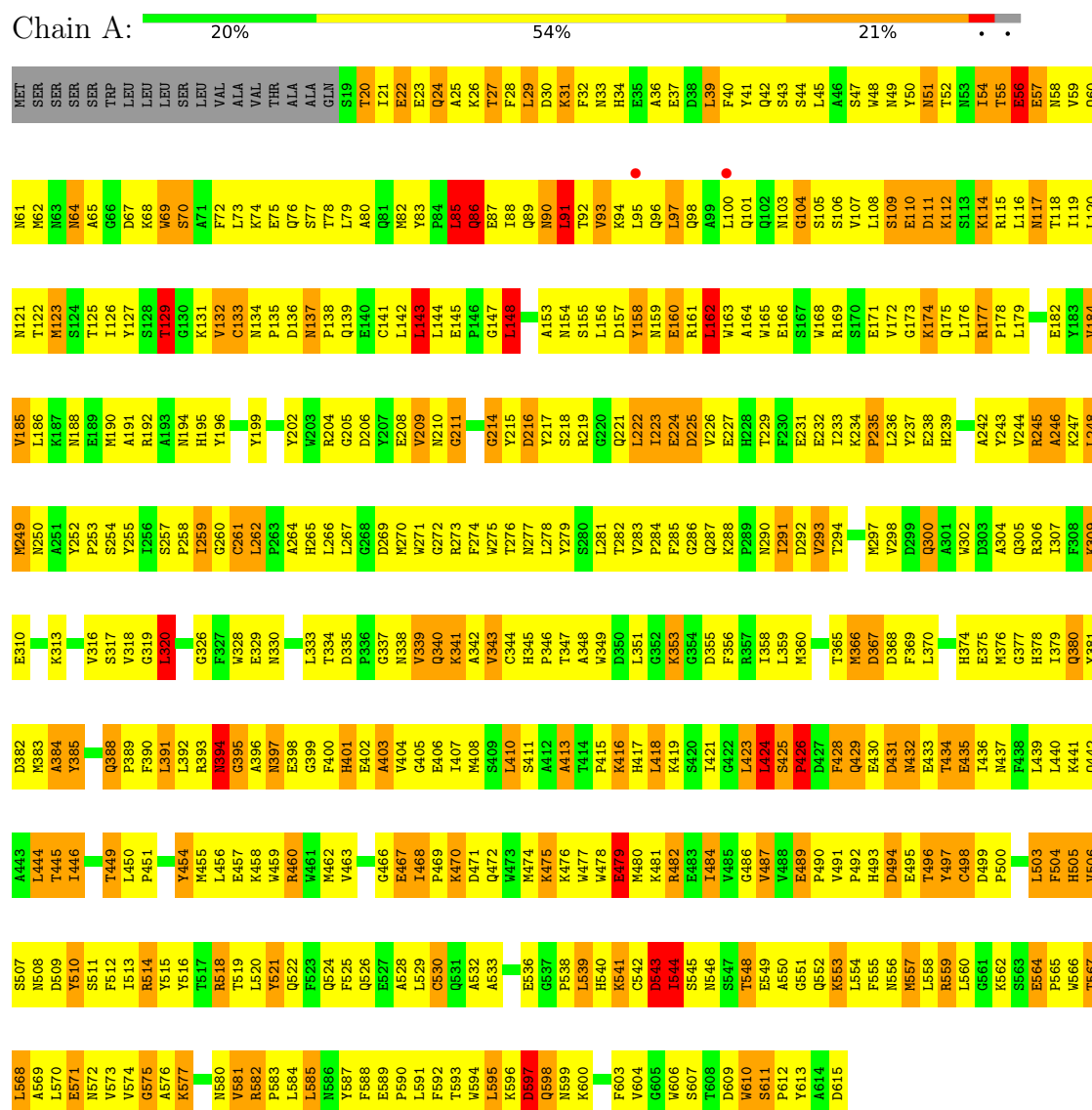
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	13	Total	O	0	0
			13	13		

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: angiotensin I converting enzyme 2



• Molecule 2: disordered segment of collectrin homology domain

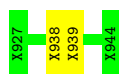
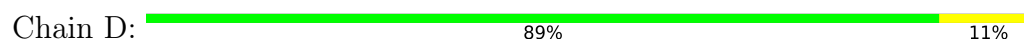




- Molecule 3: disordered segment of collectrin homology domain



- Molecule 4: disordered segment of collectrin homology domain



- Molecule 5: disordered segment of collectrin homology domain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	100.53Å 86.51Å 105.86Å 90.00° 103.65° 90.00°	Depositor
Resolution (Å)	43.26 – 3.00 43.26 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.8 (43.26-3.00) 96.8 (43.26-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.61Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, R_{free}	0.253 , 0.337 0.243 , 0.329	Depositor DCC
R_{free} test set	1730 reflections (8.11%)	wwPDB-VP
Wilson B-factor (Å ²)	60.0	Xtriage
Anisotropy	0.523	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 74.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5218	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.46% 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: CL, XX5, ZN, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.51	0/4989	1.10	48/6779 (0.7%)

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 (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	245	ARG	N-CA-C	-11.66	99.15	113.50
1	A	479	GLU	N-CA-C	-10.50	99.84	111.07
1	A	496	THR	N-CA-C	-8.22	103.39	113.41
1	A	64	ASN	N-CA-C	-8.11	102.39	113.18
1	A	160	GLU	N-CA-C	-7.83	102.69	111.07
1	A	22	GLU	N-CA-C	-7.71	102.72	113.20
1	A	541	LYS	N-CA-C	-7.65	102.84	114.16
1	A	204	ARG	N-CA-C	-7.25	104.40	113.18
1	A	148	LEU	N-CA-C	-7.00	102.86	111.33
1	A	162	LEU	N-CA-C	6.91	118.46	111.07
1	A	449	THR	N-CA-C	6.87	119.79	111.82
1	A	31	LYS	N-CA-C	-6.83	104.20	112.54
1	A	264	ALA	N-CA-C	6.79	121.17	112.34
1	A	249	MET	N-CA-C	-6.56	104.21	111.36
1	A	530	CYS	N-CA-C	-6.55	104.06	111.07
1	A	549	GLU	N-CA-C	-6.41	103.57	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	595	LEU	N-CA-C	-6.36	104.40	111.71
1	A	143	LEU	N-CA-C	-6.29	102.42	110.53
1	A	548	THR	N-CA-C	-6.18	105.22	112.89
1	A	533	ALA	N-CA-C	-6.11	103.42	113.50
1	A	70	SER	N-CA-C	-6.06	104.36	110.97
1	A	214	GLY	N-CA-C	-6.01	107.39	115.21
1	A	366	MET	N-CA-C	-6.01	105.44	112.89
1	A	69	TRP	N-CA-C	-5.97	104.85	111.71
1	A	272	GLY	N-CA-C	-5.96	106.50	115.32
1	A	320	LEU	CA-C-N	5.96	127.29	119.84
1	A	320	LEU	C-N-CA	5.96	127.29	119.84
1	A	489	GLU	CA-C-N	5.92	126.03	119.87
1	A	489	GLU	C-N-CA	5.92	126.03	119.87
1	A	582	ARG	CA-C-N	-5.86	112.83	119.28
1	A	582	ARG	C-N-CA	-5.86	112.83	119.28
1	A	57	GLU	N-CA-C	-5.82	104.28	111.33
1	A	434	THR	N-CA-C	-5.68	106.19	113.01
1	A	24	GLN	N-CA-C	-5.67	106.20	113.01
1	A	132	VAL	N-CA-C	-5.66	100.33	108.48
1	A	137	ASN	CA-C-N	5.56	126.79	119.84
1	A	137	ASN	C-N-CA	5.56	126.79	119.84
1	A	112	LYS	N-CA-C	-5.55	105.61	112.72
1	A	521	TYR	N-CA-C	-5.51	105.17	111.07
1	A	208	GLU	N-CA-C	5.45	118.35	110.28
1	A	425	SER	CA-C-N	5.33	126.50	119.84
1	A	425	SER	C-N-CA	5.33	126.50	119.84
1	A	446	ILE	N-CA-C	5.26	115.92	110.82
1	A	367	ASP	N-CA-C	-5.20	105.52	111.14
1	A	482	ARG	N-CA-C	5.10	117.62	111.40
1	A	309	LYS	N-CA-C	-5.09	106.75	113.12
1	A	468	ILE	CA-C-N	5.07	124.83	119.76
1	A	468	ILE	C-N-CA	5.07	124.83	119.76

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	510	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	4853	0	4619	615	1
2	B	31	0	9	5	0
3	C	101	0	32	12	0
4	D	91	0	21	1	0
5	E	71	0	17	3	0
6	A	28	0	26	3	0
7	A	1	0	0	1	0
8	A	1	0	0	0	0
9	A	28	0	21	1	0
10	A	13	0	0	0	0
All	All	5218	0	4745	631	1

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 63.

