



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2017 – 07:02 PM EDT

PDB ID : 3OJY
Title : Crystal Structure of Human Complement Component C8
Authors : Lovelace, L.L.; Cooper, C.L.; Sodetz, J.M.; Lebioda, L.
Deposited on : unknown
Resolution : 2.51 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

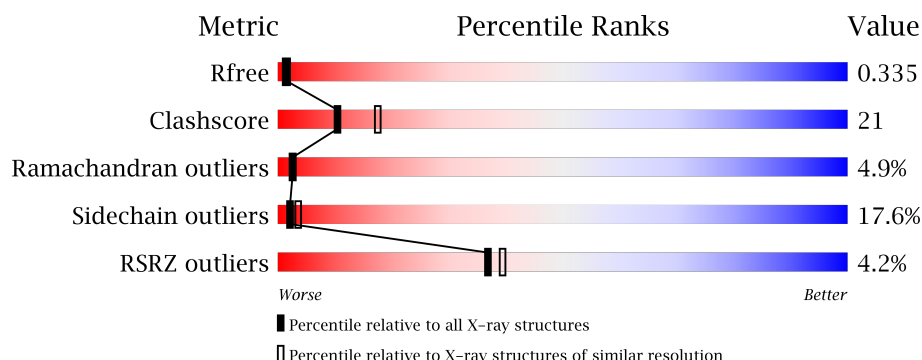
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	554	<div> <div>5%</div> <div> <div></div> <div>52%</div> <div>26%</div> <div>8%</div> <div>14%</div> </div> </div>
2	B	537	<div> <div>4%</div> <div> <div></div> <div>45%</div> <div>36%</div> <div>11%</div> <div>6%</div> </div> </div>
3	C	182	<div> <div>2%</div> <div> <div></div> <div>54%</div> <div>30%</div> <div>7%</div> <div>9%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9234 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 Complement component C8 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	478	Total	C	N	O	S	0	0	0
			3799	2359	666	736	38			

- Molecule 2 is a protein called Complement component C8 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	P S	0	0	0
			4050	2521	722	771	1 35			

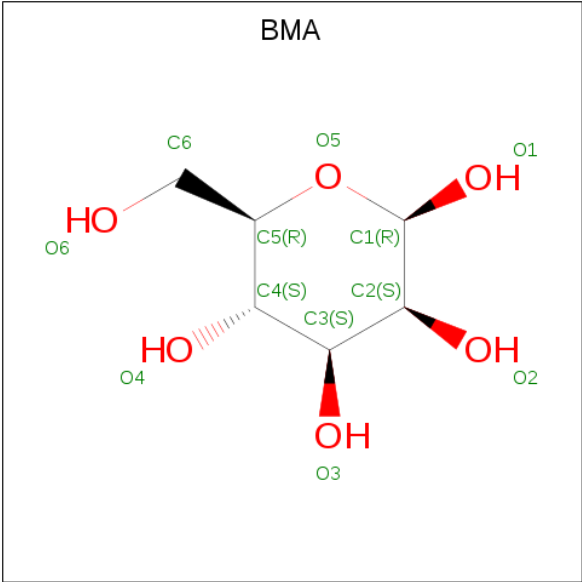
- Molecule 3 is a protein called Complement component C8 gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	165	Total	C	N	O	S	0	0	0
			1295	828	224	239	4			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C₆H₁₂O₆).

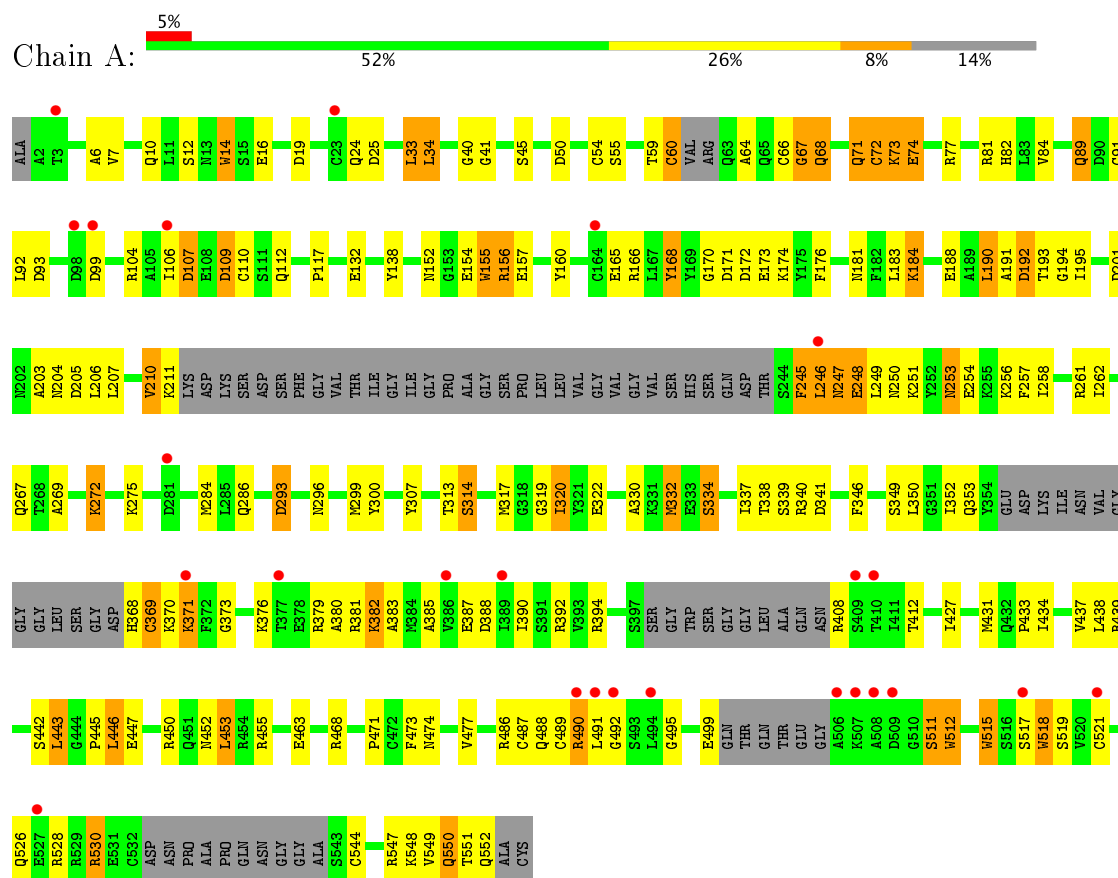


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		

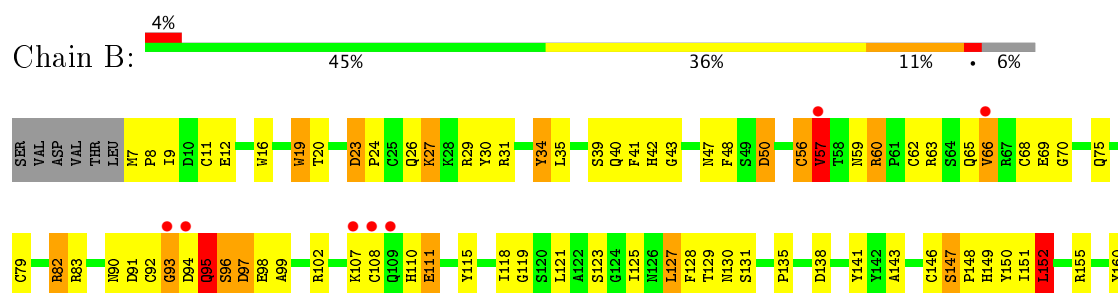
3 Residue-property plots [i](#)

