



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:52 am GMT

PDB ID : 4BTW
Title : Crystal structure of human vascular adhesion protein-1 in complex with pyridazinone inhibitors
Authors : Bligt-Linden, E.; Pihlavisto, M.; Szatmari, I.; Otwinowski, Z.; Smith, D.J.; Lazar, L.; Fulop, F.; Salminen, T.A.
Deposited on : 2013-06-19
Resolution : 2.80 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	:	trunk28620
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)	:	recalc28949

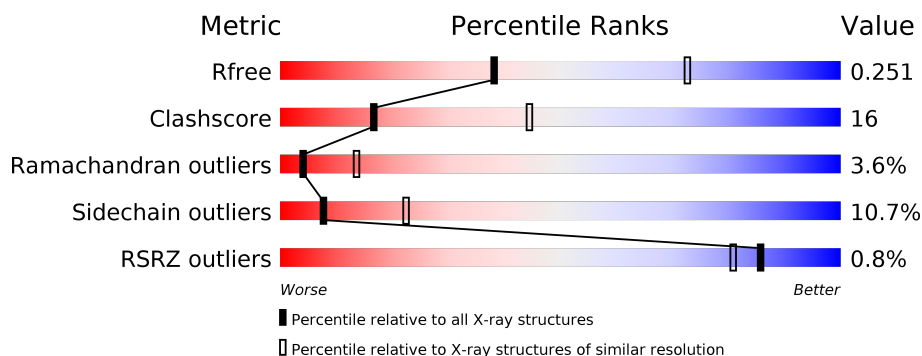
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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	737	<div> <div></div> <div>60% 30% 6% .</div> </div>
1	B	737	<div> <div></div> <div>59% 30% 6% .</div> </div>

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	1770	X	-	-	-
6	NAG	A	1771	X	-	-	-
6	NAG	B	1774	X	-	-	-
7	JW7	A	2000	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 11573 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 MEMBRANE PRIMARY AMINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	711	Total	C	N	O	S	0	0	0
			5609	3599	970	1020	20			
1	B	705	Total	C	N	O	S	0	0	0
			5562	3571	959	1012	20			

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cu	0	0
			1	1		
2	A	1	Total	Cu	0	0
			1	1		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Ca	0	0
			2	2		
3	A	2	Total	Ca	0	0
			2	2		

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

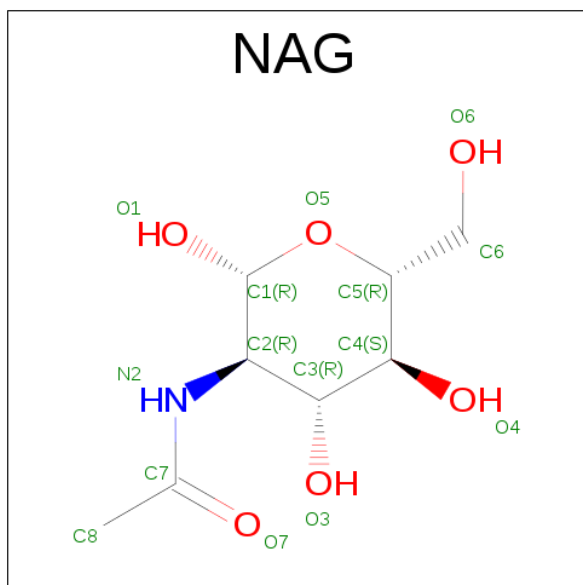
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	2	Total	C	N	O	0	0
			28	16	2	10		

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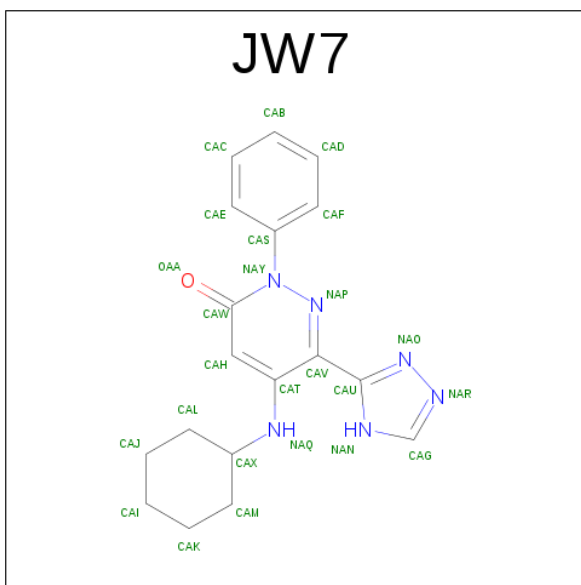
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is 5-(CYCLOHEXYLAMINO)-2-PHENYL-6-(1H-1,2,4-TRIAZOL-5-YL)-3(2H)-PYRIDAZINONE (three-letter code: JW7) (formula: $C_{18}H_{20}N_6O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total 25	C 18	N 6	O 1	0	0
7	B	1	Total 25	C 18	N 6	O 1	0	0

- Molecule 8 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	5	Total	C	N	O	0	0
			61	34	2	25		

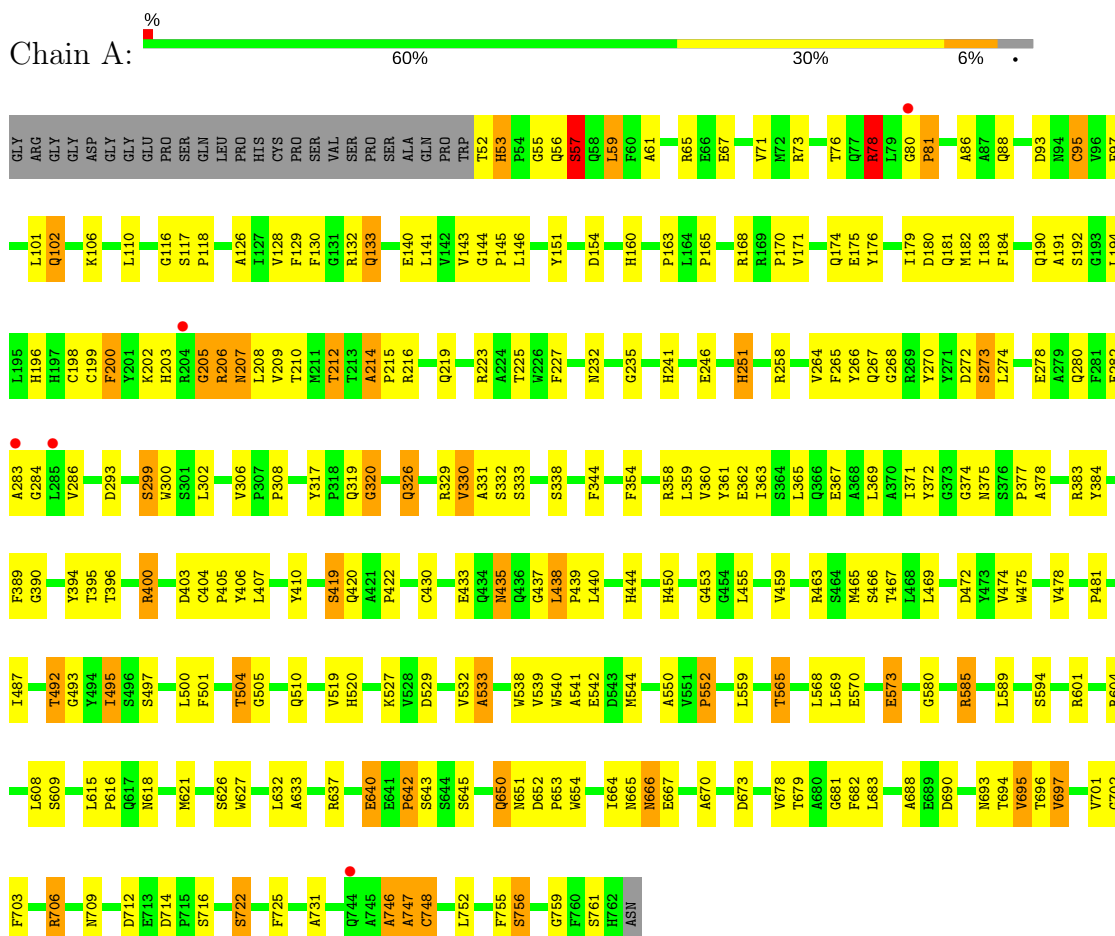
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	64	Total O 64 64	0	0
9	B	42	Total O 42 42	0	0