All (631) 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)
2:B:905:UNK:HA	3:C:907:UNK:HA	1.36	1.07
1:A:97:LEU:HD12	1:A:101:GLN:HE21	1.26	0.96
1:A:287:GLN:HE22	1:A:288:LYS:HG2	1.31	0.94
1:A:177:ARG:HB3	1:A:178:PRO:HD3	1.49	0.92
1:A:86:GLN:HE21	1:A:87:GLU:N	1.65	0.92
1:A:388:GLN:HG3	1:A:389:PRO:HD2	1.55	0.89
1:A:341:LYS:H	1:A:341:LYS:HD2	1.38	0.88
1:A:539:LEU:HD23	1:A:539:LEU:H	1.36	0.88
1:A:224:GLU:HA	1:A:227:GLU:HG3	1.56	0.87
1:A:229:THR:HG23	1:A:516:TYR:OH	1.75	0.86
1:A:406:GLU:HG3	1:A:518:ARG:HE	1.41	0.85
1:A:557:MET:O	1:A:557:MET:HE3	1.75	0.85
1:A:559:ARG:HD2	1:A:560:LEU:HD22	1.60	0.84
1:A:97:LEU:HD12	1:A:101:GLN:NE2	1.92	0.84
1:A:131:LYS:HE2	1:A:143:LEU:HD13	1.58	0.83
1:A:224:GLU:HA	1:A:227:GLU:CG	2.08	0.83
1:A:571:GLU:HG3	1:A:577:LYS:HB3	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:HIS:O	1:A:404:VAL:HG12	1.81	0.81
1:A:174:LYS:HD2	1:A:496:THR:HG23	1.62	0.80
1:A:494:ASP:OD2	1:A:495:GLU:N	2.15	0.80
1:A:79:LEU:O	1:A:79:LEU:HD23	1.82	0.80
1:A:275:TRP:O	1:A:444:LEU:HG	1.82	0.79
1:A:610:TRP:CG	1:A:611:SER:H	1.97	0.79
1:A:132:VAL:HG21	1:A:148:LEU:HD11	1.64	0.78
1:A:552:GLN:HE21	1:A:556:ASN:HD21	1.32	0.77
1:A:339:VAL:O	1:A:340:GLN:HB3	1.85	0.77
1:A:457:GLU:HG2	1:A:512:PHE:HB3	1.66	0.77
1:A:117:ASN:N	1:A:117:ASN:HD22	1.83	0.77
1:A:431:ASP:HB2	1:A:434:THR:HG23	1.67	0.76
1:A:439:LEU:HD23	1:A:591:LEU:HB2	1.67	0.76
1:A:310:GLU:OE2	1:A:421:ILE:HD11	1.84	0.76
1:A:47:SER:HA	1:A:62:MET:HG3	1.67	0.76
1:A:95:LEU:HA	1:A:98:GLN:HE21	1.50	0.76
1:A:520:LEU:HD21	1:A:581:VAL:HG23	1.68	0.76
1:A:552:GLN:NE2	1:A:556:ASN:HD21	1.83	0.75
1:A:454:TYR:CD1	1:A:454:TYR:C	2.60	0.75
1:A:91:LEU:HD13	1:A:91:LEU:H	1.51	0.74
1:A:318:VAL:O	1:A:551:GLY:HA3	1.86	0.74
1:A:458:LYS:HE3	1:A:462:MET:SD	2.28	0.73
1:A:155:SER:O	1:A:161:ARG:HD3	1.89	0.73
1:A:85:LEU:HG	1:A:86:GLN:H	1.53	0.72
1:A:476:LYS:O	1:A:480:MET:HG3	1.89	0.72
1:A:500:PRO:O	1:A:506:VAL:HG11	1.88	0.72
1:A:21:ILE:HG13	1:A:24:GLN:NE2	2.05	0.71
1:A:158:TYR:CE2	1:A:162:LEU:HD12	2.25	0.71
1:A:50:TYR:OH	1:A:125:THR:HG22	1.91	0.71
1:A:104:GLY:C	1:A:106:SER:H	1.98	0.71
1:A:125:THR:O	1:A:129:THR:HB	1.90	0.71
1:A:249:MET:SD	1:A:258:PRO:HG3	2.31	0.71
1:A:244:VAL:O	1:A:248:LEU:HB2	1.91	0.71
1:A:293:VAL:HG21	1:A:418:LEU:HD11	1.71	0.71
1:A:105:SER:OG	1:A:190:MET:HG3	1.91	0.71
1:A:418:LEU:O	1:A:421:ILE:HG22	1.91	0.71
1:A:91:LEU:HD13	1:A:91:LEU:N	2.06	0.70
1:A:454:TYR:C	1:A:454:TYR:HD1	1.97	0.70
1:A:338:ASN:O	1:A:339:VAL:HB	1.90	0.70
1:A:168:TRP:O	1:A:172:VAL:HG22	1.91	0.70
1:A:398:GLU:HB2	1:A:514:ARG:HB3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:VAL:O	1:A:574:VAL:HG23	1.91	0.70
1:A:248:LEU:HD12	1:A:262:LEU:HD23	1.73	0.69
1:A:320:LEU:HD12	1:A:380:GLN:HG3	1.74	0.69
1:A:320:LEU:H	1:A:320:LEU:HD22	1.58	0.69
1:A:459:TRP:O	1:A:463:VAL:HG23	1.92	0.69
1:A:341:LYS:HD2	1:A:341:LYS:N	2.08	0.68
1:A:610:TRP:O	1:A:611:SER:HB2	1.93	0.68
1:A:455:MET:HE1	1:A:481:LYS:NZ	2.09	0.68
1:A:26:LYS:HD3	6:A:800:NAG:O6	1.95	0.67
1:A:384:ALA:O	1:A:559:ARG:HA	1.94	0.67
1:A:245:ARG:HH12	1:A:260:GLY:N	1.91	0.67
3:C:916:UNK:O	3:C:918:UNK:N	2.28	0.67
1:A:199:TYR:O	1:A:202:TYR:HB3	1.93	0.67
1:A:396:ALA:HB1	1:A:566:TRP:HB3	1.76	0.67
1:A:388:GLN:HG3	1:A:389:PRO:CD	2.22	0.67
1:A:29:LEU:O	1:A:32:PHE:HB3	1.94	0.67
1:A:287:GLN:NE2	1:A:288:LYS:HG2	2.07	0.67
1:A:121:ASN:O	1:A:125:THR:HG23	1.95	0.66
1:A:90:ASN:O	1:A:93:VAL:HG22	1.94	0.66
1:A:169:ARG:HG3	1:A:169:ARG:HH21	1.59	0.66
1:A:425:SER:HB2	1:A:426:PRO:HD2	1.78	0.66
1:A:396:ALA:O	1:A:562:LYS:HE3	1.95	0.66
1:A:410:LEU:HD11	1:A:587:TYR:CE1	2.31	0.66
1:A:172:VAL:HG23	1:A:173:GLY:N	2.10	0.66
1:A:406:GLU:HG3	1:A:518:ARG:NE	2.09	0.66
1:A:25:ALA:HA	1:A:28:PHE:HB3	1.76	0.66
1:A:333:LEU:O	1:A:334:THR:HG23	1.97	0.66
1:A:419:LYS:HA	1:A:424:LEU:HB3	1.77	0.65
1:A:293:VAL:HG11	1:A:418:LEU:HD12	1.77	0.65
1:A:320:LEU:H	1:A:320:LEU:CD2	2.09	0.65
1:A:593:THR:HA	1:A:596:LYS:HG3	1.77	0.65
1:A:593:THR:O	1:A:596:LYS:HB2	1.96	0.65
1:A:23:GLU:O	1:A:27:THR:HG22	1.97	0.65
1:A:356:PHE:CE2	1:A:383:MET:HG2	2.32	0.65
1:A:505:HIS:O	1:A:509:ASP:O	2.14	0.65
1:A:381:TYR:OH	1:A:395:GLY:HA2	1.96	0.65
1:A:455:MET:CE	1:A:481:LYS:HZ2	2.09	0.65
1:A:21:ILE:C	1:A:23:GLU:H	2.05	0.65
1:A:554:LEU:O	1:A:558:LEU:HD13	1.97	0.64
1:A:292:ASP:O	1:A:294:THR:N	2.27	0.64
1:A:245:ARG:O	1:A:249:MET:HG3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:ALA:O	1:A:248:LEU:N	2.31	0.64
1:A:68:LYS:O	1:A:68:LYS:HD3	1.98	0.63
1:A:95:LEU:HA	1:A:98:GLN:NE2	2.13	0.63
1:A:260:GLY:HA2	1:A:607:SER:H	1.62	0.63
1:A:85:LEU:H	1:A:85:LEU:HD23	1.62	0.63
1:A:157:ASP:O	1:A:159:ASN:N	2.32	0.62
1:A:499:ASP:HB3	7:A:802:CL:CL	2.36	0.62
1:A:74:LYS:HD3	1:A:106:SER:HB2	1.81	0.62
1:A:27:THR:HG23	1:A:28:PHE:H	1.64	0.62
1:A:291:ILE:HG23	1:A:291:ILE:O	1.98	0.62
3:C:923:UNK:O	3:C:924:UNK:C	2.47	0.62
1:A:353:LYS:HE3	1:A:353:LYS:HA	1.81	0.61
1:A:552:GLN:HE21	1:A:556:ASN:ND2	1.98	0.61
3:C:923:UNK:O	3:C:925:UNK:N	2.33	0.61
1:A:245:ARG:HH12	1:A:260:GLY:C	2.08	0.61
1:A:292:ASP:C	1:A:294:THR:H	2.08	0.61
1:A:474:MET:HE1	1:A:499:ASP:HB2	1.83	0.61
1:A:503:LEU:HD22	1:A:503:LEU:O	2.00	0.61
1:A:436:ILE:HG21	1:A:594:TRP:CE2	2.35	0.61
1:A:91:LEU:HD22	1:A:92:THR:H	1.66	0.60
1:A:245:ARG:NH1	1:A:260:GLY:N	2.49	0.60
1:A:252:TYR:O	1:A:255:TYR:HB2	2.01	0.60
1:A:259:ILE:HG13	1:A:603:PHE:CE1	2.37	0.60
1:A:610:TRP:CG	1:A:611:SER:N	2.69	0.60
1:A:243:TYR:HB2	1:A:599:ASN:HD21	1.65	0.60
1:A:413:ALA:HA	1:A:418:LEU:HD23	1.84	0.60
1:A:385:TYR:CD2	1:A:393:ARG:HB2	2.37	0.60
1:A:95:LEU:HD12	1:A:96:GLN:N	2.16	0.60
1:A:209:VAL:HG22	1:A:217:TYR:N	2.17	0.59
1:A:175:GLN:O	1:A:178:PRO:HD2	2.02	0.59
1:A:209:VAL:HG22	1:A:217:TYR:H	1.68	0.59
1:A:246:ALA:O	1:A:249:MET:N	2.35	0.59
1:A:209:VAL:HG23	1:A:216:ASP:HA	1.85	0.59
1:A:25:ALA:C	1:A:27:THR:H	2.09	0.59
1:A:440:LEU:HD13	1:A:440:LEU:O	2.02	0.59
1:A:95:LEU:HA	1:A:98:GLN:HG3	1.83	0.59
1:A:514:ARG:O	1:A:518:ARG:HB3	2.02	0.59
1:A:478:TRP:CE3	1:A:489:GLU:HB3	2.38	0.59
1:A:72:PHE:HE1	1:A:76:GLN:HE21	1.50	0.59
1:A:477:TRP:CH2	1:A:500:PRO:HB3	2.38	0.59
1:A:132:VAL:HG22	1:A:148:LEU:HD21	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ARG:HB3	1:A:178:PRO:CD	2.28	0.59
1:A:131:LYS:HE2	1:A:143:LEU:CD1	2.31	0.58
1:A:339:VAL:O	1:A:340:GLN:CB	2.51	0.58
1:A:521:TYR:HB3	1:A:525:PHE:HE1	1.68	0.58
1:A:594:TRP:CH2	1:A:598:GLN:HG3	2.37	0.58
1:A:261:CYS:H	1:A:606:TRP:HB2	1.67	0.58
1:A:554:LEU:HG	1:A:558:LEU:CD1	2.33	0.58
1:A:158:TYR:O	1:A:162:LEU:HB2	2.04	0.58
1:A:242:ALA:HB1	1:A:603:PHE:O	2.04	0.58
1:A:365:THR:HG22	1:A:367:ASP:H	1.68	0.58
1:A:257:SER:C	1:A:259:ILE:H	2.11	0.58
1:A:184:VAL:O	1:A:188:ASN:HB2	2.04	0.58
1:A:380:GLN:HE21	1:A:380:GLN:HA	1.68	0.58
1:A:489:GLU:OE2	1:A:489:GLU:N	2.23	0.58
3:C:907:UNK:C	5:E:958:UNK:HA	2.33	0.58