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

• Molecule 1: Complement component C8 alpha chain



• Molecule 2: Complement component C8 beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	139.57Å 139.57Å 127.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.69 – 2.51 45.69 – 2.51	Depositor EDS
% Data completeness (in resolution range)	93.1 (45.69-2.51) 93.1 (45.69-2.51)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.249 , 0.337 0.248 , 0.335	Depositor DCC
R_{free} test set	2267 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	50.6	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.038 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9234	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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: TPO, CA, BMA

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	0.80	4/3873 (0.1%)	0.82	0/5207
2	B	0.86	5/4131 (0.1%)	0.89	3/5574 (0.1%)
3	C	0.70	0/1323	0.82	1/1794 (0.1%)
All	All	0.81	9/9327 (0.1%)	0.85	4/12575 (0.0%)

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
2	B	0	2
3	C	0	1
All	All	0	3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	16	TRP	CG-CD1	9.82	1.50	1.36
1	A	515	TRP	CG-CD1	9.75	1.50	1.36
1	A	518	TRP	CG-CD1	9.59	1.50	1.36
1	A	512	TRP	CG-CD1	9.27	1.49	1.36
2	B	497	TRP	CG-CD1	9.19	1.49	1.36
2	B	19	TRP	CG-CD1	9.09	1.49	1.36
1	A	14	TRP	CG-CD1	9.08	1.49	1.36
2	B	467	CYS	CB-SG	-7.94	1.68	1.82
2	B	500	TRP	CG-CD1	7.77	1.47	1.36

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	480	CYS	CA-CB-SG	-6.48	102.34	114.00
3	C	89	LEU	CA-CB-CG	5.43	127.78	115.30
2	B	520	GLN	N-CA-C	5.40	125.58	111.00
2	B	152	LEU	CA-CB-CG	5.18	127.22	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	107	LYS	Peptide
2	B	96	SER	Peptide
3	C	110	THR	Peptide

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	3799	0	3596	118	1
2	B	4050	0	3853	224	1
3	C	1295	0	1259	45	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	44	0	40	1	0
5	B	44	0	40	3	0
All	All	9234	0	8788	373	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 21.