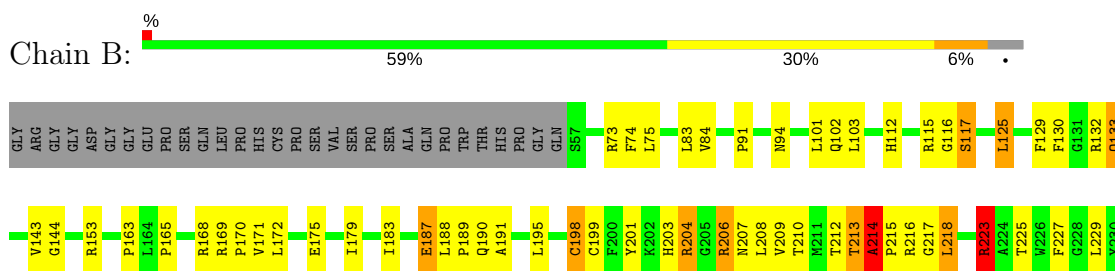
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: MEMBRANE PRIMARY AMINE OXIDASE



• Molecule 1: MEMBRANE PRIMARY AMINE OXIDASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	226.47Å 226.47Å 219.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.39 – 2.80 49.34 – 2.80	Depositor EDS
% Data completeness (in resolution range)	77.9 (49.39-2.80) 77.9 (49.34-2.80)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.205 , 0.260 0.199 , 0.251	Depositor DCC
R_{free} test set	3176 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	53.3	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11573	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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: BMA, NAG, CA, JW7, TPQ, CU, MAN

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	0.73	1/5774 (0.0%)	0.95	6/7874 (0.1%)
1	B	0.73	2/5724 (0.0%)	0.93	8/7805 (0.1%)
All	All	0.73	3/11498 (0.0%)	0.94	14/15679 (0.1%)

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	3
1	B	0	4
All	All	0	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	641	GLU	CG-CD	6.26	1.61	1.51
1	B	641	GLU	CD-OE2	5.39	1.31	1.25
1	A	540	TRP	CB-CG	-5.39	1.40	1.50

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	223	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	A	78	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	A	529	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	B	531	ASP	CB-CG-OD1	5.96	123.66	118.30
1	B	223	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	A	712	ASP	CB-CG-OD2	-5.80	113.08	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	B	572	GLU	OE1-CD-OE2	-5.64	116.53	123.30
1	A	330	VAL	CB-CA-C	-5.42	101.11	111.40
1	B	641	GLU	CA-CB-CG	5.38	125.23	113.40
1	B	641	GLU	OE1-CD-OE2	-5.21	117.04	123.30
1	B	462	VAL	CB-CA-C	-5.06	101.78	111.40
1	A	529	ASP	CB-CG-OD1	5.03	122.83	118.30
1	B	529	ASP	CB-CG-OD2	-5.00	113.80	118.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	198	CYS	Peptide
1	A	205	GLY	Peptide
1	A	437	GLY	Peptide
1	B	213	THR	Peptide
1	B	214	ALA	Peptide
1	B	512	SER	Peptide
1	B	749	ALA	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	5609	0	5351	171	1
1	B	5562	0	5313	197	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	39	0	34	1	0
5	A	28	0	25	0	0
5	B	28	0	25	0	0
6	A	28	0	26	0	0
6	B	56	0	52	2	0
7	A	25	0	20	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	25	0	20	6	0
8	B	61	0	52	3	0
9	A	64	0	0	1	0
9	B	42	0	0	8	0
All	All	11573	0	10918	353	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 16.