1:A:43:SER:HA	1:A:65:ALA:HB1	1.86	0.58
1:A:157:ASP:OD2	1:A:159:ASN:HB2	2.03	0.58
1:A:538:PRO:HB2	1:A:540:HIS:CD2	2.38	0.58
1:A:544:ILE:HD13	1:A:544:ILE:O	2.04	0.58
1:A:245:ARG:HH12	1:A:260:GLY:CA	2.17	0.58
1:A:89:GLN:O	1:A:90:ASN:C	2.47	0.58
1:A:54:ILE:HG13	1:A:341:LYS:O	2.04	0.57
1:A:115:ARG:O	1:A:119:ILE:HG13	2.04	0.57
1:A:431:ASP:C	1:A:433:GLU:H	2.12	0.57
1:A:245:ARG:NH1	1:A:260:GLY:H	2.02	0.57
1:A:388:GLN:CG	1:A:389:PRO:HD2	2.32	0.57
1:A:86:GLN:HE21	1:A:86:GLN:C	2.11	0.57
1:A:457:GLU:OE2	1:A:460:ARG:NH1	2.37	0.57
1:A:86:GLN:HE21	1:A:87:GLU:H	1.51	0.57
1:A:177:ARG:HD3	1:A:497:TYR:O	2.04	0.57
1:A:21:ILE:HG13	1:A:24:GLN:HE21	1.67	0.57
1:A:505:HIS:HE1	1:A:515:TYR:OH	1.88	0.57
1:A:494:ASP:C	1:A:496:THR:H	2.13	0.57
1:A:137:ASN:C	1:A:137:ASN:HD22	2.12	0.56
1:A:266:LEU:O	1:A:278:LEU:HD11	2.05	0.56
1:A:529:LEU:HA	1:A:532:ALA:HB3	1.87	0.56
1:A:406:GLU:CG	1:A:518:ARG:HE	2.15	0.56
1:A:525:PHE:HA	1:A:574:VAL:HG11	1.86	0.56
1:A:96:GLN:HG3	1:A:392:LEU:HD13	1.87	0.56
1:A:492:PRO:HG3	1:A:613:TYR:CE1	2.40	0.56
1:A:262:LEU:HD12	1:A:262:LEU:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:ALA:O	1:A:573:VAL:HG23	2.06	0.56
1:A:40:PHE:O	1:A:43:SER:N	2.35	0.56
1:A:104:GLY:C	1:A:106:SER:N	2.63	0.56
1:A:399:GLY:HA3	1:A:521:TYR:HE2	1.70	0.56
1:A:613:TYR:C	1:A:615:ASP:H	2.13	0.56
1:A:397:ASN:N	1:A:397:ASN:HD22	2.04	0.56
1:A:592:PHE:O	1:A:596:LYS:HG2	2.06	0.56
1:A:192:ARG:HA	1:A:196:TYR:O	2.05	0.56
1:A:222:LEU:O	1:A:226:VAL:HG23	2.06	0.56
1:A:22:GLU:O	1:A:22:GLU:HG2	2.05	0.56
1:A:359:LEU:C	1:A:359:LEU:HD23	2.31	0.56
1:A:441:LYS:O	1:A:444:LEU:HB2	2.06	0.56
1:A:597:ASP:O	1:A:598:GLN:C	2.49	0.56
1:A:122:THR:O	1:A:123:MET:C	2.49	0.55
1:A:411:SER:OG	1:A:544:ILE:HG22	2.06	0.55
2:B:905:UNK:CA	3:C:907:UNK:HA	2.22	0.55
1:A:62:MET:C	1:A:64:ASN:H	2.14	0.55
1:A:214:GLY:O	1:A:577:LYS:HE2	2.07	0.55
1:A:246:ALA:C	1:A:248:LEU:H	2.13	0.55
1:A:554:LEU:O	1:A:557:MET:HB3	2.06	0.55
1:A:90:ASN:O	1:A:92:THR:N	2.39	0.55
1:A:403:ALA:HB2	1:A:518:ARG:HA	1.89	0.55
1:A:521:TYR:HB3	1:A:525:PHE:CE1	2.41	0.55
1:A:246:ALA:HA	1:A:249:MET:HE2	1.89	0.55
1:A:554:LEU:HG	1:A:558:LEU:HD13	1.88	0.55
1:A:23:GLU:OE2	1:A:23:GLU:HA	2.07	0.55
1:A:454:TYR:HD1	1:A:454:TYR:O	1.90	0.55
1:A:20:THR:HG22	1:A:22:GLU:H	1.71	0.55
1:A:103:ASN:OD1	6:A:801:NAG:C2	2.56	0.54
1:A:293:VAL:HB	1:A:423:LEU:HB3	1.89	0.54
1:A:595:LEU:O	1:A:599:ASN:HB2	2.07	0.54
1:A:25:ALA:C	1:A:27:THR:N	2.66	0.54
1:A:51:ASN:O	1:A:359:LEU:HD11	2.07	0.54
1:A:109:SER:O	1:A:110:GLU:C	2.50	0.54
1:A:182:GLU:O	1:A:186:LEU:HD23	2.07	0.54
1:A:210:ASN:O	1:A:211:GLY:C	2.50	0.54
1:A:525:PHE:O	1:A:529:LEU:HG	2.07	0.54
1:A:445:THR:HG22	1:A:446:ILE:N	2.23	0.54
1:A:594:TRP:CZ3	1:A:598:GLN:HG3	2.43	0.54
1:A:85:LEU:HG	1:A:86:GLN:CD	2.33	0.54
1:A:317:SER:O	1:A:546:ASN:HA	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:SER:OG	1:A:543:ASP:O	2.21	0.54
1:A:309:LYS:HD2	1:A:328:TRP:CZ2	2.43	0.53
1:A:458:LYS:O	1:A:462:MET:HG2	2.09	0.53
1:A:543:ASP:OD2	1:A:543:ASP:N	2.25	0.53
1:A:78:THR:C	1:A:80:ALA:H	2.16	0.53
1:A:215:TYR:O	1:A:567:THR:HG21	2.09	0.53
1:A:259:ILE:HG13	1:A:603:PHE:CD1	2.44	0.53
1:A:277:ASN:C	1:A:279:TYR:H	2.16	0.53
1:A:122:THR:HG22	1:A:126:ILE:HG12	1.89	0.53
1:A:432:ASN:HD22	1:A:433:GLU:N	2.07	0.53
1:A:221:GLN:O	1:A:222:LEU:C	2.51	0.53
1:A:391:LEU:HD12	1:A:391:LEU:C	2.33	0.53
1:A:431:ASP:C	1:A:433:GLU:N	2.65	0.53
1:A:22:GLU:CD	1:A:89:GLN:H	2.17	0.53
1:A:570:LEU:HD23	1:A:574:VAL:HG22	1.90	0.53
1:A:261:CYS:HB2	1:A:487:VAL:HA	1.91	0.52
1:A:284:PRO:HG2	1:A:437:ASN:OD1	2.09	0.52
1:A:497:TYR:O	1:A:498:CYS:HB2	2.07	0.52
1:A:500:PRO:O	1:A:506:VAL:HG21	2.08	0.52
1:A:584:LEU:HD23	1:A:584:LEU:C	2.34	0.52
1:A:137:ASN:HD21	1:A:139:GLN:HE21	1.58	0.52
1:A:169:ARG:HG3	1:A:169:ARG:NH2	2.25	0.52
1:A:293:VAL:O	1:A:297:MET:HG3	2.10	0.52
1:A:398:GLU:O	1:A:399:GLY:C	2.52	0.52
1:A:269:ASP:O	1:A:271:TRP:N	2.42	0.52
1:A:466:GLY:O	1:A:468:ILE:N	2.43	0.52
1:A:556:ASN:O	1:A:560:LEU:HD21	2.09	0.52
1:A:88:ILE:HD12	1:A:94:LYS:HA	1.92	0.52
1:A:320:LEU:HD22	1:A:320:LEU:N	2.25	0.52
1:A:335:ASP:C	1:A:337:GLY:H	2.17	0.52
1:A:479:GLU:O	1:A:482:ARG:HB2	2.10	0.52
1:A:455:MET:HE1	1:A:481:LYS:HZ3	1.74	0.52
1:A:609:ASP:O	1:A:610:TRP:O	2.28	0.52
1:A:480:MET:C	1:A:482:ARG:N	2.66	0.52
1:A:88:ILE:HD11	1:A:94:LYS:HG3	1.92	0.52
1:A:157:ASP:C	1:A:159:ASN:N	2.68	0.52
1:A:410:LEU:HD23	1:A:522:GLN:NE2	2.25	0.52
1:A:492:PRO:HG3	1:A:613:TYR:CZ	2.44	0.52
1:A:326:GLY:O	1:A:330:ASN:OD1	2.27	0.51
1:A:402:GLU:HB2	1:A:518:ARG:HB2	1.92	0.51
1:A:209:VAL:CG2	1:A:216:ASP:HA	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:VAL:C	1:A:300:GLN:H	2.18	0.51
1:A:428:PHE:O	1:A:429:GLN:C	2.52	0.51
1:A:466:GLY:C	1:A:468:ILE:H	2.17	0.51
1:A:86:GLN:O	1:A:88:ILE:HG12	2.11	0.51
1:A:478:TRP:CZ3	1:A:489:GLU:HB3	2.46	0.51
1:A:540:HIS:CD2	1:A:541:LYS:HG2	2.46	0.51
1:A:436:ILE:N	1:A:436:ILE:HD12	2.25	0.51
1:A:494:ASP:OD2	1:A:494:ASP:C	2.54	0.51
1:A:559:ARG:CD	1:A:560:LEU:HD22	2.38	0.51
5:E:956:UNK:O	5:E:957:UNK:C	2.58	0.51
1:A:24:GLN:C	1:A:83:TYR:HE2	2.17	0.51
1:A:176:LEU:O	1:A:177:ARG:C	2.54	0.51
1:A:246:ALA:C	1:A:248:LEU:N	2.69	0.51
1:A:593:THR:HA	1:A:596:LYS:CG	2.41	0.51
1:A:27:THR:HG23	1:A:28:PHE:N	2.25	0.51
1:A:234:LYS:O	1:A:235:PRO:C	2.54	0.51
1:A:306:ARG:HG2	1:A:306:ARG:HH11	1.76	0.51
1:A:455:MET:CE	1:A:481:LYS:NZ	2.71	0.51
1:A:504:PHE:CD1	1:A:508:ASN:ND2	2.79	0.51
1:A:137:ASN:O	1:A:139:GLN:N	2.44	0.51
1:A:192:ARG:C	1:A:194:ASN:H	2.19	0.51
1:A:418:LEU:HD12	1:A:423:LEU:HB2	1.93	0.50
1:A:285:PHE:CD1	1:A:433:GLU:HG2	2.47	0.50
1:A:539:LEU:H	1:A:539:LEU:CD2	2.16	0.50
1:A:257:SER:OG	1:A:259:ILE:HG22	2.11	0.50
1:A:339:VAL:O	1:A:339:VAL:HG12	2.11	0.50
1:A:399:GLY:HA3	1:A:521:TYR:CE2	2.45	0.50
1:A:457:GLU:HG3	1:A:513:ILE:N	2.27	0.50
1:A:543:ASP:O	1:A:544:ILE:HG22	2.12	0.50
1:A:560:LEU:HD22	1:A:560:LEU:H	1.76	0.50
1:A:40:PHE:HB2	1:A:69:TRP:CZ3	2.47	0.50
1:A:103:ASN:OD1	6:A:801:NAG:H2	2.12	0.50
1:A:117:ASN:N	1:A:117:ASN:ND2	2.53	0.50
1:A:374:HIS:HD2	1:A:375:GLU:OE2	1.95	0.50
1:A:390:PHE:O	1:A:393:ARG:HG2	2.11	0.50
1:A:239:HIS:CE1	1:A:596:LYS:HD2	2.47	0.50
1:A:430:GLU:O	1:A:431:ASP:C	2.53	0.50
1:A:110:GLU:C	1:A:112:LYS:H	2.19	0.50
1:A:369:PHE:CD1	1:A:370:LEU:HD23	2.47	0.50
1:A:439:LEU:HD23	1:A:591:LEU:CB	2.39	0.50
1:A:48:TRP:HB2	1:A:349:TRP:CZ3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:VAL:CG2	1:A:173:GLY:N	2.75	0.50
1:A:528:ALA:CB	1:A:574:VAL:HG12	2.42	0.50
1:A:137:ASN:C	1:A:137:ASN:ND2	2.69	0.49
1:A:302:TRP:CZ2	1:A:306:ARG:NH2	2.80	0.49
1:A:445:THR:HG22	1:A:446:ILE:HG13	1.93	0.49
1:A:559:ARG:HH11	1:A:559:ARG:HB2	1.77	0.49
1:A:597:ASP:O	1:A:600:LYS:HG2	2.12	0.49
1:A:106:SER:C	1:A:108:LEU:H	2.20	0.49
1:A:114:LYS:NZ	1:A:114:LYS:CB	2.75	0.49