All (373) 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:93:GLY:O	2:B:261:TYR:CD2	2.04	1.09
2:B:520:GLN:NE2	2:B:520:GLN:HA	1.52	1.08
1:A:322:GLU:HB3	1:A:392:ARG:HB2	1.34	1.08
2:B:516:ASN:O	2:B:518:PRO:HD3	1.56	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:146:CYS:O	2:B:148:PRO:HD3	1.58	1.03
2:B:485:ARG:HG2	2:B:485:ARG:HH11	1.19	1.02
1:A:156:ARG:HD2	2:B:404:TYR:CE2	1.98	0.99
1:A:25:ASP:HB3	1:A:54:CYS:O	1.64	0.97
2:B:26:GLN:O	2:B:27:LYS:HG2	1.63	0.97
3:C:155:THR:H	3:C:158:GLN:HE21	1.12	0.96
1:A:368:HIS:HE1	1:A:370:LYS:HG3	1.30	0.94
2:B:82:ARG:H	2:B:82:ARG:HH11	1.11	0.94
2:B:490:ILE:HB	2:B:518:PRO:HD2	1.49	0.94
2:B:489:PRO:HB3	2:B:520:GLN:HG2	1.50	0.92
2:B:520:GLN:NE2	2:B:520:GLN:CA	2.34	0.91
2:B:94:ASP:O	2:B:95:GLN:HG3	1.72	0.90
2:B:187:GLU:HG3	2:B:190:VAL:HG22	1.52	0.89
2:B:266:ARG:NH1	2:B:285:ASP:OD2	2.09	0.86
2:B:41:PHE:CE2	2:B:479:ALA:HB2	2.12	0.85
2:B:349:CYS:O	2:B:351:GLY:N	2.13	0.81
2:B:457:ASN:HD21	2:B:491:ASP:H	1.25	0.81
1:A:257:PHE:HE1	1:A:387:GLU:HG3	1.46	0.81
1:A:7:VAL:O	1:A:41:GLY:HA3	1.82	0.79
2:B:457:ASN:ND2	2:B:491:ASP:H	1.79	0.79
3:C:78:GLN:HB2	3:C:171:ALA:CB	2.13	0.79
1:A:74:GLU:HA	1:A:74:GLU:OE2	1.80	0.78
2:B:353:LEU:HD23	2:B:353:LEU:O	1.83	0.78
1:A:550:GLN:OE1	1:A:550:GLN:HA	1.83	0.77
1:A:191:ALA:HB3	2:B:220:ARG:HG2	1.67	0.76
2:B:349:CYS:SG	2:B:350:ARG:HG3	2.25	0.76
1:A:495:GLY:HA3	1:A:499:GLU:OE1	1.85	0.76
2:B:217:GLN:O	2:B:218:SER:O	2.03	0.75
3:C:155:THR:H	3:C:158:GLN:NE2	1.84	0.75
2:B:82:ARG:NH1	2:B:82:ARG:H	1.82	0.75
3:C:101:GLY:HA3	3:C:122:ARG:HE	1.52	0.74
1:A:257:PHE:CE1	1:A:387:GLU:HG3	2.23	0.73
2:B:503:CYS:C	2:B:505:GLY:H	1.91	0.73
2:B:520:GLN:HE21	2:B:520:GLN:HA	1.52	0.72
2:B:187:GLU:HG3	2:B:190:VAL:CG2	2.18	0.71
2:B:519:PRO:O	2:B:520:GLN:NE2	2.21	0.71
2:B:352:ILE:C	2:B:354:ASN:H	1.94	0.71
2:B:82:ARG:HH11	2:B:82:ARG:N	1.88	0.70
2:B:260:HIS:HD2	2:B:262:GLU:H	1.39	0.70
2:B:485:ARG:HG2	2:B:485:ARG:NH1	1.96	0.70
1:A:512:TRP:CE3	1:A:530:ARG:HG3	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:381:ILE:HG23	2:B:386:TYR:HD1	1.57	0.70
2:B:93:GLY:HA2	2:B:94:ASP:HB3	1.73	0.70
1:A:368:HIS:CE1	1:A:370:LYS:HG3	2.21	0.70
2:B:380:HIS:CE1	2:B:397:GLU:HG3	2.28	0.69
2:B:500:TRP:CE3	2:B:508:LYS:HG3	2.28	0.69
2:B:270:LEU:HD11	2:B:282:LEU:HD22	1.74	0.68
2:B:489:PRO:HB3	2:B:520:GLN:CG	2.22	0.67
1:A:59:THR:O	1:A:60:CYS:HB2	1.94	0.67
3:C:78:GLN:HB2	3:C:171:ALA:HB2	1.74	0.66
2:B:19:TRP:CZ2	2:B:31:ARG:HD2	2.31	0.66
1:A:445:PRO:O	1:A:446:LEU:HG	1.95	0.66
2:B:349:CYS:C	2:B:351:GLY:H	1.98	0.66
2:B:94:ASP:C	2:B:95:GLN:HG3	2.14	0.66
2:B:414:GLU:HG3	2:B:418:GLU:HG3	1.77	0.65
2:B:379:GLU:OE2	2:B:379:GLU:HA	1.97	0.65
2:B:143:ALA:HB2	2:B:160:TYR:CD1	2.31	0.65
2:B:70:GLY:HA2	2:B:82:ARG:CZ	2.27	0.65
2:B:444:LYS:HG2	5:B:541:BMA:O6	1.98	0.64
2:B:352:ILE:C	2:B:354:ASN:N	2.51	0.64
2:B:394:LEU:O	2:B:394:LEU:HG	1.97	0.64
3:C:41:ARG:O	3:C:44:GLN:HG2	1.98	0.64
3:C:110:THR:OG1	3:C:111:ASP:O	2.15	0.64
2:B:355:GLU:O	2:B:359:ARG:HD3	1.98	0.64
2:B:364:TPO:HA	2:B:364:TPO:O2P	1.98	0.64
3:C:46:GLN:HB3	3:C:49:ARG:HD3	1.80	0.64
3:C:41:ARG:HA	3:C:44:GLN:HE21	1.63	0.63
2:B:69:GLU:OE1	2:B:69:GLU:HA	1.98	0.63
1:A:512:TRP:CH2	1:A:548:LYS:HB3	2.34	0.62
2:B:213:GLY:O	2:B:214:ILE:C	2.38	0.62
3:C:57:VAL:HG13	3:C:64:MET:HE3	1.80	0.62
2:B:390:PRO:HG2	2:B:391:THR:H	1.65	0.62
2:B:293:GLU:HB2	2:B:412:LYS:HB2	1.80	0.62
1:A:490:ARG:N	1:A:490:ARG:HE	1.98	0.62
2:B:96:SER:C	2:B:98:GLU:H	2.03	0.61
2:B:214:ILE:O	2:B:218:SER:OG	2.13	0.61
1:A:322:GLU:HB3	1:A:392:ARG:CB	2.22	0.61
2:B:317:THR:O	2:B:320:ASN:HB2	2.01	0.61
3:C:146:GLU:O	3:C:149:VAL:HG12	2.00	0.61
2:B:269:ARG:HH11	2:B:269:ARG:CB	2.15	0.60
1:A:249:LEU:C	1:A:251:LYS:H	2.06	0.60
2:B:9:ILE:O	2:B:43:GLY:HA3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:190:VAL:C	2:B:192:GLU:H	2.04	0.59
2:B:490:ILE:CB	2:B:518:PRO:HD2	2.28	0.59
2:B:503:CYS:C	2:B:505:GLY:N	2.54	0.59
2:B:352:ILE:O	2:B:354:ASN:N	2.36	0.59
2:B:298:GLY:HA2	2:B:374:ARG:O	2.03	0.59
1:A:204:ASN:HD22	1:A:490:ARG:HD2	1.68	0.59
2:B:90:ASN:ND2	2:B:94:ASP:HB2	2.18	0.59
2:B:93:GLY:O	2:B:261:TYR:CE2	2.55	0.59
1:A:138:TYR:HB3	1:A:181:ASN:HD22	1.69	0.58
2:B:246:GLU:OE1	2:B:249:HIS:NE2	2.25	0.58
3:C:47:GLY:O	3:C:49:ARG:N	2.37	0.58
2:B:349:CYS:SG	2:B:350:ARG:N	2.76	0.58
2:B:290:TYR:CZ	2:B:419:LEU:HD13	2.39	0.57
2:B:40:GLN:OE1	2:B:452:ALA:HB3	2.03	0.57
2:B:427:TYR:O	2:B:428:SER:C	2.41	0.57
2:B:512:ARG:HH22	2:B:527:SER:HA	1.69	0.57
2:B:66:VAL:O	2:B:66:VAL:HG23	2.04	0.57
2:B:92:CYS:O	2:B:93:GLY:C	2.42	0.57
2:B:115:TYR:OH	2:B:149:HIS:HD2	1.87	0.57
2:B:453:PRO:HB3	2:B:515:ASN:HB2	1.87	0.57
2:B:123:SER:HA	2:B:135:PRO:HA	1.86	0.57
2:B:506:ARG:CZ	5:B:542:BMA:O2	2.53	0.57
1:A:261:ARG:NH2	1:A:322:GLU:OE2	2.24	0.56
2:B:466:ARG:HG3	2:B:467:CYS:N	2.19	0.56
2:B:179:GLU:HG3	2:B:322:HIS:HD2	1.68	0.56
1:A:154:GLU:O	1:A:156:ARG:N	2.39	0.56
1:A:275:LYS:NZ	2:B:285:ASP:OD2	2.28	0.56
3:C:45:GLU:C	3:C:47:GLY:H	2.09	0.56
2:B:349:CYS:HB2	2:B:353:LEU:HD13	1.87	0.56
3:C:47:GLY:C	3:C:49:ARG:H	2.10	0.55
1:A:284:MET:HG3	1:A:307:TYR:CD1	2.42	0.55
2:B:485:ARG:HH11	2:B:485:ARG:CG	2.06	0.55
1:A:258:ILE:CD1	1:A:339:SER:HB3	2.36	0.55
2:B:216:SER:OG	2:B:217:GLN:N	2.40	0.55
2:B:478:LEU:C	2:B:480:CYS:H	2.10	0.54
1:A:511:SER:N	1:A:544:CYS:SG	2.80	0.54
3:C:78:GLN:HB2	3:C:171:ALA:HB3	1.87	0.54
1:A:547:ARG:NH2	2:B:12:GLU:OE2	2.41	0.54