All (353) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:GLU:OE2	1:A:645:SER:OG	1.75	1.04
1:A:492:THR:HG21	1:B:441:ARG:HA	1.42	1.01
1:A:80:GLY:O	1:A:81:PRO:O	1.90	0.90
1:B:620:SER:HG	1:B:654:TRP:HD1	1.11	0.90
1:A:495:ILE:HB	9:A:2046:HOH:O	1.70	0.89
7:B:2000:JW7:HAH	7:B:2000:JW7:HAM1	1.59	0.85
1:A:265:PHE:HD2	1:A:270:TYR:CE1	1.95	0.85
1:A:469:LEU:HD21	7:A:2000:JW7:CAD	2.07	0.84
1:A:585:ARG:NH1	1:B:611:ALA:O	2.11	0.83
1:B:500:LEU:HD11	1:B:504:THR:HG21	1.60	0.83
8:B:1767:BMA:HO4	8:B:1768:BMA:HO2	1.14	0.82
1:A:102:GLN:HA	1:A:102:GLN:HE21	1.45	0.79
1:B:214:ALA:CB	1:B:382:THR:HA	2.12	0.79
1:A:519:VAL:HG13	1:B:562:LEU:HD23	1.63	0.79
1:B:271:TYR:CE2	1:B:277:LEU:HD13	2.18	0.79
1:A:86:ALA:HA	1:A:95:CYS:SG	2.25	0.76
1:A:214:ALA:CB	1:A:215:PRO:HD3	2.16	0.75
1:B:214:ALA:HB2	1:B:382:THR:HA	1.67	0.75
1:B:163:PRO:HB3	8:B:1765:NAG:H82	1.69	0.74
1:B:381:THR:O	1:B:383:ARG:HD3	1.87	0.74
1:A:191:ALA:HA	1:A:278:GLU:HG2	1.70	0.73
1:A:472:ASP:OD2	1:B:443:HIS:ND1	2.20	0.72
1:B:407:LEU:HD21	1:B:752:LEU:HD23	1.72	0.72
1:B:251:HIS:HA	1:B:259:TRP:CD1	2.25	0.71
1:B:214:ALA:CB	1:B:215:PRO:CD	2.68	0.71
1:B:214:ALA:CB	1:B:215:PRO:HD2	2.21	0.71
1:A:214:ALA:HB1	1:A:215:PRO:HD3	1.73	0.70
1:B:683:LEU:HD12	1:B:684:HIS:N	2.06	0.70
1:A:191:ALA:HA	1:A:278:GLU:CG	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:2000:JW7:OAA	7:B:2000:JW7:HAF	1.91	0.69
1:A:130:PHE:HB3	1:A:133:GLN:OE1	1.93	0.69
1:A:212:THR:OG1	1:A:216:ARG:NH2	2.26	0.69
1:B:474:VAL:HB	1:B:490:TYR:HB2	1.74	0.68
1:B:115:ARG:O	1:B:117:SER:N	2.26	0.68
1:B:214:ALA:HB1	1:B:215:PRO:CD	2.24	0.68
1:A:171:VAL:HG13	1:A:175:GLU:HB3	1.77	0.67
1:B:360:VAL:HG12	1:B:530:LEU:HA	1.77	0.66
1:B:525:HIS:CE1	1:B:644:SER:HG	2.13	0.66
1:A:492:THR:HG22	1:A:694:THR:O	1.96	0.65
1:B:478:VAL:HG22	1:B:486:GLU:HB3	1.78	0.65
1:B:349:ILE:HD11	1:B:363:ILE:HB	1.77	0.65
1:A:440:LEU:HD23	1:A:455:LEU:HD23	1.79	0.65
1:B:271:TYR:CD2	1:B:277:LEU:HD13	2.31	0.65
1:B:229:LEU:CD1	1:B:245:LEU:HD23	2.28	0.64
1:A:214:ALA:CB	1:A:215:PRO:CD	2.75	0.64
1:B:366:GLN:HG3	1:B:644:SER:HB2	1.80	0.64
1:B:496:SER:O	1:B:518:THR:HG22	1.98	0.64
1:B:214:ALA:HB1	1:B:383:ARG:H	1.63	0.63
1:A:78:ARG:HB2	1:A:78:ARG:HH11	1.63	0.63
1:B:469:LEU:HD21	7:B:2000:JW7:CAC	2.28	0.63
1:B:615:LEU:HD12	1:B:616:PRO:HD2	1.79	0.62
1:A:403:ASP:HB3	1:A:465:MET:HE3	1.81	0.62
1:A:394:TYR:CE1	7:A:2000:JW7:HAE	2.34	0.62
1:A:67:GLU:O	1:A:71:VAL:HG23	1.99	0.62
1:B:575:ALA:HB1	1:B:634:VAL:HG23	1.81	0.62
1:B:129:PHE:CZ	1:B:169:ARG:HB2	2.34	0.62
1:B:214:ALA:HB3	1:B:215:PRO:HD2	1.81	0.62
1:A:52:THR:OG1	1:A:53:HIS:CD2	2.53	0.61
1:B:382:THR:C	1:B:383:ARG:HD3	2.21	0.61
1:B:683:LEU:HD12	1:B:684:HIS:H	1.66	0.61
1:B:690:ASP:OD1	1:B:694:THR:HG23	1.99	0.61
1:A:369:LEU:HD12	1:A:384:TYR:O	2.01	0.61
1:B:419:SER:OG	1:B:420:GLN:N	2.34	0.60
1:B:542:GLU:HA	1:B:565:THR:O	2.01	0.60
1:A:640:GLU:C	1:A:642:PRO:HD3	2.22	0.60
1:B:468:LEU:O	1:B:471:TPQ:H6	2.01	0.60
1:A:344:PHE:HA	1:A:390:GLY:HA2	1.83	0.60
1:A:265:PHE:CD2	1:A:270:TYR:CE1	2.84	0.60
1:B:551:VAL:HG23	1:B:557:HIS:O	2.02	0.60
1:A:246:GLU:OE1	1:A:377:PRO:HD2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:GLU:O	1:B:274:LEU:HD13	2.01	0.59
1:B:716:SER:O	1:B:719:SER:HB2	2.02	0.59
1:A:495:ILE:N	1:A:495:ILE:HD12	2.17	0.59
1:B:212:THR:HG21	1:B:216:ARG:HH21	1.67	0.59
1:B:738:PRO:HA	1:B:741:CYS:SG	2.42	0.59
1:B:175:GLU:O	1:B:179:ILE:HG13	2.02	0.59
1:A:266:TYR:O	1:A:268:GLY:N	2.34	0.58
1:A:205:GLY:O	1:A:207:ASN:N	2.36	0.58
1:A:403:ASP:OD2	1:B:442:ARG:NH1	2.35	0.58
1:A:209:VAL:HG23	1:A:232:ASN:HB2	1.85	0.58
1:B:212:THR:HG21	1:B:216:ARG:NH2	2.19	0.58
1:A:265:PHE:HD2	1:A:270:TYR:HE1	1.48	0.58
1:A:241:HIS:NE2	1:A:299:SER:O	2.35	0.58
1:A:308:PRO:HA	1:B:720:ALA:O	2.04	0.58
1:B:229:LEU:HD13	1:B:245:LEU:HD23	1.87	0.57
1:B:187:GLU:HG3	1:B:274:LEU:HD12	1.86	0.57
1:A:102:GLN:CA	1:A:102:GLN:HE21	2.14	0.57
1:A:532:VAL:O	1:A:533:ALA:C	2.42	0.57
1:B:213:THR:HB	1:B:382:THR:OG1	2.05	0.57
1:B:214:ALA:HB2	1:B:382:THR:CA	2.35	0.57
1:B:187:GLU:CG	1:B:274:LEU:HD12	2.34	0.57
1:B:383:ARG:HD3	1:B:383:ARG:N	2.19	0.57
1:B:611:ALA:O	1:B:613:GLU:N	2.37	0.57
1:A:265:PHE:CD2	1:A:270:TYR:HE1	2.23	0.56
1:A:371:ILE:O	1:A:520:HIS:HA	2.04	0.56
1:A:59:LEU:HD23	1:A:59:LEU:N	2.20	0.56
1:B:716:SER:O	1:B:719:SER:CB	2.52	0.56
1:A:319:GLN:O	1:A:320:GLY:O	2.23	0.56
1:B:252:LYS:HD3	1:B:252:LYS:O	2.05	0.56
1:B:204:ARG:H	1:B:206:ARG:HH22	1.54	0.56
1:B:276:GLN:HG3	9:B:2014:HOH:O	2.06	0.56
1:A:372:TYR:CD1	1:A:520:HIS:HB3	2.40	0.55
1:A:403:ASP:HB3	1:A:465:MET:CE	2.36	0.55
1:A:492:THR:CG2	1:B:441:ARG:HA	2.27	0.55
1:B:500:LEU:CD1	1:B:504:THR:HG21	2.34	0.55
1:B:714:ASP:OD2	1:B:716:SER:OG	2.24	0.55
1:A:493:GLY:O	1:A:693:ASN:HA	2.07	0.55
1:A:57:SER:HB3	1:A:59:LEU:HD22	1.89	0.55
1:A:374:GLY:O	1:B:561:ARG:NH2	2.36	0.55
1:B:204:ARG:H	1:B:206:ARG:NH2	2.05	0.54
1:B:445:SER:HB3	1:B:451:TYR:CE1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:GLY:O	1:B:724:TYR:OH	2.23	0.54
1:A:214:ALA:HB3	1:A:215:PRO:HD3	1.90	0.54
1:B:214:ALA:HB1	1:B:215:PRO:HD2	1.86	0.54
1:A:440:LEU:HD23	1:A:455:LEU:CD2	2.37	0.54
1:A:200:PHE:N	1:A:200:PHE:CD1	2.75	0.54
1:A:627:TRP:CE3	1:A:679:THR:HG23	2.43	0.54