1:A:184:VAL:CG2	1:A:185:VAL:N	2.75	0.49
1:A:209:VAL:HG21	1:A:215:TYR:O	2.12	0.49
1:A:504:PHE:O	1:A:505:HIS:C	2.54	0.49
1:A:106:SER:C	1:A:108:LEU:N	2.71	0.49
1:A:108:LEU:HD11	1:A:190:MET:HB2	1.94	0.49
1:A:398:GLU:HB2	1:A:514:ARG:HG2	1.93	0.49
1:A:591:LEU:HG	1:A:595:LEU:HD13	1.93	0.49
1:A:162:LEU:O	1:A:162:LEU:HD23	2.12	0.49
1:A:396:ALA:HB1	1:A:566:TRP:CB	2.42	0.49
1:A:21:ILE:C	1:A:23:GLU:N	2.71	0.49
1:A:391:LEU:HD12	1:A:391:LEU:O	2.12	0.49
1:A:574:VAL:O	1:A:575:GLY:C	2.55	0.49
1:A:232:GLU:OE2	1:A:582:ARG:NH1	2.45	0.49
1:A:50:TYR:C	1:A:52:THR:H	2.20	0.49
1:A:165:TRP:HZ3	1:A:493:HIS:HE2	1.56	0.49
2:B:902:UNK:O	3:C:909:UNK:HA	2.13	0.49
1:A:32:PHE:CZ	1:A:100:LEU:HD21	2.47	0.49
1:A:202:TYR:O	1:A:205:GLY:N	2.39	0.49
1:A:346:PRO:HG3	1:A:360:MET:HG3	1.94	0.49
1:A:396:ALA:C	1:A:562:LYS:HE3	2.38	0.49
1:A:109:SER:O	1:A:111:ASP:N	2.46	0.48
1:A:300:GLN:HB3	1:A:302:TRP:HD1	1.77	0.48
1:A:341:LYS:N	1:A:341:LYS:CD	2.75	0.48
1:A:574:VAL:O	1:A:574:VAL:CG2	2.59	0.48
1:A:613:TYR:C	1:A:615:ASP:N	2.69	0.48
1:A:52:THR:O	1:A:52:THR:HG22	2.13	0.48
1:A:319:GLY:O	1:A:320:LEU:O	2.31	0.48
3:C:922:UNK:O	3:C:924:UNK:N	2.46	0.48
1:A:172:VAL:O	1:A:173:GLY:C	2.56	0.48
1:A:503:LEU:O	1:A:504:PHE:C	2.56	0.48
1:A:545:SER:O	1:A:546:ASN:HB2	2.13	0.48
1:A:265:HIS:ND1	1:A:490:PRO:HG2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:ASP:O	1:A:294:THR:HG22	2.14	0.48
1:A:493:HIS:ND1	1:A:497:TYR:CZ	2.82	0.48
1:A:555:PHE:C	1:A:557:MET:H	2.22	0.48
1:A:221:GLN:O	1:A:223:ILE:N	2.47	0.48
1:A:242:ALA:HA	1:A:245:ARG:HD2	1.96	0.48
1:A:555:PHE:C	1:A:555:PHE:CD1	2.92	0.48
1:A:388:GLN:O	1:A:389:PRO:C	2.56	0.48
1:A:587:TYR:HD2	1:A:588:PHE:CE2	2.32	0.48
1:A:59:VAL:O	1:A:62:MET:HB3	2.14	0.47
1:A:137:ASN:ND2	1:A:139:GLN:HE21	2.12	0.47
1:A:253:PRO:O	1:A:254:SER:CB	2.61	0.47
1:A:257:SER:HB2	1:A:610:TRP:NE1	2.29	0.47
1:A:267:LEU:C	1:A:278:LEU:HD11	2.39	0.47
1:A:555:PHE:O	1:A:559:ARG:HG3	2.14	0.47
1:A:559:ARG:HD2	1:A:560:LEU:CD2	2.39	0.47
1:A:117:ASN:HD22	1:A:117:ASN:H	1.58	0.47
1:A:302:TRP:HH2	1:A:310:GLU:HG2	1.80	0.47
1:A:457:GLU:CG	1:A:512:PHE:HB3	2.40	0.47
1:A:253:PRO:O	1:A:254:SER:OG	2.28	0.47
1:A:374:HIS:O	1:A:377:GLY:N	2.47	0.47
1:A:504:PHE:O	1:A:506:VAL:N	2.47	0.47
1:A:85:LEU:HD23	1:A:85:LEU:N	2.28	0.47
1:A:119:ILE:HG23	1:A:179:LEU:HB3	1.95	0.47
1:A:153:ALA:HB1	1:A:277:ASN:OD1	2.15	0.47
1:A:291:ILE:HA	1:A:291:ILE:HD12	1.60	0.47
1:A:540:HIS:CD2	1:A:540:HIS:C	2.91	0.47
1:A:61:ASN:HD22	1:A:61:ASN:N	2.12	0.47
1:A:74:LYS:HD3	1:A:106:SER:CB	2.43	0.47
1:A:91:LEU:N	1:A:91:LEU:CD1	2.77	0.47
1:A:157:ASP:O	1:A:158:TYR:C	2.58	0.47
1:A:440:LEU:HD13	1:A:440:LEU:C	2.39	0.47
1:A:50:TYR:CE1	1:A:59:VAL:HG22	2.50	0.47
1:A:60:GLN:O	1:A:61:ASN:C	2.58	0.47
1:A:229:THR:OG1	1:A:520:LEU:HD21	2.14	0.47
1:A:239:HIS:CD2	1:A:604:VAL:HG11	2.49	0.47
1:A:589:GLU:N	1:A:590:PRO:CD	2.78	0.47
1:A:26:LYS:HE2	1:A:93:VAL:HG11	1.96	0.47
1:A:48:TRP:HA	1:A:349:TRP:CH2	2.49	0.47
1:A:119:ILE:O	1:A:123:MET:HG3	2.14	0.47
1:A:552:GLN:O	1:A:553:LYS:C	2.57	0.47
1:A:236:LEU:HA	1:A:592:PHE:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ASN:ND2	1:A:250:ASN:O	2.48	0.46
1:A:293:VAL:CG2	1:A:423:LEU:HD13	2.45	0.46
1:A:329:GLU:O	1:A:329:GLU:HG2	2.15	0.46
1:A:147:GLY:O	1:A:148:LEU:C	2.58	0.46
1:A:432:ASN:HD22	1:A:432:ASN:N	2.11	0.46
1:A:21:ILE:N	1:A:21:ILE:HD12	2.29	0.46
1:A:32:PHE:CE2	1:A:100:LEU:HD21	2.50	0.46
1:A:141:CYS:O	1:A:142:LEU:HD23	2.16	0.46
1:A:245:ARG:HE	1:A:245:ARG:HB2	1.35	0.46
1:A:526:GLN:O	1:A:530:CYS:SG	2.74	0.46
5:E:945:UNK:O	5:E:946:UNK:C	2.63	0.46
1:A:154:ASN:O	1:A:155:SER:C	2.57	0.46
1:A:292:ASP:C	1:A:294:THR:N	2.73	0.46
1:A:305:GLN:O	1:A:306:ARG:C	2.58	0.46
1:A:385:TYR:CE2	1:A:393:ARG:HB2	2.51	0.46
1:A:472:GLN:OE1	1:A:475:LYS:HG3	2.15	0.46
1:A:243:TYR:C	1:A:243:TYR:CD2	2.94	0.46
1:A:281:LEU:N	1:A:281:LEU:CD1	2.79	0.46
1:A:319:GLY:O	1:A:320:LEU:C	2.58	0.46
1:A:435:GLU:CD	1:A:541:LYS:HE2	2.40	0.46
1:A:514:ARG:H	1:A:514:ARG:HG3	1.53	0.46
1:A:550:ALA:O	1:A:551:GLY:C	2.59	0.46
1:A:174:LYS:CD	1:A:496:THR:HG23	2.41	0.46
1:A:374:HIS:O	1:A:375:GLU:C	2.59	0.46
1:A:376:MET:O	1:A:379:ILE:N	2.49	0.46
1:A:394:ASN:O	1:A:395:GLY:O	2.32	0.46
1:A:442:GLN:HE21	1:A:442:GLN:HA	1.81	0.46
1:A:524:GLN:HG2	1:A:583:PRO:HG3	1.98	0.46
1:A:36:ALA:O	1:A:40:PHE:N	2.40	0.46
1:A:91:LEU:CD2	1:A:92:THR:H	2.29	0.46
1:A:505:HIS:CE1	1:A:515:TYR:OH	2.68	0.46
1:A:109:SER:HB3	1:A:112:LYS:HB3	1.98	0.45
1:A:174:LYS:NZ	1:A:496:THR:HG21	2.31	0.45
1:A:273:ARG:HG2	1:A:274:PHE:CE1	2.51	0.45
1:A:51:ASN:O	1:A:342:ALA:HB1	2.15	0.45
1:A:345:HIS:O	1:A:347:THR:HG23	2.17	0.45
1:A:585:LEU:O	1:A:589:GLU:HG2	2.16	0.45
1:A:316:VAL:HA	1:A:320:LEU:O	2.17	0.45
1:A:353:LYS:HE3	1:A:353:LYS:CA	2.46	0.45
1:A:43:SER:HA	1:A:65:ALA:CB	2.47	0.45
1:A:257:SER:C	1:A:259:ILE:N	2.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:ARG:O	1:A:394:ASN:OD1	2.34	0.45
1:A:67:ASP:O	1:A:70:SER:HB3	2.16	0.45
1:A:86:GLN:HB2	1:A:87:GLU:H	1.47	0.45
1:A:145:GLU:HG2	1:A:344:CYS:CB	2.46	0.45
1:A:234:LYS:HB2	1:A:235:PRO:HD3	1.99	0.45
1:A:503:LEU:O	1:A:505:HIS:N	2.50	0.45
1:A:402:GLU:HA	1:A:402:GLU:OE1	2.17	0.45
1:A:435:GLU:C	1:A:437:ASN:N	2.73	0.45
1:A:456:LEU:HD22	1:A:512:PHE:CD1	2.51	0.45
1:A:505:HIS:CD2	1:A:505:HIS:H	2.35	0.45
1:A:570:LEU:HD23	1:A:574:VAL:CG2	2.47	0.45
3:C:920:UNK:O	3:C:921:UNK:C	2.64	0.45
1:A:30:ASP:O	1:A:34:HIS:HD2	1.99	0.45
1:A:380:GLN:HA	1:A:380:GLN:NE2	2.30	0.45
1:A:442:GLN:HA	1:A:442:GLN:NE2	2.31	0.45
1:A:503:LEU:HD22	1:A:503:LEU:C	2.42	0.45
1:A:132:VAL:CG2	1:A:148:LEU:HD11	2.42	0.45
1:A:261:CYS:HB2	1:A:487:VAL:CA	2.47	0.45
1:A:418:LEU:C	1:A:421:ILE:HG22	2.41	0.45
1:A:145:GLU:HG2	1:A:344:CYS:HB3	1.99	0.45
1:A:267:LEU:C	1:A:278:LEU:CD1	2.91	0.45
1:A:39:LEU:HD11	1:A:68:LYS:HG3	1.98	0.44
1:A:144:LEU:HD22	1:A:168:TRP:CZ2	2.52	0.44
1:A:194:ASN:O	1:A:195:HIS:HB2	2.17	0.44
1:A:226:VAL:HA	1:A:229:THR:HG22	1.98	0.44
1:A:512:PHE:O	1:A:515:TYR:HD2	2.01	0.44
1:A:157:ASP:C	1:A:159:ASN:H	2.25	0.44
1:A:215:TYR:CD2	1:A:568:LEU:HB2	2.53	0.44
1:A:471:ASP:O	1:A:472:GLN:NE2	2.50	0.44
1:A:313:LYS:O	1:A:316:VAL:HG12	2.17	0.44
1:A:125:THR:O	1:A:126:ILE:C	2.60	0.44
1:A:166:GLU:OE1	1:A:493:HIS:HE1	2.00	0.44
1:A:318:VAL:O	1:A:318:VAL:HG23	2.17	0.44
1:A:365:THR:HG22	1:A:366:MET:N	2.32	0.44
1:A:398:GLU:HB2	1:A:514:ARG:CB	2.46	0.44
1:A:469:PRO:O	1:A:470:LYS:C	2.60	0.44
1:A:477:TRP:CZ2	1:A:500:PRO:HB3	2.53	0.44
1:A:480:MET:O	1:A:481:LYS:C	2.59	0.44
1:A:85:LEU:HG	1:A:86:GLN:HG3	1.99	0.44
1:A:252:TYR:N	1:A:253:PRO:CD	2.81	0.44
1:A:109:SER:HB3	1:A:112:LYS:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:MET:HE2	1:A:408:MET:HA	1.99	0.44
1:A:564:GLU:O	1:A:565:PRO:C	2.59	0.44
1:A:49:ASN:HB3	1:A:58:ASN:HD22	1.82	0.44
1:A:120:LEU:HD23	1:A:120:LEU:HA	1.74	0.44