1:A:296:ASN:O	1:A:300:TYR:HD1	1.91	0.54
2:B:179:GLU:HG3	2:B:322:HIS:CD2	2.43	0.54
1:A:195:ILE:HD12	1:A:195:ILE:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:LYS:O	1:A:385:ALA:N	2.38	0.54
2:B:24:PRO:HB2	2:B:62:CYS:HB2	1.89	0.54
1:A:160:TYR:OH	1:A:165:GLU:OE1	2.26	0.54
2:B:20:THR:O	2:B:29:ARG:HB2	2.08	0.54
3:C:78:GLN:CB	3:C:171:ALA:CB	2.84	0.54
1:A:473:PHE:O	1:A:474:ASN:HB2	2.08	0.53
2:B:97:ASP:N	2:B:97:ASP:OD2	2.41	0.53
2:B:365:MET:O	2:B:365:MET:HG2	2.09	0.53
2:B:400:ASP:CG	2:B:401:ALA:N	2.61	0.53
2:B:93:GLY:N	2:B:94:ASP:HA	2.23	0.53
2:B:269:ARG:HH11	2:B:269:ARG:HB2	1.71	0.53
2:B:179:GLU:H	2:B:179:GLU:CD	2.10	0.53
2:B:352:ILE:HG22	2:B:356:ILE:N	2.24	0.53
1:A:254:GLU:HG2	1:A:256:LYS:HG2	1.90	0.52
1:A:296:ASN:OD1	1:A:299:MET:HG2	2.09	0.52
1:A:191:ALA:HB3	2:B:220:ARG:CG	2.39	0.52
2:B:96:SER:CA	2:B:98:GLU:H	2.23	0.52
1:A:33:LEU:HB3	1:A:468:ARG:HH12	1.75	0.52
2:B:181:GLU:HA	2:B:237:VAL:HG22	1.92	0.52
2:B:150:TYR:CZ	2:B:155:ARG:HG3	2.44	0.52
1:A:486:ARG:O	1:A:487:CYS:SG	2.68	0.52
2:B:128:PHE:CE2	2:B:443:GLN:HG3	2.44	0.52
2:B:93:GLY:HA2	2:B:94:ASP:CB	2.38	0.52
2:B:221:GLY:O	2:B:225:ILE:HG12	2.10	0.51
1:A:82:HIS:NE2	2:B:95:GLN:CB	2.73	0.51
3:C:38:SER:HB2	3:C:127:SER:HB3	1.93	0.51
2:B:352:ILE:HB	2:B:356:ILE:HB	1.92	0.51
1:A:300:TYR:CE2	1:A:452:ASN:HB3	2.45	0.51
1:A:59:THR:O	1:A:60:CYS:CB	2.59	0.51
2:B:348:LYS:O	2:B:348:LYS:HG3	2.09	0.51
1:A:73:LYS:HB2	1:A:93:ASP:OD2	2.11	0.51
2:B:59:ASN:O	2:B:60:ARG:C	2.48	0.51
3:C:172:ASP:O	3:C:174:PHE:N	2.44	0.51
1:A:190:LEU:O	1:A:190:LEU:HD23	2.11	0.51
1:A:191:ALA:O	1:A:193:THR:HG23	2.11	0.51
1:A:434:ILE:O	1:A:437:VAL:HG12	2.11	0.51
1:A:521:CYS:SG	1:A:526:GLN:NE2	2.82	0.51
3:C:81:GLN:NE2	3:C:94:LEU:HD21	2.26	0.51
3:C:16:ILE:O	3:C:91:ARG:NH2	2.43	0.51
2:B:381:ILE:HG23	2:B:386:TYR:CD1	2.42	0.51
2:B:352:ILE:O	2:B:356:ILE:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:478:LEU:O	2:B:479:ALA:HB3	2.11	0.50
3:C:128:VAL:HG23	3:C:145:PHE:HE1	1.77	0.50
2:B:121:LEU:HD11	2:B:296:LEU:HD11	1.93	0.50
2:B:380:HIS:HE1	2:B:397:GLU:HG3	1.73	0.50
2:B:381:ILE:HG22	2:B:382:THR:N	2.27	0.50
2:B:93:GLY:O	2:B:261:TYR:CG	2.61	0.50
3:C:128:VAL:HG23	3:C:145:PHE:CE1	2.47	0.50
1:A:269:ALA:HB3	1:A:317:MET:HB2	1.92	0.50
2:B:500:TRP:CD2	2:B:508:LYS:HG3	2.46	0.50
3:C:41:ARG:HG2	3:C:42:PHE:H	1.76	0.50
2:B:518:PRO:HB2	2:B:519:PRO:HD3	1.94	0.50
1:A:166:ARG:HG2	1:A:168:TYR:CD2	2.45	0.50
3:C:155:THR:HG23	3:C:158:GLN:NE2	2.27	0.50
3:C:21:ASN:O	3:C:22:PHE:C	2.48	0.50
1:A:293:ASP:OD2	1:A:293:ASP:N	2.45	0.50
2:B:260:HIS:CD2	2:B:262:GLU:H	2.24	0.49
2:B:59:ASN:O	2:B:60:ARG:O	2.30	0.49
2:B:8:PRO:HB3	2:B:43:GLY:HA2	1.94	0.49
1:A:25:ASP:OD1	1:A:55:SER:HA	2.11	0.49
2:B:481:GLU:N	2:B:481:GLU:OE1	2.42	0.49
3:C:169:GLU:CG	3:C:170:ALA:H	2.25	0.49
1:A:155:TRP:HB3	1:A:174:LYS:HA	1.94	0.49
1:A:518:TRP:CH2	1:A:552:GLN:HB2	2.47	0.49
1:A:195:ILE:H	1:A:195:ILE:HD12	1.78	0.49
3:C:57:VAL:CG1	3:C:64:MET:HE3	2.43	0.49
2:B:269:ARG:NH1	2:B:269:ARG:HB3	2.28	0.49
1:A:515:TRP:CZ3	1:A:530:ARG:HD2	2.47	0.48
2:B:75:GLN:H	2:B:95:GLN:NE2	2.11	0.48
1:A:368:HIS:HE1	1:A:370:LYS:CG	2.14	0.48
2:B:91:ASP:C	2:B:93:GLY:N	2.66	0.48
1:A:247:ASN:C	1:A:249:LEU:H	2.17	0.48
1:A:267:GLN:HG2	1:A:427:ILE:HD11	1.95	0.48
2:B:19:TRP:CH2	2:B:31:ARG:HD2	2.48	0.48
2:B:352:ILE:O	2:B:355:GLU:N	2.47	0.48
2:B:247:VAL:CG1	2:B:403:GLN:NE2	2.76	0.48
2:B:141:TYR:CD2	2:B:258:MET:HG2	2.48	0.48
2:B:485:ARG:NH1	2:B:485:ARG:CG	2.72	0.48
2:B:512:ARG:NH2	2:B:527:SER:HA	2.28	0.48
3:C:135:LEU:HA	3:C:136:PRO:C	2.33	0.48
2:B:489:PRO:HB3	2:B:520:GLN:CB	2.44	0.48
1:A:184:LYS:HG2	1:A:272:LYS:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:320:ASN:O	2:B:324:CYS:HB2	2.13	0.48
1:A:431:MET:HE2	2:B:47:ASN:HD22	1.79	0.48
2:B:500:TRP:HB3	2:B:506:ARG:HG2	1.96	0.48
1:A:371:LYS:HG3	1:A:380:ALA:HA	1.95	0.48
2:B:270:LEU:HD13	2:B:279:TYR:CE2	2.49	0.48
2:B:187:GLU:CG	2:B:190:VAL:HG22	2.36	0.48
1:A:313:THR:O	1:A:314:SER:HB3	2.14	0.48
2:B:377:ALA:HB1	2:B:381:ILE:HD11	1.96	0.48
2:B:429:SER:O	2:B:433:GLN:HG2	2.14	0.48
2:B:208:GLY:H	2:B:412:LYS:NZ	2.12	0.47
1:A:518:TRP:CZ3	1:A:528:ARG:HB2	2.49	0.47
2:B:348:LYS:NZ	2:B:351:GLY:HA2	2.30	0.47
2:B:226:ARG:NH1	2:B:471:CYS:HB2	2.29	0.47
2:B:355:GLU:HA	2:B:358:ASP:HB2	1.96	0.47
3:C:109:GLU:O	3:C:110:THR:HB	2.14	0.47
2:B:269:ARG:NH1	2:B:269:ARG:CB	2.78	0.47
2:B:484:TYR:O	2:B:485:ARG:HB2	2.15	0.47
2:B:489:PRO:HB3	2:B:520:GLN:HB2	1.96	0.47
1:A:191:ALA:O	1:A:193:THR:N	2.48	0.47
1:A:71:GLN:HB3	1:A:71:GLN:HE21	1.60	0.47
2:B:189:ASN:OD1	2:B:240:HIS:CE1	2.68	0.47
1:A:82:HIS:NE2	2:B:95:GLN:HB2	2.29	0.46
1:A:107:ASP:C	1:A:109:ASP:H	2.19	0.46
1:A:68:GLN:O	1:A:81:ARG:NE	2.38	0.46
3:C:41:ARG:O	3:C:44:GLN:CG	2.62	0.46
3:C:79:VAL:HG13	3:C:177:LEU:HB3	1.98	0.46
1:A:138:TYR:HB3	1:A:181:ASN:ND2	2.30	0.46
1:A:6:ALA:HB1	1:A:40:GLY:H	1.80	0.46
2:B:512:ARG:NH2	2:B:527:SER:OG	2.48	0.46
1:A:262:ILE:O	1:A:322:GLU:HA	2.15	0.46
2:B:348:LYS:HZ1	2:B:351:GLY:HA2	1.79	0.46
2:B:210:PHE:HE2	2:B:413:VAL:HG22	1.81	0.46
1:A:82:HIS:NE2	2:B:95:GLN:HB3	2.31	0.46
1:A:154:GLU:C	1:A:156:ARG:H	2.19	0.46
1:A:14:TRP:CH2	1:A:50:ASP:HB2	2.51	0.46
2:B:29:ARG:HD3	2:B:56:CYS:SG	2.56	0.46
2:B:96:SER:HB2	2:B:99:ALA:N	2.30	0.46
2:B:226:ARG:HG2	2:B:471:CYS:O	2.16	0.46
2:B:151:ILE:HG22	2:B:152:LEU:HG	1.98	0.45
2:B:70:GLY:HA2	2:B:82:ARG:NH1	2.30	0.45