1:B:371:ILE:HG12	1:B:383:ARG:HB3	1.90	0.54
7:A:2000:JW7:HAE	7:A:2000:JW7:OAA	2.08	0.53
1:B:623:ARG:HD3	1:B:659:ASP:OD2	2.08	0.53
1:A:332:SER:OG	1:A:333:SER:N	2.42	0.53
1:A:52:THR:HG1	1:A:53:HIS:CD2	2.25	0.53
1:A:550:ALA:O	1:A:552:PRO:HD3	2.09	0.53
1:A:678:VAL:HG11	1:A:703:PHE:CD2	2.43	0.53
1:A:171:VAL:HG11	1:A:176:TYR:CE1	2.43	0.53
1:B:256:PRO:HA	1:B:259:TRP:CE2	2.44	0.52
1:B:445:SER:CB	1:B:451:TYR:CE1	2.92	0.52
1:B:349:ILE:CD1	1:B:363:ILE:HB	2.39	0.52
6:B:1774:NAG:O3	6:B:1774:NAG:H82	2.09	0.52
1:A:264:VAL:HG12	1:A:265:PHE:N	2.24	0.52
1:A:67:GLU:HB3	1:A:146:LEU:HD22	1.90	0.52
1:A:144:GLY:O	1:A:151:TYR:CD1	2.63	0.52
1:B:366:GLN:CG	1:B:644:SER:HB2	2.39	0.52
1:B:383:ARG:CD	1:B:383:ARG:N	2.72	0.52
1:A:544:MET:SD	1:B:613:GLU:HB3	2.50	0.52
1:A:495:ILE:HD12	1:A:495:ILE:H	1.74	0.52
1:B:281:PHE:HA	1:B:286:VAL:HB	1.91	0.52
1:B:214:ALA:HB1	1:B:383:ARG:N	2.23	0.52
1:A:453:GLY:HA3	1:B:302:LEU:HD13	1.92	0.51
1:A:219:GLN:O	1:A:654:TRP:CE3	2.63	0.51
1:A:209:VAL:HG13	1:B:448:TYR:CE2	2.46	0.51
1:B:102:GLN:OE1	1:B:125:LEU:HD12	2.11	0.51
1:A:141:LEU:HD23	1:A:154:ASP:HA	1.93	0.51
1:B:223:ARG:CG	1:B:223:ARG:HH11	2.24	0.51
1:A:106:LYS:HG3	1:A:361:TYR:CZ	2.46	0.51
1:B:352:VAL:HB	1:B:360:VAL:CG2	2.40	0.51
1:A:179:ILE:HD11	1:A:251:HIS:ND1	2.26	0.50
1:A:696:THR:HG21	1:B:439:PRO:O	2.11	0.50
1:A:192:SER:O	1:A:196:HIS:CD2	2.64	0.50
1:B:409:THR:O	1:B:430:CYS:HA	2.11	0.50
1:A:539:VAL:HB	1:A:589:LEU:CD2	2.42	0.50
1:B:372:TYR:CD1	1:B:520:HIS:HB3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:706:ARG:NH2	1:B:699:ASN:OD1	2.45	0.50
1:A:71:VAL:HG13	1:A:143:VAL:HG11	1.94	0.50
1:A:652:ASP:N	1:A:653:PRO:HD3	2.26	0.50
1:A:701:VAL:CG1	1:A:702:GLY:N	2.75	0.49
1:A:665:ASN:O	1:A:667:GLU:N	2.46	0.49
1:B:532:VAL:HG21	1:B:589:LEU:O	2.13	0.49
1:B:266:TYR:O	1:B:268:GLY:N	2.45	0.49
1:A:214:ALA:HB2	1:A:384:TYR:HA	1.94	0.49
8:B:1767:BMA:O4	8:B:1768:BMA:O2	1.97	0.49
1:A:214:ALA:O	1:A:215:PRO:C	2.50	0.49
1:A:241:HIS:CE1	1:A:300:TRP:CZ3	3.00	0.49
1:A:272:ASP:O	1:A:273:SER:HB3	2.13	0.49
1:B:404:CYS:HB2	1:B:410:TYR:OH	2.12	0.49
1:B:571:MET:O	1:B:573:GLU:N	2.45	0.49
1:A:59:LEU:H	1:A:59:LEU:HD23	1.77	0.49
1:A:568:LEU:HD23	1:A:570:GLU:CG	2.42	0.48
1:A:585:ARG:NH1	1:B:613:GLU:HB2	2.28	0.48
1:A:438:LEU:HD12	1:A:439:PRO:HD2	1.95	0.48
7:B:2000:JW7:OAA	7:B:2000:JW7:CAF	2.61	0.48
1:A:214:ALA:HB1	1:A:215:PRO:CD	2.42	0.48
1:B:337:PHE:CE2	1:B:479:PHE:CE2	3.02	0.48
1:A:372:TYR:CE1	1:A:520:HIS:HB3	2.49	0.48
1:A:97:PHE:CG	1:A:129:PHE:CZ	3.01	0.48
1:A:469:LEU:HD21	7:A:2000:JW7:CAF	2.42	0.48
1:A:573:GLU:OE2	1:A:666:ASN:HA	2.14	0.48
1:B:386:ASP:HB3	1:B:468:LEU:CD1	2.44	0.48
1:B:469:LEU:HD21	7:B:2000:JW7:CAE	2.44	0.48
1:B:640:GLU:C	1:B:642:PRO:HD3	2.34	0.48
1:B:497:SER:HB2	1:B:515:THR:HG22	1.95	0.48
1:A:317:TYR:N	1:A:317:TYR:CD1	2.80	0.47
1:B:275:ALA:O	1:B:276:GLN:C	2.52	0.47
1:B:214:ALA:HB2	1:B:382:THR:HG23	1.96	0.47
1:B:744:GLN:NE2	9:B:2041:HOH:O	2.47	0.47
1:B:129:PHE:CE1	1:B:169:ARG:HB2	2.49	0.47
1:B:556:GLU:HA	1:B:556:GLU:OE1	2.14	0.47
1:B:571:MET:HB2	1:B:574:GLN:HG3	1.96	0.47
1:A:110:LEU:HD22	1:A:358:ARG:NH1	2.29	0.47
1:A:354:PHE:HB2	1:A:359:LEU:HD11	1.96	0.47
1:A:65:ARG:NH2	1:A:422:PRO:O	2.48	0.47
1:A:688:ALA:O	1:B:713:GLU:HA	2.14	0.47
1:A:330:VAL:HG12	1:A:331:ALA:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:THR:HG21	1:B:444:HIS:O	2.14	0.47
1:A:601:ARG:HA	1:A:709:ASN:O	2.15	0.47
1:B:132:ARG:O	1:B:133:GLN:HB3	2.14	0.47
1:A:126:ALA:HB3	1:A:141:LEU:HB2	1.96	0.47
1:B:620:SER:OG	1:B:654:TRP:CD1	2.62	0.47
1:B:447:LEU:O	1:B:449:SER:N	2.42	0.47
1:B:593:HIS:HE1	6:B:1773:NAG:H82	1.79	0.47
1:B:486:GLU:HG3	1:B:704:PHE:CE1	2.50	0.47
1:B:258:ARG:HB2	1:B:258:ARG:NH1	2.30	0.47
1:A:278:GLU:HA	1:A:278:GLU:OE1	2.15	0.47
1:B:463:ARG:HB2	1:B:476:ASP:OD1	2.15	0.47
1:A:214:ALA:HB3	1:A:215:PRO:CD	2.46	0.46
1:A:495:ILE:HD11	1:A:690:ASP:O	2.15	0.46
1:A:400:ARG:HG2	1:A:406:TYR:CD1	2.51	0.46
1:A:181:GLN:O	1:A:182:MET:C	2.52	0.46
1:B:191:ALA:HA	1:B:278:GLU:HB2	1.96	0.46
1:B:742:LEU:HA	9:B:2041:HOH:O	2.16	0.46
1:B:91:PRO:HB2	1:B:254:LEU:HA	1.97	0.46
1:A:280:GLN:HB3	1:A:286:VAL:CG2	2.45	0.46
1:A:487:ILE:HG12	1:A:703:PHE:CE1	2.51	0.46
1:B:339:PHE:HA	1:B:349:ILE:HG22	1.97	0.46
1:B:440:LEU:HD12	1:B:440:LEU:O	2.15	0.46
1:A:695:VAL:HG13	1:B:440:LEU:CD1	2.45	0.46
1:B:381:THR:HG21	9:B:2012:HOH:O	2.16	0.46
1:B:512:SER:HB3	1:B:515:THR:HB	1.98	0.46
1:A:140:GLU:OE1	1:A:160:HIS:NE2	2.47	0.46
1:B:246:GLU:OE1	1:B:376:SER:HB2	2.16	0.46
1:B:417:LEU:O	1:B:418:GLU:C	2.54	0.46
1:A:117:SER:HB3	1:A:118:PRO:CD	2.46	0.46
1:A:225:THR:HB	1:A:227:PHE:CE2	2.50	0.46
1:B:258:ARG:HB2	1:B:258:ARG:HH11	1.81	0.46
1:A:492:THR:HB	1:A:493:GLY:H	1.47	0.45
1:A:746:ALA:O	1:A:747:ALA:C	2.55	0.45
1:B:382:THR:HG21	1:B:384:TYR:CE1	2.51	0.45
1:B:501:PHE:O	1:B:503:ALA:N	2.48	0.45
1:A:683:LEU:HD13	1:B:544:MET:CE	2.46	0.45
1:A:419:SER:OG	1:A:420:GLN:N	2.49	0.45
1:B:212:THR:CG2	1:B:216:ARG:HH21	2.28	0.45
1:B:488:ARG:NH2	1:B:608:LEU:HD22	2.31	0.45
1:B:478:VAL:HG22	1:B:486:GLU:CB	2.46	0.45
1:A:106:LYS:HZ3	1:A:673:ASP:CG	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:VAL:HG13	1:B:175:GLU:HB3	1.98	0.45