1:A:307:ILE:C	1:A:309:LYS:H	2.25	0.44
1:A:548:THR:O	1:A:552:GLN:CB	2.65	0.44
1:A:20:THR:HG22	1:A:21:ILE:N	2.32	0.44
1:A:462:MET:SD	1:A:467:GLU:OE1	2.75	0.44
1:A:504:PHE:C	1:A:508:ASN:HD22	2.26	0.44
1:A:515:TYR:HD1	1:A:518:ARG:NH2	2.16	0.44
1:A:109:SER:O	1:A:112:LYS:N	2.50	0.44
1:A:226:VAL:HA	1:A:229:THR:CG2	2.48	0.44
1:A:232:GLU:HB3	1:A:585:LEU:HD21	2.00	0.44
1:A:385:TYR:CD2	1:A:385:TYR:C	2.96	0.44
1:A:430:GLU:O	1:A:431:ASP:O	2.35	0.44
1:A:543:ASP:O	1:A:544:ILE:CB	2.65	0.44
1:A:257:SER:O	1:A:259:ILE:N	2.50	0.43
1:A:259:ILE:HG12	1:A:259:ILE:O	2.18	0.43
1:A:402:GLU:HG3	1:A:514:ARG:HB2	2.00	0.43
1:A:410:LEU:HD11	1:A:587:TYR:HE1	1.82	0.43
1:A:460:ARG:NH1	1:A:460:ARG:HG2	2.33	0.43
1:A:50:TYR:C	1:A:52:THR:N	2.76	0.43
1:A:52:THR:HA	1:A:342:ALA:CB	2.48	0.43
1:A:225:ASP:O	1:A:229:THR:HG22	2.19	0.43
1:A:300:GLN:HB3	1:A:302:TRP:CD1	2.53	0.43
1:A:436:ILE:HD12	1:A:436:ILE:H	1.83	0.43
1:A:127:TYR:CZ	1:A:504:PHE:HB2	2.53	0.43
1:A:134:ASN:OD1	1:A:136:ASP:OD1	2.36	0.43
1:A:261:CYS:CB	1:A:486:GLY:C	2.92	0.43
1:A:74:LYS:O	1:A:77:SER:HB3	2.19	0.43
1:A:137:ASN:C	1:A:139:GLN:H	2.25	0.43
1:A:351:LEU:HD13	1:A:355:ASP:OD1	2.18	0.43
4:D:938:UNK:O	4:D:939:UNK:C	2.65	0.43
1:A:115:ARG:NH2	1:A:119:ILE:HG13	2.33	0.43
1:A:304:ALA:O	1:A:305:GLN:C	2.61	0.43
1:A:343:VAL:O	1:A:359:LEU:HD21	2.18	0.43
1:A:435:GLU:OE2	1:A:541:LYS:NZ	2.46	0.43
3:C:912:UNK:O	3:C:920:UNK:CB	2.66	0.43
1:A:48:TRP:HE3	1:A:349:TRP:CD2	2.36	0.43
1:A:56:GLU:O	1:A:59:VAL:N	2.51	0.43
1:A:539:LEU:O	1:A:542:CYS:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:THR:O	1:A:125:THR:N	2.51	0.43
1:A:237:TYR:CZ	1:A:451:PRO:HG3	2.54	0.43
1:A:276:THR:HB	1:A:445:THR:OG1	2.19	0.43
1:A:450:LEU:HD21	1:A:519:THR:HG21	2.01	0.43
1:A:97:LEU:CD1	1:A:101:GLN:HG3	2.48	0.43
1:A:114:LYS:HB2	1:A:114:LYS:HZ2	1.83	0.43
3:C:925:UNK:O	3:C:926:UNK:C	2.66	0.43
1:A:36:ALA:O	1:A:37:GLU:C	2.61	0.43
1:A:108:LEU:O	1:A:110:GLU:N	2.51	0.43
1:A:285:PHE:CD2	1:A:433:GLU:CD	2.97	0.43
1:A:390:PHE:C	1:A:392:LEU:H	2.27	0.43
1:A:431:ASP:O	1:A:433:GLU:N	2.52	0.42
1:A:489:GLU:O	1:A:613:TYR:HE2	2.01	0.42
1:A:568:LEU:CD2	1:A:572:ASN:OD1	2.67	0.42
1:A:587:TYR:CD2	1:A:588:PHE:CE2	3.07	0.42
3:C:918:UNK:O	3:C:919:UNK:CB	2.67	0.42
1:A:76:GLN:O	1:A:80:ALA:HB2	2.19	0.42
1:A:302:TRP:CE3	1:A:306:ARG:HG3	2.54	0.42
1:A:381:TYR:O	1:A:382:ASP:C	2.62	0.42
1:A:610:TRP:O	1:A:611:SER:CB	2.62	0.42
1:A:368:ASP:OD2	9:A:804:XX5:CL24	2.74	0.42
1:A:397:ASN:HD21	1:A:400:PHE:HD1	1.66	0.42
1:A:442:GLN:HE21	1:A:442:GLN:CA	2.32	0.42
1:A:444:LEU:HD12	1:A:444:LEU:HA	1.94	0.42
1:A:594:TRP:HE3	1:A:595:LEU:HD12	1.84	0.42
1:A:28:PHE:HZ	1:A:80:ALA:HB2	1.83	0.42
1:A:215:TYR:HE2	1:A:568:LEU:HA	1.84	0.42
1:A:375:GLU:O	1:A:378:HIS:HB2	2.20	0.42
1:A:285:PHE:CE1	1:A:433:GLU:HG2	2.54	0.42
1:A:390:PHE:C	1:A:390:PHE:CD2	2.98	0.42
1:A:177:ARG:HA	1:A:177:ARG:HD2	1.83	0.42
1:A:226:VAL:CA	1:A:229:THR:HG22	2.50	0.42
1:A:490:PRO:C	1:A:491:VAL:HG23	2.45	0.42
1:A:571:GLU:HA	1:A:576:ALA:O	2.19	0.42
1:A:134:ASN:HA	1:A:135:PRO:HD3	1.92	0.42
1:A:282:THR:O	1:A:283:VAL:C	2.63	0.42
1:A:391:LEU:HD13	1:A:391:LEU:HA	1.83	0.42
1:A:484:ILE:H	1:A:484:ILE:HG13	1.67	0.42
1:A:566:TRP:O	1:A:570:LEU:HB2	2.20	0.42
1:A:390:PHE:O	1:A:393:ARG:CG	2.67	0.42
1:A:554:LEU:HG	1:A:558:LEU:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:THR:C	1:A:80:ALA:N	2.77	0.42
1:A:86:GLN:C	1:A:88:ILE:HG12	2.45	0.42
1:A:242:ALA:O	1:A:245:ARG:HG2	2.20	0.42
1:A:407:ILE:HG23	1:A:526:GLN:NE2	2.35	0.42
1:A:591:LEU:O	1:A:595:LEU:HD13	2.19	0.42
1:A:56:GLU:O	1:A:59:VAL:HB	2.19	0.42
1:A:156:LEU:N	1:A:156:LEU:HD12	2.35	0.42
1:A:237:TYR:O	1:A:238:GLU:C	2.63	0.42
1:A:335:ASP:C	1:A:337:GLY:N	2.78	0.42
1:A:408:MET:O	1:A:411:SER:N	2.53	0.42
1:A:506:VAL:O	1:A:508:ASN:N	2.53	0.42
1:A:597:ASP:O	1:A:600:LYS:N	2.40	0.42
1:A:73:LEU:HA	1:A:73:LEU:HD12	1.80	0.41
1:A:92:THR:O	1:A:94:LYS:N	2.53	0.41
1:A:160:GLU:O	1:A:161:ARG:C	2.63	0.41
1:A:374:HIS:HA	1:A:405:GLY:HA3	2.01	0.41
1:A:277:ASN:C	1:A:279:TYR:N	2.78	0.41
1:A:441:LYS:O	1:A:444:LEU:CB	2.67	0.41
1:A:493:HIS:ND1	1:A:497:TYR:CE1	2.88	0.41
1:A:511:SER:O	1:A:514:ARG:HD2	2.20	0.41
1:A:615:ASP:OXT	2:B:901:UNK:N	2.53	0.41
1:A:117:ASN:ND2	1:A:117:ASN:H	2.16	0.41
1:A:174:LYS:HZ3	1:A:496:THR:HG21	1.85	0.41
1:A:348:ALA:HA	1:A:358:ILE:HG12	2.02	0.41
1:A:456:LEU:CD1	1:A:503:LEU:HD12	2.51	0.41
1:A:466:GLY:C	1:A:468:ILE:N	2.77	0.41
1:A:553:LYS:O	1:A:554:LEU:C	2.61	0.41
1:A:555:PHE:C	1:A:557:MET:N	2.76	0.41
1:A:555:PHE:C	1:A:555:PHE:HD1	2.29	0.41
1:A:55:THR:O	1:A:56:GLU:HB2	2.19	0.41
1:A:95:LEU:CD1	1:A:392:LEU:HD11	2.50	0.41
1:A:377:GLY:O	1:A:378:HIS:C	2.62	0.41
1:A:107:VAL:O	1:A:107:VAL:HG12	2.20	0.41
1:A:116:LEU:O	1:A:119:ILE:HB	2.20	0.41
1:A:320:LEU:CD2	1:A:320:LEU:N	2.78	0.41
1:A:539:LEU:C	1:A:541:LYS:H	2.28	0.41
1:A:80:ALA:C	1:A:82:MET:H	2.28	0.41
1:A:217:TYR:OH	1:A:222:LEU:HA	2.21	0.41
1:A:417:HIS:O	1:A:418:LEU:C	2.64	0.41
1:A:41:TYR:O	1:A:45:LEU:HB2	2.20	0.41
1:A:131:LYS:HG2	1:A:143:LEU:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:TRP:O	1:A:164:ALA:C	2.64	0.41
1:A:44:SER:HB3	1:A:351:LEU:HD23	2.02	0.41
1:A:191:ALA:O	1:A:194:ASN:HB2	2.21	0.41
1:A:524:GLN:NE2	1:A:580:ASN:H	2.19	0.41
1:A:117:ASN:O	1:A:118:THR:C	2.63	0.41
1:A:119:ILE:HD13	1:A:182:GLU:HB2	2.03	0.41
1:A:137:ASN:ND2	1:A:139:GLN:H	2.18	0.41
1:A:237:TYR:CE1	1:A:451:PRO:HG3	2.55	0.41
1:A:285:PHE:O	1:A:287:GLN:N	2.54	0.41
1:A:489:GLU:HA	1:A:490:PRO:HD3	1.81	0.41
1:A:21:ILE:HA	1:A:24:GLN:HE21	1.86	0.41
1:A:33:ASN:N	1:A:33:ASN:HD22	2.18	0.41
1:A:133:CYS:HA	1:A:141:CYS:HA	2.03	0.41
1:A:284:PRO:HG2	1:A:285:PHE:CD1	2.56	0.41
1:A:474:MET:HE1	1:A:499:ASP:CB	2.50	0.41
1:A:474:MET:CE	1:A:499:ASP:H	2.34	0.41
1:A:115:ARG:NH2	1:A:119:ILE:CG1	2.85	0.40
1:A:184:VAL:HG23	1:A:185:VAL:N	2.37	0.40
1:A:425:SER:O	1:A:426:PRO:C	2.63	0.40
2:B:905:UNK:O	2:B:906:UNK:CB	2.70	0.40
1:A:25:ALA:O	1:A:27:THR:N	2.54	0.40
1:A:29:LEU:HD11	1:A:97:LEU:CD2	2.51	0.40
1:A:28:PHE:CE2	1:A:80:ALA:HA	2.56	0.40
1:A:205:GLY:HA2	1:A:219:ARG:HD3	2.02	0.40
1:A:307:ILE:C	1:A:309:LYS:N	2.79	0.40
1:A:512:PHE:O	1:A:515:TYR:CD2	2.75	0.40
1:A:521:TYR:O	1:A:522:GLN:C	2.64	0.40
1:A:22:GLU:OE1	1:A:89:GLN:N	2.46	0.40
1:A:137:ASN:C	1:A:139:GLN:N	2.80	0.40
1:A:313:LYS:C	1:A:316:VAL:HG12	2.47	0.40
1:A:376:MET:O	1:A:377:GLY:C	2.64	0.40
1:A:415:PRO:O	1:A:416:LYS:C	2.65	0.40
1:A:610:TRP:CH2	1:A:612:PRO:HB3	2.56	0.40
1:A:56:GLU:O	1:A:57:GLU:C	2.63	0.40
1:A:112:LYS:C	1:A:114:LYS:N	2.78	0.40
1:A:224:GLU:HA	1:A:227:GLU:HG2	1.98	0.40
1:A:231:GLU:C	1:A:233:ILE:N	2.79	0.40
1:A:406:GLU:CD	1:A:518:ARG:HH11	2.29	0.40
1:A:424:LEU:O	1:A:425:SER:C	2.65	0.40
1:A:599:ASN:O	1:A:600:LYS:C	2.65	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:ARG:NH1	1:A:582:ARG:NH1[2_655]	2.02	0.18