2:B:502:SER:HA	2:B:506:ARG:CG	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:327:ASN:CG	2:B:328:ASP:N	2.70	0.45
2:B:56:CYS:O	2:B:57:VAL:HG13	2.16	0.45
3:C:16:ILE:N	3:C:16:ILE:HD13	2.31	0.45
2:B:299:ILE:O	2:B:398:TRP:CH2	2.69	0.45
1:A:107:ASP:OD1	1:A:107:ASP:N	2.49	0.45
1:A:89:GLN:HG3	1:A:91:CYS:O	2.17	0.45
2:B:23:ASP:HA	2:B:24:PRO:HD3	1.85	0.45
2:B:173:TYR:O	2:B:174:GLU:C	2.53	0.45
2:B:183:TYR:O	2:B:186:PHE:HB3	2.16	0.45
1:A:443:LEU:HG	1:A:443:LEU:H	1.63	0.45
1:A:447:GLU:HG3	1:A:450:ARG:HH21	1.82	0.45
1:A:16:GLU:HA	1:A:16:GLU:OE1	2.16	0.44
1:A:350:LEU:HA	1:A:412:THR:HG22	1.98	0.44
2:B:235:LYS:O	2:B:308:LYS:HB2	2.16	0.44
2:B:129:THR:HB	2:B:217:GLN:HG2	1.98	0.44
2:B:162:VAL:HG22	2:B:250:TYR:HE1	1.83	0.44
1:A:165:GLU:O	3:C:70:ARG:NH2	2.50	0.44
2:B:383:THR:HA	2:B:388:GLU:OE2	2.18	0.44
2:B:516:ASN:OD1	2:B:516:ASN:N	2.25	0.44
1:A:34:LEU:HD12	1:A:34:LEU:HA	1.80	0.44
2:B:96:SER:C	2:B:98:GLU:N	2.64	0.44
1:A:66:CYS:O	1:A:67:GLY:C	2.55	0.44
2:B:23:ASP:OD2	2:B:272:LEU:HG	2.18	0.44
1:A:452:ASN:OD1	1:A:455:ARG:NH2	2.51	0.44
2:B:371:VAL:HG21	2:B:385:ALA:O	2.17	0.44
2:B:408:ILE:HG22	2:B:411:VAL:HG23	2.00	0.44
2:B:316:TYR:CD2	2:B:353:LEU:HD12	2.53	0.44
1:A:353:GLN:NE2	2:B:387:GLN:OE1	2.44	0.43
2:B:50:ASP:OD1	2:B:50:ASP:N	2.36	0.43
2:B:11:CYS:HB2	2:B:39:SER:HB3	2.00	0.43
2:B:349:CYS:C	2:B:351:GLY:N	2.67	0.43
2:B:355:GLU:C	2:B:357:LYS:N	2.71	0.43
1:A:253:ASN:N	1:A:253:ASN:OD1	2.37	0.43
2:B:204:PHE:HE2	2:B:443:GLN:NE2	2.16	0.43
1:A:152:ASN:O	1:A:155:TRP:HD1	2.01	0.43
1:A:168:TYR:CD2	1:A:168:TYR:N	2.86	0.43
1:A:319:GLY:C	1:A:320:ILE:HG12	2.38	0.43
3:C:71:LYS:HA	3:C:75:ILE:O	2.19	0.43
2:B:325:ALA:C	2:B:327:ASN:H	2.22	0.43
2:B:520:GLN:HE21	2:B:520:GLN:CA	2.17	0.43
1:A:192:ASP:OD2	2:B:227:ARG:NH2	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:PRO:HD3	1:A:176:PHE:CD2	2.54	0.43
2:B:141:TYR:CG	2:B:258:MET:HG2	2.54	0.43
2:B:190:VAL:C	2:B:192:GLU:N	2.72	0.43
2:B:34:TYR:HB2	2:B:445:GLU:OE2	2.19	0.43
2:B:478:LEU:O	2:B:481:GLU:OE1	2.36	0.43
1:A:245:PHE:HD1	1:A:390:ILE:HG21	1.84	0.43
3:C:37:GLY:HA3	3:C:128:VAL:HG22	2.00	0.43
2:B:183:TYR:HB3	2:B:234:THR:HB	2.00	0.43
2:B:127:LEU:HD12	2:B:127:LEU:HA	1.80	0.42
2:B:151:ILE:HD13	2:B:167:PRO:HG3	2.01	0.42
1:A:170:GLY:C	1:A:172:ASP:H	2.23	0.42
1:A:337:ILE:HG23	1:A:341:ASP:HB2	2.01	0.42
1:A:528:ARG:NH2	5:A:558:BMA:O5	2.52	0.42
2:B:283:PHE:CZ	2:B:439:LEU:HD13	2.54	0.42
3:C:104:HIS:O	3:C:120:LEU:HA	2.19	0.42
2:B:205:LYS:CE	2:B:418:GLU:OE1	2.68	0.42
2:B:209:ILE:HG13	2:B:209:ILE:H	1.44	0.42
2:B:457:ASN:HD21	2:B:491:ASP:N	2.03	0.42
2:B:506:ARG:CZ	5:B:542:BMA:HO2	2.31	0.42
2:B:514:CYS:O	2:B:515:ASN:CB	2.68	0.42
2:B:212:LEU:C	2:B:214:ILE:H	2.23	0.42
3:C:34:VAL:HG21	3:C:137:VAL:HG21	2.00	0.42
2:B:30:TYR:CE1	2:B:271:PRO:HG3	2.55	0.42
1:A:81:ARG:O	1:A:84:VAL:HB	2.20	0.42
2:B:130:ASN:HD22	2:B:216:SER:HB2	1.84	0.42
2:B:118:ILE:HG23	2:B:119:GLY:N	2.35	0.42
2:B:201:SER:O	2:B:202:PHE:O	2.37	0.42
1:A:211:LYS:HE2	1:A:477:VAL:HG22	2.01	0.41
1:A:368:HIS:CG	1:A:369:CYS:N	2.88	0.41
2:B:179:GLU:O	2:B:180:TYR:CG	2.73	0.41
2:B:42:HIS:H	2:B:466:ARG:HH22	1.67	0.41
3:C:78:GLN:HB3	3:C:176:VAL:HB	2.02	0.41
1:A:155:TRP:CB	1:A:174:LYS:HA	2.50	0.41
1:A:512:TRP:HH2	1:A:548:LYS:HB3	1.84	0.41
2:B:187:GLU:CG	2:B:190:VAL:CG2	2.94	0.41
1:A:518:TRP:CZ2	1:A:528:ARG:HD2	2.55	0.41
2:B:408:ILE:CG2	2:B:411:VAL:HG23	2.50	0.41
2:B:441:GLU:HA	2:B:444:LYS:NZ	2.35	0.41
3:C:169:GLU:HG3	3:C:170:ALA:H	1.85	0.41
2:B:243:SER:O	2:B:299:ILE:O	2.39	0.41
2:B:427:TYR:O	2:B:429:SER:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:128:PHE:CD2	2:B:443:GLN:HG3	2.55	0.41
3:C:44:GLN:HG3	3:C:45:GLU:OE1	2.20	0.41
3:C:47:GLY:C	3:C:49:ARG:N	2.73	0.41
1:A:246:LEU:HD21	1:A:488:GLN:OE1	2.21	0.41
1:A:379:ARG:H	1:A:379:ARG:HG3	1.67	0.41
1:A:284:MET:HE3	1:A:434:ILE:HD11	2.03	0.41
1:A:33:LEU:N	1:A:463:GLU:OE1	2.28	0.41
2:B:416:LEU:HA	2:B:416:LEU:HD12	1.85	0.41
3:C:41:ARG:HG2	3:C:42:PHE:N	2.35	0.41
2:B:356:ILE:HG13	2:B:364:TPO:O	2.20	0.41
2:B:381:ILE:HG13	2:B:386:TYR:CE1	2.56	0.41
1:A:249:LEU:C	1:A:251:LYS:N	2.72	0.41
2:B:208:GLY:HA2	2:B:412:LYS:HE2	2.02	0.41
3:C:119:TYR:CD1	3:C:128:VAL:HG12	2.56	0.41
1:A:332:MET:SD	1:A:338:THR:HA	2.61	0.41
2:B:108:CYS:C	2:B:110:HIS:H	2.23	0.41
2:B:327:ASN:CG	2:B:328:ASP:H	2.24	0.41
1:A:330:ALA:O	1:A:334:SER:OG	2.35	0.41
1:A:490:ARG:NE	1:A:490:ARG:N	2.67	0.41
1:A:72:CYS:SG	1:A:77:ARG:HB3	2.61	0.41
2:B:247:VAL:HG13	2:B:403:GLN:HE22	1.86	0.41
1:A:550:GLN:HG3	1:A:551:THR:H	1.86	0.41
2:B:79:CYS:SG	2:B:79:CYS:O	2.79	0.41
1:A:438:LEU:HD11	1:A:453:LEU:HD12	2.03	0.40
2:B:230:ARG:HB2	2:B:230:ARG:HE	1.59	0.40
3:C:105:VAL:HG13	3:C:120:LEU:HG	2.03	0.40
3:C:55:LEU:HD22	3:C:131:TYR:CZ	2.56	0.40
1:A:170:GLY:O	1:A:172:ASP:N	2.54	0.40
2:B:130:ASN:HD22	2:B:216:SER:CB	2.34	0.40
2:B:383:THR:HB	2:B:384:LEU:HD12	2.02	0.40
1:A:160:TYR:OH	1:A:165:GLU:CD	2.59	0.40
1:A:346:PHE:O	1:A:349:SER:OG	2.39	0.40
2:B:75:GLN:N	2:B:95:GLN:NE2	2.69	0.40
1:A:207:LEU:HD23	1:A:490:ARG:HG2	2.03	0.40
2:B:138:ASP:HB2	2:B:260:HIS:HA	2.03	0.40
2:B:111:GLU:HG3	2:B:155:ARG:HH12	1.86	0.40
1:A:433:PRO:HD3	2:B:48:PHE:HA	2.02	0.40
1:A:515:TRP:CH2	1:A:530:ARG:HD2	2.57	0.40
2:B:150:TYR:CE2	2:B:155:ARG:HG3	2.56	0.40
2:B:179:GLU:CG	2:B:322:HIS:HD2	2.34	0.40
1:A:431:MET:CE	2:B:47:ASN:HD22	2.34	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:GLN:NE2	2:B:520:GLN:O[2_545]	2.07	0.13