1:B:335:TRP:HZ2	1:B:480:HIS:O	1.99	0.45
1:B:195:LEU:HB3	1:B:201:TYR:HB2	1.97	0.45
1:B:394:TYR:HA	9:B:2020:HOH:O	2.16	0.45
1:B:509:ASN:HB2	1:B:686:PRO:O	2.16	0.45
1:B:451:TYR:N	1:B:451:TYR:CD1	2.85	0.44
1:A:375:ASN:ND2	1:A:501:PHE:O	2.48	0.44
1:B:508:GLY:HA3	1:B:517:GLY:O	2.16	0.44
1:A:61:ALA:O	1:A:101:LEU:HD22	2.17	0.44
1:B:195:LEU:CB	1:B:201:TYR:HB2	2.47	0.44
1:A:459:VAL:CG1	1:A:478:VAL:CG1	2.95	0.44
1:A:627:TRP:HE3	1:A:679:THR:HG23	1.83	0.44
1:B:225:THR:HB	1:B:227:PHE:CE1	2.52	0.44
1:B:266:TYR:O	1:B:267:GLN:C	2.56	0.44
1:A:440:LEU:HD22	1:A:481:PRO:HG2	1.99	0.44
1:A:714:ASP:HB2	1:B:689:GLU:O	2.17	0.44
1:B:212:THR:HG22	1:B:213:THR:N	2.31	0.44
1:B:474:VAL:O	1:B:489:PHE:HA	2.18	0.44
1:B:551:VAL:HG23	1:B:557:HIS:C	2.37	0.44
1:B:716:SER:O	1:B:719:SER:N	2.51	0.44
1:B:74:PHE:O	1:B:75:LEU:C	2.55	0.44
1:B:537:ASN:HA	1:B:590:ALA:O	2.18	0.44
1:B:659:ASP:OD1	1:B:659:ASP:C	2.56	0.44
1:A:407:LEU:HD21	1:A:752:LEU:HD22	1.99	0.44
1:B:188:LEU:N	1:B:189:PRO:CD	2.81	0.44
1:A:199:CYS:C	1:A:200:PHE:HD1	2.21	0.44
1:A:633:ALA:HB1	1:A:664:ILE:HD11	1.99	0.44
1:B:281:PHE:O	1:B:284:GLY:N	2.47	0.44
1:B:231:TYR:HE2	1:B:291:ILE:HG22	1.83	0.44
1:B:251:HIS:HA	1:B:259:TRP:CG	2.53	0.43
1:A:88:GLN:HA	1:A:174:GLN:HG2	2.00	0.43
1:A:171:VAL:HG11	1:A:176:TYR:CD1	2.54	0.43
1:A:400:ARG:HG2	1:A:406:TYR:CE1	2.54	0.43
1:A:542:GLU:HA	1:A:565:THR:O	2.18	0.43
1:B:183:ILE:HG22	1:B:188:LEU:HG	1.99	0.43
1:B:650:GLN:HA	1:B:650:GLN:OE1	2.18	0.43
1:B:453:GLY:HA2	1:B:723:ILE:O	2.18	0.43
1:A:117:SER:HB3	1:A:118:PRO:HD2	2.00	0.43
1:A:465:MET:HE2	1:A:474:VAL:HG22	2.00	0.43
1:A:214:ALA:HB1	1:A:383:ARG:O	2.18	0.43
1:A:538:TRP:CD1	1:A:670:ALA:HA	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:GLN:NE2	1:B:527:LYS:HB2	2.34	0.43
1:B:393:LYS:HG3	1:B:417:LEU:HD13	2.01	0.43
1:A:209:VAL:CG2	1:A:232:ASN:HB2	2.48	0.43
1:B:256:PRO:HA	1:B:259:TRP:CD2	2.53	0.43
1:B:367:GLU:OE2	1:B:387:GLY:N	2.44	0.43
1:A:344:PHE:HA	1:A:390:GLY:CA	2.48	0.43
1:B:195:LEU:HD12	1:B:201:TYR:CD2	2.54	0.43
1:B:502:GLY:O	1:B:504:THR:N	2.52	0.43
1:A:171:VAL:HG22	1:A:223:ARG:HH21	1.84	0.43
1:A:78:ARG:HB2	1:A:78:ARG:NH1	2.32	0.43
1:B:498:ALA:HB3	1:B:516:LEU:HB3	2.01	0.43
1:B:737:ASN:C	1:B:737:ASN:OD1	2.57	0.43
1:A:163:PRO:HB3	4:A:1765:NAG:H82	2.01	0.42
1:A:395:THR:HA	1:A:466:SER:HA	2.01	0.42
1:B:245:LEU:HD12	1:B:265:PHE:O	2.19	0.42
1:A:395:THR:CG2	1:A:396:THR:N	2.83	0.42
1:A:435:ASN:C	1:A:435:ASN:OD1	2.57	0.42
1:A:179:ILE:HG22	1:A:180:ASP:N	2.35	0.42
1:A:365:LEU:HD21	1:A:475:TRP:CZ2	2.54	0.42
1:A:389:PHE:HB3	1:A:394:TYR:CE2	2.54	0.42
1:A:306:VAL:HG21	1:B:718:TYR:O	2.19	0.42
1:B:749:ALA:CB	1:B:750:PRO:CD	2.97	0.42
1:A:504:THR:HG22	1:A:505:GLY:N	2.35	0.42
1:B:165:PRO:HD2	1:B:168:ARG:NH1	2.34	0.42
1:A:403:ASP:O	1:A:404:CYS:SG	2.77	0.42
1:A:205:GLY:O	1:A:207:ASN:ND2	2.41	0.42
1:A:696:THR:O	1:A:697:VAL:C	2.58	0.42
1:B:94:ASN:OD1	1:B:130:PHE:HA	2.20	0.42
1:B:360:VAL:CG1	1:B:530:LEU:HD23	2.50	0.42
1:A:183:ILE:HG22	1:A:184:PHE:N	2.34	0.42
1:A:444:HIS:O	1:B:467:THR:HG21	2.20	0.42
1:A:500:LEU:HD22	1:A:510:GLN:HG3	2.01	0.42
1:A:541:ALA:HB2	1:A:569:LEU:HD11	2.01	0.42
1:B:297:GLY:O	1:B:299:SER:N	2.49	0.42
1:A:282:GLU:C	1:A:284:GLY:H	2.22	0.42
1:B:198:CYS:HB2	1:B:266:TYR:OH	2.20	0.42
1:B:112:HIS:CD2	1:B:112:HIS:C	2.91	0.41
1:B:587:LEU:O	1:B:587:LEU:HD23	2.20	0.41
1:A:695:VAL:HG13	1:B:440:LEU:HD12	2.00	0.41
1:A:725:PHE:CD2	1:A:731:ALA:HB2	2.54	0.41
1:A:755:PHE:CD1	1:A:756:SER:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:VAL:HG12	1:B:144:GLY:N	2.34	0.41
1:A:539:VAL:HB	1:A:589:LEU:HD22	2.02	0.41
7:B:2000:JW7:CAH	7:B:2000:JW7:HAM1	2.40	0.41
1:B:203:HIS:HA	1:B:204:ARG:HA	1.78	0.41
1:A:93:ASP:HA	1:A:132:ARG:NH2	2.35	0.41
1:B:101:LEU:HD23	1:B:103:LEU:HD23	2.03	0.41
1:B:187:GLU:O	1:B:274:LEU:CD1	2.67	0.41
1:A:144:GLY:C	1:A:151:TYR:CE1	2.94	0.41
1:A:405:PRO:O	1:A:410:TYR:OH	2.31	0.41
1:A:615:LEU:HA	1:A:616:PRO:HD2	1.82	0.41
1:B:633:ALA:O	1:B:677:TRP:N	2.48	0.41
1:B:524:ALA:O	1:B:679:THR:HA	2.20	0.41
1:A:362:GLU:OE1	1:A:527:LYS:HE2	2.21	0.41
1:A:56:GLN:O	1:A:57:SER:C	2.58	0.41
1:B:722:SER:O	1:B:723:ILE:HD13	2.20	0.41
1:B:153:ARG:HD2	9:B:2005:HOH:O	2.21	0.41
1:B:217:GLY:C	1:B:218:LEU:HD13	2.41	0.41
1:B:352:VAL:HB	1:B:360:VAL:HG23	2.01	0.41
1:B:388:GLY:HA3	1:B:650:GLN:HB2	2.01	0.41
1:B:564:VAL:HG12	1:B:565:THR:N	2.36	0.41
1:B:501:PHE:CD2	1:B:501:PHE:O	2.74	0.41
1:B:242:HIS:HD2	1:B:499:PHE:H	1.68	0.41
1:B:342:GLY:O	1:B:343:ALA:C	2.58	0.41
1:B:571:MET:HE2	9:B:2037:HOH:O	2.21	0.41
1:A:430:CYS:SG	1:A:463:ARG:HB3	2.60	0.41
1:B:497:SER:HB2	1:B:515:THR:CG2	2.51	0.41
1:B:499:PHE:CD1	1:B:500:LEU:N	2.88	0.41
1:A:681:GLY:O	1:A:682:PHE:HB3	2.21	0.40
1:B:330:VAL:O	1:B:336:THR:HA	2.21	0.40
1:B:352:VAL:HB	1:B:360:VAL:HG22	2.03	0.40
1:A:383:ARG:HD3	1:A:621:MET:SD	2.62	0.40
1:A:433:GLU:HA	1:A:459:VAL:O	2.20	0.40
1:B:399:THR:HA	9:B:2022:HOH:O	2.21	0.40
1:B:425:ILE:HG22	1:B:425:ILE:O	2.20	0.40
1:B:480:HIS:HA	1:B:481:PRO:HD2	1.92	0.40
1:B:215:PRO:HG3	1:B:621:MET:SD	2.61	0.40
1:A:650:GLN:HG3	1:A:651:ASN:OD1	2.22	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:326:GLN:OE1	1:A:326:GLN:OE1[10_665]	1.91	0.29