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	595/615 (97%)	400 (67%)	129 (22%)	66 (11%)	0 1

All (66) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	THR
1	A	85	LEU
1	A	86	GLN
1	A	91	LEU
1	A	110	GLU
1	A	129	THR
1	A	158	TYR
1	A	211	GLY
1	A	261	CYS
1	A	270	MET
1	A	293	VAL
1	A	320	LEU
1	A	394	ASN
1	A	395	GLY
1	A	426	PRO
1	A	428	PHE
1	A	431	ASP
1	A	498	CYS
1	A	505	HIS
1	A	510	TYR
1	A	544	ILE

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Mol	Chain	Res	Type
1	A	575	GLY
1	A	610	TRP
1	A	611	SER
1	A	56	GLU
1	A	109	SER
1	A	206	ASP
1	A	223	ILE
1	A	247	LYS
1	A	286	GLY
1	A	424	LEU
1	A	467	GLU
1	A	504	PHE
1	A	506	VAL
1	A	507	SER
1	A	543	ASP
1	A	597	ASP
1	A	20	THR
1	A	138	PRO
1	A	222	LEU
1	A	340	GLN
1	A	413	ALA
1	A	429	GLN
1	A	470	LYS
1	A	51	ASN
1	A	90	ASN
1	A	104	GLY
1	A	177	ARG
1	A	224	GLU
1	A	246	ALA
1	A	339	VAL
1	A	384	ALA
1	A	403	ALA
1	A	475	LYS
1	A	497	TYR
1	A	553	LYS
1	A	93	VAL
1	A	111	ASP
1	A	259	ILE
1	A	300	GLN
1	A	423	LEU
1	A	123	MET
1	A	598	GLN