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	464/554 (84%)	386 (83%)	55 (12%)	23 (5%)	2	2
2	B	495/537 (92%)	412 (83%)	55 (11%)	28 (6%)	2	2
3	C	161/182 (88%)	146 (91%)	11 (7%)	4 (2%)	6	10
All	All	1120/1273 (88%)	944 (84%)	121 (11%)	55 (5%)	2	2

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	194	GLY
1	A	369	CYS
2	B	202	PHE
2	B	218	SER
2	B	350	ARG
2	B	363	ASP
2	B	519	PRO
3	C	48	HIS
3	C	173	GLN
1	A	24	GLN
1	A	67	GLY
1	A	73	LYS
1	A	155	TRP
1	A	192	ASP
2	B	57	VAL
2	B	66	VAL

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Mol	Chain	Res	Type
2	B	93	GLY
2	B	214	ILE
2	B	215	SER
2	B	326	LYS
2	B	327	ASN
2	B	353	LEU
2	B	388	GLU
2	B	485	ARG
3	C	46	GLN
3	C	169	GLU
1	A	157	GLU
1	A	171	ASP
1	A	210	VAL
1	A	250	ASN
1	A	371	LYS
1	A	471	PRO
1	A	492	GLY
2	B	174	GLU
2	B	351	GLY
2	B	381	ILE
2	B	383	THR
2	B	390	PRO
1	A	248	GLU
2	B	60	ARG
2	B	95	GLN
2	B	173	TYR
2	B	503	CYS
1	A	64	ALA
1	A	110	CYS
1	A	203	ALA
1	A	383	ALA
1	A	446	LEU
1	A	491	LEU
2	B	147	SER
2	B	378	SER
2	B	428	SER
1	A	314	SER
2	B	191	THR
1	A	373	GLY