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	708/737 (96%)	599 (85%)	82 (12%)	27 (4%)	4	12
1	B	702/737 (95%)	607 (86%)	71 (10%)	24 (3%)	4	15
All	All	1410/1474 (96%)	1206 (86%)	153 (11%)	51 (4%)	4	13

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	PRO
1	A	116	GLY
1	A	206	ARG
1	A	214	ALA
1	A	267	GLN
1	A	504	THR
1	A	697	VAL
1	A	747	ALA
1	B	214	ALA
1	B	267	GLN
1	B	502	GLY
1	B	744	GLN
1	B	747	ALA
1	B	749	ALA
1	A	57	SER
1	A	273	SER
1	A	283	ALA
1	A	320	GLY
1	A	378	ALA
1	A	580	GLY

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Mol	Chain	Res	Type
1	A	666	ASN
1	A	748	CYS
1	A	759	GLY
1	B	116	GLY
1	B	280	GLN
1	B	418	GLU
1	B	448	TYR
1	B	503	ALA
1	B	572	GLU
1	B	612	GLY
1	A	274	LEU
1	B	513	GLU
1	B	740	ALA
1	A	190	GLN
1	A	533	ALA
1	A	722	SER
1	A	746	ALA
1	B	117	SER
1	B	405	PRO
1	B	618	ASN
1	B	628	GLU
1	A	165	PRO
1	B	170	PRO
1	B	481	PRO
1	B	750	PRO
1	A	438	LEU
1	A	642	PRO
1	B	133	GLN
1	B	641	GLU
1	A	55	GLY
1	A	145	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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	590/610 (97%)	530 (90%)	60 (10%)	8 25
1	B	585/610 (96%)	519 (89%)	66 (11%)	7 20
All	All	1175/1220 (96%)	1049 (89%)	126 (11%)	8 22

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	HIS
1	A	57	SER
1	A	59	LEU
1	A	73	ARG
1	A	76	THR
1	A	78	ARG
1	A	95	CYS
1	A	102	GLN
1	A	128	VAL
1	A	133	GLN
1	A	170	PRO
1	A	194	LEU
1	A	200	PHE
1	A	202	LYS
1	A	203	HIS
1	A	206	ARG
1	A	207	ASN
1	A	208	LEU
1	A	210	THR
1	A	212	THR
1	A	251	HIS
1	A	258	ARG
1	A	293	ASP
1	A	299	SER
1	A	302	LEU
1	A	326	GLN
1	A	329	ARG
1	A	338	SER
1	A	360	VAL
1	A	363	ILE
1	A	400	ARG
1	A	419	SER

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Mol	Chain	Res	Type
1	A	435	ASN
1	A	450	HIS
1	A	492	THR
1	A	495	ILE
1	A	497	SER
1	A	552	PRO
1	A	559	LEU
1	A	565	THR
1	A	573	GLU
1	A	585	ARG
1	A	594	SER
1	A	604	ARG
1	A	608	LEU
1	A	609	SER
1	A	618	ASN
1	A	626	SER
1	A	632	LEU
1	A	637	ARG
1	A	640	GLU
1	A	643	SER
1	A	650	GLN
1	A	695	VAL
1	A	706	ARG
1	A	716	SER
1	A	722	SER
1	A	748	CYS
1	A	756	SER
1	A	761	SER
1	B	73	ARG
1	B	83	LEU
1	B	84	VAL
1	B	125	LEU
1	B	172	LEU
1	B	187	GLU
1	B	190	GLN
1	B	198	CYS
1	B	199	CYS
1	B	204	ARG
1	B	206	ARG
1	B	207	ASN
1	B	208	LEU
1	B	209	VAL