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Mol	Chain	Res	Type
1	A	54	ILE
1	A	484	ILE
1	A	185	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	523/542 (96%)	451 (86%)	72 (14%)	3 17

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	THR
1	A	29	LEU
1	A	31	LYS
1	A	39	LEU
1	A	42	GLN
1	A	56	GLU
1	A	75	GLU
1	A	85	LEU
1	A	86	GLN
1	A	91	LEU
1	A	97	LEU
1	A	114	LYS
1	A	117	ASN
1	A	129	THR
1	A	133	CYS
1	A	143	LEU
1	A	148	LEU
1	A	162	LEU
1	A	171	GLU
1	A	174	LYS
1	A	184	VAL
1	A	209	VAL
1	A	216	ASP

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Mol	Chain	Res	Type
1	A	218	SER
1	A	225	ASP
1	A	235	PRO
1	A	248	LEU
1	A	262	LEU
1	A	290	ASN
1	A	291	ILE
1	A	341	LYS
1	A	343	VAL
1	A	353	LYS
1	A	380	GLN
1	A	385	TYR
1	A	388	GLN
1	A	391	LEU
1	A	394	ASN
1	A	397	ASN
1	A	401	HIS
1	A	410	LEU
1	A	416	LYS
1	A	418	LEU
1	A	424	LEU
1	A	426	PRO
1	A	432	ASN
1	A	435	GLU
1	A	444	LEU
1	A	445	THR
1	A	449	THR
1	A	454	TYR
1	A	460	ARG
1	A	479	GLU
1	A	487	VAL
1	A	494	ASP
1	A	503	LEU
1	A	514	ARG
1	A	518	ARG
1	A	536	GLU
1	A	539	LEU
1	A	543	ASP
1	A	544	ILE
1	A	557	MET
1	A	559	ARG
1	A	564	GLU

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Mol	Chain	Res	Type
1	A	567	THR
1	A	568	LEU
1	A	571	GLU
1	A	577	LYS
1	A	581	VAL
1	A	585	LEU
1	A	597	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	33	ASN
1	A	34	HIS
1	A	42	GLN
1	A	53	ASN
1	A	60	GLN
1	A	61	ASN
1	A	64	ASN
1	A	76	GLN
1	A	86	GLN
1	A	98	GLN
1	A	101	GLN
1	A	117	ASN
1	A	137	ASN
1	A	139	GLN
1	A	149	ASN
1	A	154	ASN
1	A	159	ASN
1	A	239	HIS
1	A	250	ASN
1	A	277	ASN
1	A	287	GLN
1	A	290	ASN
1	A	330	ASN
1	A	373	HIS
1	A	388	GLN
1	A	394	ASN
1	A	397	ASN
1	A	417	HIS
1	A	432	ASN
1	A	442	GLN

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Mol	Chain	Res	Type
1	A	505	HIS
1	A	508	ASN
1	A	522	GLN
1	A	524	GLN
1	A	526	GLN
1	A	531	GLN
1	A	540	HIS
1	A	546	ASN
1	A	552	GLN
1	A	580	ASN
1	A	586	ASN
1	A	599	ASN

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 ⓘ

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

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	$\# Z > 2$
9	XX5	A	804	8	29,29,29	2.21	12 (41%)	36,40,40	2.24	10 (27%)
6	NAG	A	801	1	14,14,15	0.60	0	17,19,21	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	800	1	14,14,15	0.81	1 (7%)	17,19,21	0.77	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	XX5	A	804	8	-	7/24/24/24	0/2/2/2
6	NAG	A	801	1	-	5/6/23/26	0/1/1/1
6	NAG	A	800	1	1/1/5/7	5/6/23/26	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	804	XX5	C26-C27	4.94	1.46	1.38
9	A	804	XX5	C22-C23	4.35	1.45	1.38
9	A	804	XX5	C20-N19	3.53	1.53	1.47
9	A	804	XX5	C16-C15	3.51	1.41	1.36
9	A	804	XX5	C26-C21	3.51	1.45	1.39
9	A	804	XX5	C20-C21	2.63	1.56	1.51
9	A	804	XX5	C16-N17	-2.60	1.33	1.37
9	A	804	XX5	O3-C2	-2.59	1.22	1.30
6	A	800	NAG	C1-C2	2.57	1.55	1.52
9	A	804	XX5	C25-C23	2.45	1.42	1.38
9	A	804	XX5	C27-CL28	2.44	1.80	1.74
9	A	804	XX5	C22-C21	2.42	1.43	1.39
9	A	804	XX5	O12-C11	-2.34	1.23	1.30

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	804	XX5	C16-C15-N19	8.01	109.88	105.08
9	A	804	XX5	C21-C20-N19	5.77	121.78	112.84
9	A	804	XX5	C18-N19-C15	-3.75	101.58	106.30
9	A	804	XX5	C26-C27-CL28	2.40	122.18	119.17
9	A	804	XX5	C20-N19-C15	2.38	128.99	126.50
9	A	804	XX5	C20-N19-C18	2.36	129.43	126.32
9	A	804	XX5	C6-C5-C4	2.26	121.47	115.40
9	A	804	XX5	C27-C26-C21	2.15	121.91	119.71
9	A	804	XX5	C5-C4-C2	2.06	116.47	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	804	XX5	O3-C2-C4	2.00	120.29	113.51