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	412/466 (88%)	351 (85%)	61 (15%)	3	6
2	B	446/472 (94%)	356 (80%)	90 (20%)	1	2
3	C	134/149 (90%)	110 (82%)	24 (18%)	2	3
All	All	992/1087 (91%)	817 (82%)	175 (18%)	2	3

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	SER
1	A	19	ASP
1	A	33	LEU
1	A	34	LEU
1	A	45	SER
1	A	60	CYS
1	A	68	GLN
1	A	71	GLN
1	A	72	CYS
1	A	74	GLU
1	A	89	GLN
1	A	92	LEU
1	A	99	ASP
1	A	104	ARG
1	A	106	ILE
1	A	107	ASP
1	A	109	ASP
1	A	112	GLN
1	A	132	GLU
1	A	156	ARG
1	A	168	TYR
1	A	173	GLU
1	A	183	LEU
1	A	184	LYS
1	A	188	GLU
1	A	190	LEU

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Mol	Chain	Res	Type
1	A	201	ASP
1	A	205	ASP
1	A	206	LEU
1	A	210	VAL
1	A	245	PHE
1	A	246	LEU
1	A	247	ASN
1	A	248	GLU
1	A	253	ASN
1	A	272	LYS
1	A	286	GLN
1	A	293	ASP
1	A	320	ILE
1	A	332	MET
1	A	334	SER
1	A	340	ARG
1	A	352	ILE
1	A	376	LYS
1	A	381	ARG
1	A	382	LYS
1	A	388	ASP
1	A	394	ARG
1	A	408	ARG
1	A	439	ARG
1	A	442	SER
1	A	443	LEU
1	A	453	LEU
1	A	489	CYS
1	A	490	ARG
1	A	511	SER
1	A	517	SER
1	A	519	SER
1	A	530	ARG
1	A	549	VAL
1	A	550	GLN
2	B	7	MET
2	B	23	ASP
2	B	27	LYS
2	B	34	TYR
2	B	35	LEU
2	B	50	ASP
2	B	56	CYS

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Mol	Chain	Res	Type
2	B	57	VAL
2	B	63	ARG
2	B	65	GLN
2	B	68	CYS
2	B	82	ARG
2	B	83	ARG
2	B	95	GLN
2	B	97	ASP
2	B	102	ARG
2	B	111	GLU
2	B	125	ILE
2	B	127	LEU
2	B	131	SER
2	B	147	SER
2	B	152	LEU
2	B	163	GLU
2	B	164	SER
2	B	169	THR
2	B	170	GLN
2	B	173	TYR
2	B	179	GLU
2	B	187	GLU
2	B	188	ARG
2	B	192	GLU
2	B	201	SER
2	B	209	ILE
2	B	215	SER
2	B	217	GLN
2	B	218	SER
2	B	220	ARG
2	B	222	LYS
2	B	227	ARG
2	B	229	LYS
2	B	230	ARG
2	B	234	THR
2	B	236	SER
2	B	237	VAL
2	B	250	TYR
2	B	255	ARG
2	B	266	ARG
2	B	269	ARG
2	B	273	GLU

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Mol	Chain	Res	Type
2	B	281	ASP
2	B	303	THR
2	B	315	ASP
2	B	345	SER
2	B	350	ARG
2	B	352	ILE
2	B	356	ILE
2	B	358	ASP
2	B	359	ARG
2	B	361	LYS
2	B	362	ARG
2	B	365	MET
2	B	368	ASP
2	B	379	GLU
2	B	383	THR
2	B	386	TYR
2	B	388	GLU
2	B	394	LEU
2	B	396	GLN
2	B	400	ASP
2	B	405	ASN
2	B	408	ILE
2	B	410	LYS
2	B	411	VAL
2	B	419	LEU
2	B	423	THR
2	B	429	SER
2	B	440	GLU
2	B	457	ASN
2	B	462	LEU
2	B	463	LYS
2	B	466	ARG
2	B	468	ASP
2	B	484	TYR
2	B	485	ARG
2	B	486	LYS
2	B	503	CYS
2	B	507	ARG
2	B	513	GLN
2	B	515	ASN
2	B	520	GLN
3	C	16	ILE

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Mol	Chain	Res	Type
3	C	19	LYS
3	C	32	LEU
3	C	41	ARG
3	C	45	GLU
3	C	54	THR
3	C	62	THR
3	C	67	SER
3	C	70	ARG
3	C	82	LEU
3	C	85	ASP
3	C	86	THR
3	C	95	GLN
3	C	105	VAL
3	C	121	GLU
3	C	127	SER
3	C	134	SER
3	C	135	LEU
3	C	138	SER
3	C	146	GLU
3	C	150	GLN
3	C	169	GLU
3	C	172	ASP
3	C	176	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	71	GLN
1	A	89	GLN
1	A	146	GLN
1	A	270	HIS
1	A	368	HIS
1	A	474	ASN
2	B	47	ASN
2	B	95	GLN
2	B	130	ASN
2	B	149	HIS
2	B	170	GLN
2	B	223	HIS
2	B	260	HIS
2	B	320	ASN