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Mol	Chain	Res	Type
1	B	210	THR
1	B	218	LEU
1	B	223	ARG
1	B	258	ARG
1	B	260	THR
1	B	261	ILE
1	B	273	SER
1	B	276	GLN
1	B	280	GLN
1	B	299	SER
1	B	301	SER
1	B	319	GLN
1	B	345	SER
1	B	358	ARG
1	B	376	SER
1	B	381	THR
1	B	383	ARG
1	B	405	PRO
1	B	409	THR
1	B	419	SER
1	B	425	ILE
1	B	438	LEU
1	B	440	LEU
1	B	442	ARG
1	B	455	LEU
1	B	458	THR
1	B	478	VAL
1	B	489	PHE
1	B	539	VAL
1	B	544	MET
1	B	567	LYS
1	B	568	LEU
1	B	583	THR
1	B	596	LYS
1	B	608	LEU
1	B	613	GLU
1	B	626	SER
1	B	634	VAL
1	B	637	ARG
1	B	640	GLU
1	B	644	SER
1	B	645	SER

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Mol	Chain	Res	Type
1	B	646	SER
1	B	650	GLN
1	B	659	ASP
1	B	661	SER
1	B	668	THR
1	B	687	HIS
1	B	694	THR
1	B	713	GLU
1	B	735	GLU
1	B	742	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	HIS
1	A	102	GLN
1	B	112	HIS
1	B	593	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	TPQ	A	471	1	14,14,15	1.57	3 (21%)	17,19,21	1.54	3 (17%)
1	TPQ	B	471	1	14,14,15	1.37	2 (14%)	17,19,21	1.68	3 (17%)

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
1	TPQ	A	471	1	-	0/4/22/24	0/1/1/1
1	TPQ	B	471	1	-	0/4/22/24	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	471	TPQ	CA-C	-2.04	1.47	1.50
1	B	471	TPQ	C6-C1	2.46	1.41	1.34
1	A	471	TPQ	C6-C1	2.56	1.41	1.34
1	B	471	TPQ	C3-C4	2.88	1.40	1.35
1	A	471	TPQ	C3-C4	3.70	1.41	1.35

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	471	TPQ	CB-CA-C	-4.22	103.29	111.41
1	A	471	TPQ	CB-CA-C	-3.08	105.47	111.41
1	B	471	TPQ	O5-C5-C4	2.32	123.27	119.32
1	A	471	TPQ	C6-C1-C2	2.77	120.77	118.54
1	A	471	TPQ	O5-C5-C4	3.46	125.22	119.32
1	B	471	TPQ	C6-C1-C2	3.52	121.38	118.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	471	TPQ	1	0

5.5 Carbohydrates

12 carbohydrates 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
4	NAG	A	1765	1,4	14,14,15	0.72	0	15,19,21	1.65	4 (26%)
4	NAG	A	1766	4	14,14,15	0.82	1 (7%)	15,19,21	1.79	4 (26%)
4	BMA	A	1767	4	11,11,12	0.61	0	13,15,17	1.42	2 (15%)
5	NAG	A	1768	1,5	14,14,15	0.60	0	15,19,21	1.57	3 (20%)
5	NAG	A	1769	5	14,14,15	0.78	1 (7%)	15,19,21	1.39	2 (13%)
8	NAG	B	1765	1,8	14,14,15	0.57	0	15,19,21	1.15	1 (6%)
8	NAG	B	1766	8	14,14,15	0.48	0	15,19,21	1.71	3 (20%)
8	BMA	B	1767	8	11,11,12	0.79	0	13,15,17	2.23	3 (23%)
8	BMA	B	1768	8	11,11,12	0.68	0	13,15,17	2.32	5 (38%)
8	MAN	B	1769	8	11,11,12	0.53	0	13,15,17	2.62	3 (23%)
5	NAG	B	1770	1,5	14,14,15	0.83	0	15,19,21	2.21	5 (33%)
5	NAG	B	1771	5	14,14,15	0.64	0	15,19,21	1.59	3 (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
4	NAG	A	1765	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1766	4	-	0/6/23/26	0/1/1/1
4	BMA	A	1767	4	-	0/2/19/22	0/1/1/1
5	NAG	A	1768	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1769	5	-	0/6/23/26	0/1/1/1
8	NAG	B	1765	1,8	-	0/6/23/26	0/1/1/1
8	NAG	B	1766	8	-	0/6/23/26	0/1/1/1
8	BMA	B	1767	8	-	0/2/19/22	0/1/1/1
8	BMA	B	1768	8	-	0/2/19/22	0/1/1/1
8	MAN	B	1769	8	-	0/2/19/22	0/1/1/1
5	NAG	B	1770	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	1771	5	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1766	NAG	O5-C1	-2.08	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1769	NAG	C1-C2	2.06	1.55	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1767	BMA	O4-C4-C3	-5.01	99.46	110.36
8	B	1766	NAG	C2-N2-C7	-4.04	117.06	122.94
5	B	1770	NAG	C1-C2-N2	-3.89	103.84	110.49
4	A	1766	NAG	O4-C4-C3	-3.74	102.22	110.36
5	B	1770	NAG	O5-C1-C2	-3.42	106.71	111.47
5	A	1768	NAG	C1-C2-N2	-3.34	104.79	110.49
4	A	1766	NAG	O5-C1-C2	-3.25	106.95	111.47
4	A	1765	NAG	O4-C4-C3	-3.08	103.66	110.36
5	A	1768	NAG	C4-C3-C2	-2.85	106.83	111.02
4	A	1767	BMA	O5-C1-C2	-2.81	106.38	110.79
4	A	1765	NAG	C1-C2-N2	-2.78	105.73	110.49
8	B	1768	BMA	O2-C2-C3	-2.75	104.77	110.17
5	B	1771	NAG	O7-C7-C8	-2.57	117.38	122.06
8	B	1767	BMA	O5-C1-C2	-2.54	106.81	110.79
5	B	1770	NAG	O7-C7-C8	-2.29	117.90	122.06
5	A	1769	NAG	O7-C7-C8	-2.25	117.95	122.06
4	A	1767	BMA	O4-C4-C3	-2.21	105.55	110.36
4	A	1766	NAG	O7-C7-C8	-2.21	118.04	122.06
8	B	1766	NAG	C1-C2-N2	-2.13	106.86	110.49
8	B	1765	NAG	O4-C4-C3	2.05	114.81	110.36
4	A	1765	NAG	C1-O5-C5	2.16	115.14	112.17
5	B	1771	NAG	C1-O5-C5	2.22	115.23	112.17
8	B	1768	BMA	O2-C2-C1	2.29	113.83	109.18
8	B	1768	BMA	C3-C4-C5	2.44	114.51	110.22
5	A	1768	NAG	O3-C3-C2	2.70	115.18	109.39
5	B	1770	NAG	O7-C7-N2	2.76	127.23	121.92
8	B	1769	MAN	C3-C4-C5	2.90	115.33	110.22
5	B	1771	NAG	C1-C2-N2	2.91	115.46	110.49
8	B	1769	MAN	O5-C1-C2	2.96	115.43	110.79
5	A	1769	NAG	C1-O5-C5	3.00	116.31	112.17
4	A	1766	NAG	O4-C4-C5	3.20	117.35	109.28
4	A	1765	NAG	O3-C3-C2	3.38	116.64	109.39
8	B	1766	NAG	C1-O5-C5	3.61	117.14	112.17
8	B	1768	BMA	C1-O5-C5	4.55	118.44	112.17
8	B	1768	BMA	C1-C2-C3	4.92	115.89	109.65
5	B	1770	NAG	C2-N2-C7	5.23	130.58	122.94
8	B	1767	BMA	C3-C4-C5	5.37	119.68	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1769	MAN	C1-O5-C5	8.23	123.50	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1765	NAG	1	0
8	B	1765	NAG	1	0
8	B	1767	BMA	2	0
8	B	1768	BMA	2	0