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	800	NAG	C1

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	800	NAG	C3-C2-N2-C7
6	A	800	NAG	C8-C7-N2-C2
6	A	800	NAG	O7-C7-N2-C2
6	A	801	NAG	C8-C7-N2-C2
6	A	801	NAG	O7-C7-N2-C2
9	A	804	XX5	C2-C4-C5-C6
9	A	804	XX5	C10-C14-C15-N19
9	A	804	XX5	N9-C4-C5-C6
6	A	801	NAG	O5-C5-C6-O6
6	A	801	NAG	C4-C5-C6-O6
9	A	804	XX5	N9-C10-C11-O12
9	A	804	XX5	N9-C10-C11-O13
6	A	800	NAG	C4-C5-C6-O6
6	A	800	NAG	O5-C5-C6-O6
9	A	804	XX5	C10-C14-C15-C16
6	A	801	NAG	C3-C2-N2-C7
9	A	804	XX5	C11-C10-N9-C4

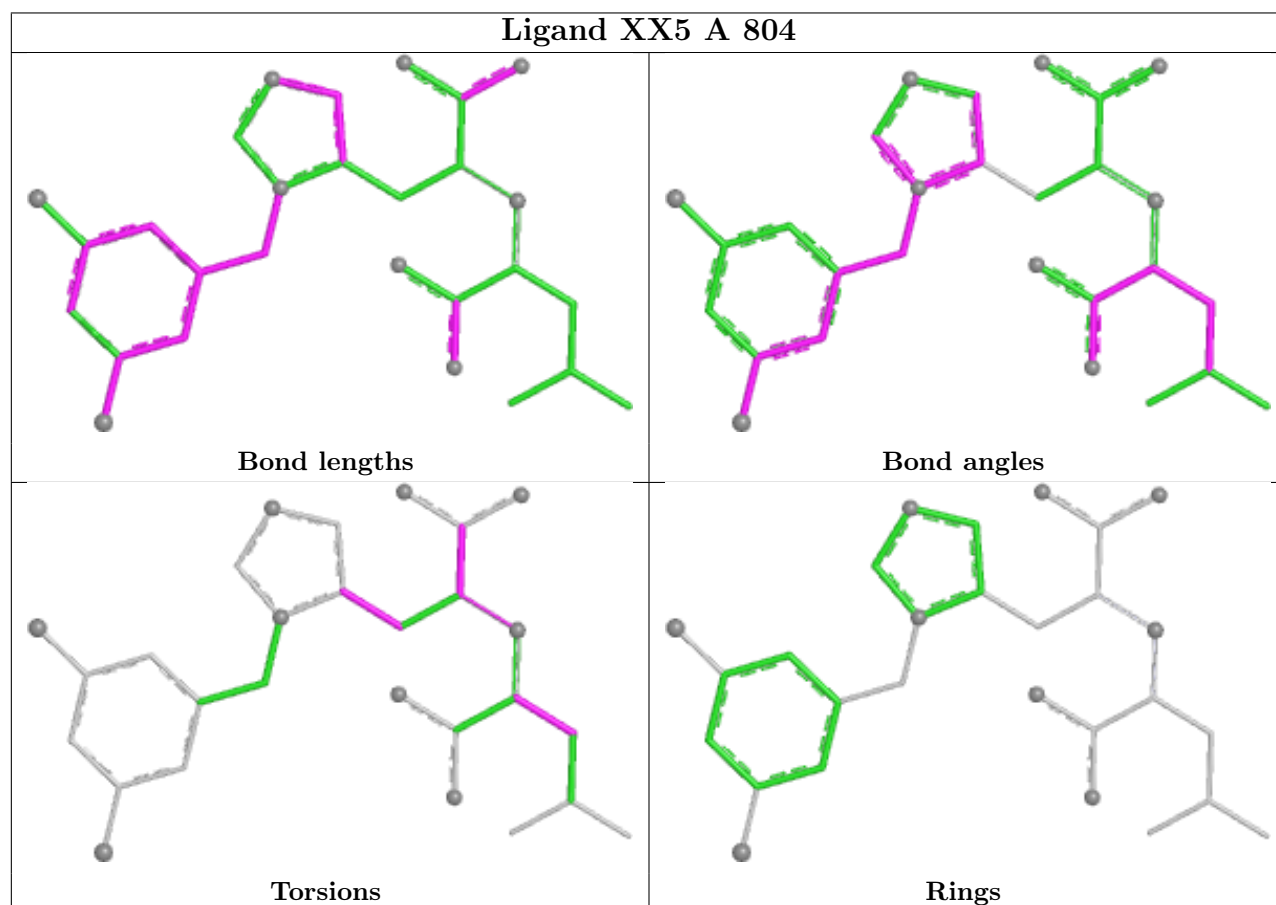
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	804	XX5	1	0
6	A	801	NAG	2	0
6	A	800	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	597/615 (97%)	-0.22	2 (0%) 90 79	35, 68, 111, 154	0
2	B	0/6	-	-	-	-
3	C	0/20	-	-	-	-
4	D	0/18	-	-	-	-
5	E	0/14	-	-	-	-
All	All	597/673 (88%)	-0.22	2 (0%) 90 79	35, 68, 111, 154	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	100	LEU	2.1
1	A	95	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

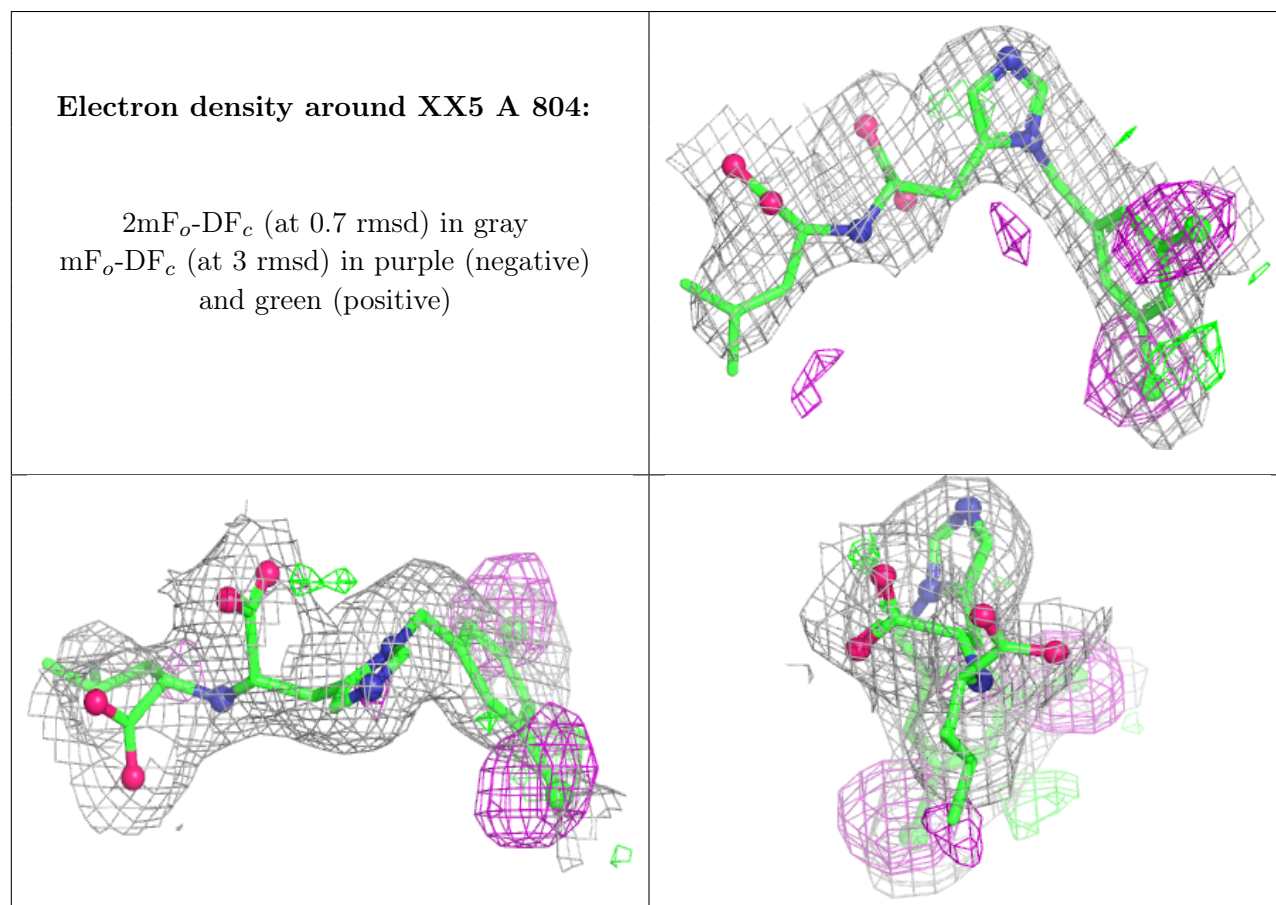
There are no oligosaccharides in this entry.

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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	A	800	14/15	0.67	0.12	128,131,133,134	0
6	NAG	A	801	14/15	0.79	0.09	115,122,128,129	0
9	XX5	A	804	28/28	0.83	0.13	34,43,51,52	0
7	CL	A	802	1/1	0.96	0.04	54,54,54,54	0
8	ZN	A	803	1/1	1.00	0.01	37,37,37,37	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.