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Mol	Chain	Res	Type
2	B	322	HIS
2	B	327	ASN
2	B	403	GLN
2	B	405	ASN
2	B	457	ASN
2	B	499	ASN
2	B	515	ASN
3	C	44	GLN
3	C	81	GLN
3	C	95	GLN
3	C	125	GLN
3	C	158	GLN
3	C	175	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	TPO	B	364	2	9,10,11	1.44	2 (22%)	10,14,16	2.15	2 (20%)

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	TPO	B	364	2	-	0/8/11/13	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	364	TPO	P-OG1	2.43	1.63	1.59
2	B	364	TPO	CA-C	2.86	1.54	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	364	TPO	O-C-CA	-2.31	119.76	125.15
2	B	364	TPO	C-CA-N	5.64	121.25	109.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	364	TPO	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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
5	BMA	A	556	1	11,11,12	0.68	0	13,15,17	1.54	3 (23%)
5	BMA	A	557	1	11,11,12	0.74	0	13,15,17	1.84	2 (15%)
5	BMA	A	558	1	11,11,12	0.72	0	13,15,17	1.46	2 (15%)
5	BMA	A	559	1	11,11,12	1.04	1 (9%)	13,15,17	2.92	4 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BMA	B	539	2	11,11,12	0.51	0	13,15,17	1.19	1 (7%)
5	BMA	B	540	2	11,11,12	0.72	0	13,15,17	1.62	2 (15%)
5	BMA	B	541	2	11,11,12	0.71	0	13,15,17	1.26	1 (7%)
5	BMA	B	542	2	11,11,12	0.83	0	13,15,17	0.79	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
5	BMA	A	556	1	-	0/2/19/22	0/1/1/1
5	BMA	A	557	1	-	0/2/19/22	0/1/1/1
5	BMA	A	558	1	-	0/2/19/22	0/1/1/1
5	BMA	A	559	1	-	0/2/19/22	0/1/1/1
5	BMA	B	539	2	-	0/2/19/22	0/1/1/1
5	BMA	B	540	2	-	0/2/19/22	0/1/1/1
5	BMA	B	541	2	-	0/2/19/22	0/1/1/1
5	BMA	B	542	2	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	559	BMA	C2-C3	2.23	1.55	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	559	BMA	C1-O5-C5	-7.94	101.22	112.17
5	A	557	BMA	C1-O5-C5	-4.99	105.29	112.17
5	A	558	BMA	C1-O5-C5	-3.63	107.17	112.17
5	B	540	BMA	C1-C2-C3	-3.50	105.21	109.65
5	B	541	BMA	O3-C3-C4	-2.27	105.41	110.36
5	A	556	BMA	O4-C4-C3	-2.15	105.67	110.36
5	B	540	BMA	C3-C4-C5	-2.02	106.65	110.22
5	A	556	BMA	O2-C2-C3	-2.00	106.25	110.17
5	B	539	BMA	O2-C2-C1	2.28	113.81	109.18
5	A	557	BMA	C3-C4-C5	2.31	114.29	110.22
5	A	558	BMA	C3-C4-C5	2.57	114.75	110.22
5	A	556	BMA	O2-C2-C1	2.76	114.79	109.18
5	A	559	BMA	O2-C2-C1	3.26	115.81	109.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	559	BMA	C2-C3-C4	3.51	117.00	110.88
5	A	559	BMA	C3-C4-C5	4.17	117.57	110.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	558	BMA	1	0
5	B	541	BMA	1	0
5	B	542	BMA	2	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	478/554 (86%)	0.42	25 (5%)	28 29	23, 54, 79, 94	1 (0%)
2	B	503/537 (93%)	0.29	19 (3%)	41 43	26, 48, 74, 86	0
3	C	165/182 (90%)	0.14	4 (2%)	59 61	28, 53, 77, 83	0
All	All	1146/1273 (90%)	0.32	48 (4%)	37 39	23, 50, 77, 94	1 (0%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	108	CYS	8.4
1	A	281	ASP	6.6
1	A	491	LEU	5.7
1	A	492	GLY	4.5
2	B	216	SER	4.3
2	B	93	GLY	4.3
1	A	3	THR	4.2
1	A	371	LYS	4.0
2	B	109	GLN	4.0
1	A	507	LYS	3.9
2	B	502	SER	3.8
1	A	409	SER	3.8
1	A	527	GLU	3.6
2	B	346	VAL	3.6
1	A	521	CYS	3.5
2	B	345	SER	3.3
1	A	509	ASP	3.2
1	A	494	LEU	3.1
1	A	164	CYS	3.0
1	A	410	THR	3.0
2	B	66	VAL	3.0
1	A	506	ALA	3.0
2	B	234	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	386	VAL	2.8
2	B	57	VAL	2.8
1	A	99	ASP	2.7
3	C	173	GLN	2.7
2	B	192	GLU	2.7
1	A	490	ARG	2.6
1	A	23	CYS	2.5
1	A	377	THR	2.4
2	B	94	ASP	2.4
1	A	517	SER	2.4
1	A	389	ILE	2.4
2	B	170	GLN	2.3
2	B	173	TYR	2.3
1	A	106	ILE	2.2
1	A	98	ASP	2.2
2	B	107	LYS	2.2
2	B	389	LEU	2.2
2	B	505	GLY	2.2
2	B	315	ASP	2.2
3	C	174	PHE	2.2
2	B	503	CYS	2.2
1	A	246	LEU	2.1
1	A	508	ALA	2.1
3	C	42	PHE	2.1
3	C	16	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	TPO	B	364	11/12	0.69	0.23	-	69,71,79,79	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	BMA	B	542	11/12	0.59	0.29	0.87	56,60,62,62	0
4	CA	B	538	1/1	0.96	0.15	0.53	38,38,38,38	0
5	BMA	A	557	11/12	0.94	0.18	0.32	58,61,61,62	0
5	BMA	A	556	11/12	0.91	0.14	0.14	47,51,56,59	0
5	BMA	B	541	11/12	0.95	0.12	-1.01	39,42,44,46	0
5	BMA	A	558	11/12	0.93	0.12	-1.49	63,65,67,67	0
4	CA	A	555	1/1	0.99	0.09	-1.93	45,45,45,45	0
5	BMA	A	559	11/12	0.66	0.32	-	79,81,81,82	0
5	BMA	B	539	11/12	0.94	0.14	-	56,59,62,64	0
5	BMA	B	540	11/12	0.83	0.34	-	63,67,67,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.