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 6 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	$\# Z > 2$
6	NAG	A	1770	1	14,14,15	1.18	2 (14%)	15,19,21	2.20	4 (26%)
6	NAG	A	1771	1	14,14,15	1.82	3 (21%)	15,19,21	3.57	8 (53%)
7	JW7	A	2000	-	23,28,28	1.83	3 (13%)	23,38,38	4.08	6 (26%)
6	NAG	B	1772	-	14,14,15	0.76	0	15,19,21	1.20	1 (6%)
6	NAG	B	1773	1	14,14,15	1.02	1 (7%)	15,19,21	2.93	5 (33%)
6	NAG	B	1774	1	14,14,15	1.50	1 (7%)	15,19,21	2.65	6 (40%)
6	NAG	B	1775	1	14,14,15	0.71	0	15,19,21	1.51	3 (20%)
7	JW7	B	2000	-	23,28,28	2.02	4 (17%)	23,38,38	4.24	8 (34%)

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
6	NAG	A	1770	1	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	A	1771	1	1/1/5/7	0/6/23/26	0/1/1/1
7	JW7	A	2000	-	-	0/10/20/20	0/4/4/4
6	NAG	B	1772	-	-	0/6/23/26	0/1/1/1
6	NAG	B	1773	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1774	1	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	B	1775	1	-	0/6/23/26	0/1/1/1
7	JW7	B	2000	-	-	0/10/20/20	0/4/4/4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	2000	JW7	CAS-NAY	-5.22	1.33	1.44
7	B	2000	JW7	CAV-CAU	-5.11	1.39	1.49
7	A	2000	JW7	CAV-CAU	-4.61	1.40	1.49
7	A	2000	JW7	CAS-NAY	-4.46	1.34	1.44
6	A	1770	NAG	C1-C2	2.19	1.55	1.52
6	A	1770	NAG	C4-C5	2.30	1.57	1.53
7	B	2000	JW7	NAR-NAO	2.32	1.42	1.37
6	A	1771	NAG	C3-C2	2.54	1.58	1.52
6	A	1771	NAG	C2-N2	2.93	1.51	1.46
6	B	1773	NAG	C1-C2	3.09	1.56	1.52
6	B	1774	NAG	C1-C2	4.76	1.59	1.52
7	A	2000	JW7	OAA-CAW	4.92	1.36	1.24
6	A	1771	NAG	C1-C2	5.11	1.59	1.52
7	B	2000	JW7	OAA-CAW	5.12	1.37	1.24

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2000	JW7	NAN-CAU-NAO	-10.55	105.96	114.75
7	B	2000	JW7	NAN-CAU-NAO	-8.71	107.49	114.75
6	A	1771	NAG	O5-C1-C2	-7.06	101.64	111.47
7	B	2000	JW7	CAM-CAX-CAL	-3.87	104.62	110.85
6	B	1773	NAG	O7-C7-C8	-3.87	115.02	122.06
6	A	1771	NAG	O7-C7-C8	-3.86	115.02	122.06
6	B	1773	NAG	O5-C1-C2	-3.80	106.19	111.47
6	B	1774	NAG	O7-C7-C8	-3.28	116.09	122.06
7	A	2000	JW7	CAT-CAV-NAP	-2.89	117.92	121.09
7	B	2000	JW7	CAU-CAV-NAP	-2.58	114.08	117.31
7	A	2000	JW7	CAF-CAS-CAE	-2.53	117.40	121.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1770	NAG	O7-C7-C8	-2.29	117.88	122.06
6	B	1775	NAG	O5-C1-C2	-2.02	108.67	111.47
6	B	1774	NAG	C3-C4-C5	2.09	113.90	110.22
6	A	1771	NAG	O7-C7-N2	2.13	126.01	121.92
6	B	1772	NAG	O5-C1-C2	2.14	114.45	111.47
6	B	1775	NAG	O4-C4-C5	2.16	114.74	109.28
6	B	1773	NAG	C8-C7-N2	2.19	120.06	116.11
7	A	2000	JW7	CAD-CAF-CAS	2.34	121.64	118.66
7	B	2000	JW7	CAJ-CAL-CAX	2.59	114.92	111.11
7	A	2000	JW7	CAE-CAS-NAY	2.65	123.33	119.49
6	A	1770	NAG	C1-C2-N2	2.68	115.07	110.49
6	A	1771	NAG	O3-C3-C2	2.82	115.42	109.39
7	B	2000	JW7	CAF-CAS-NAY	3.04	123.89	119.49
6	B	1774	NAG	C1-C2-N2	3.18	115.92	110.49
6	A	1770	NAG	O4-C4-C5	3.37	117.78	109.28
7	B	2000	JW7	CAI-CAJ-CAL	3.55	118.77	111.42
6	B	1774	NAG	C8-C7-N2	3.72	122.83	116.11
6	B	1773	NAG	C1-C2-N2	3.78	116.95	110.49
6	B	1775	NAG	C1-O5-C5	4.02	117.71	112.17
6	A	1771	NAG	C4-C3-C2	4.22	117.20	111.02
7	B	2000	JW7	CAM-CAX-NAQ	4.28	117.88	110.55
6	B	1774	NAG	C2-N2-C7	4.38	129.34	122.94
6	A	1771	NAG	C1-O5-C5	4.67	118.61	112.17
6	A	1771	NAG	C1-C2-N2	5.12	119.24	110.49
6	A	1770	NAG	C1-O5-C5	5.50	119.74	112.17
6	A	1771	NAG	C2-N2-C7	6.25	132.06	122.94
6	B	1774	NAG	C1-O5-C5	6.34	120.91	112.17
6	B	1773	NAG	C1-O5-C5	8.32	123.64	112.17
7	A	2000	JW7	CAG-NAN-CAU	15.04	110.11	101.49
7	B	2000	JW7	CAG-NAN-CAU	15.83	110.56	101.49

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	1770	NAG	C1
6	B	1774	NAG	C1
6	A	1771	NAG	C1

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	2000	JW7	4	0
6	B	1773	NAG	1	0
6	B	1774	NAG	1	0
7	B	2000	JW7	6	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	710/737 (96%)	-0.49	5 (0%) 87 83	39, 58, 82, 138	0
1	B	704/737 (95%)	-0.41	7 (0%) 82 77	38, 59, 91, 153	0
All	All	1414/1474 (95%)	-0.45	12 (0%) 86 81	38, 59, 86, 153	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	746	ALA	5.4
1	B	747	ALA	5.0
1	B	745	ALA	4.3
1	B	748	CYS	2.9
1	B	735	GLU	2.8
1	A	283	ALA	2.7
1	B	742	LEU	2.6
1	A	285	LEU	2.6
1	A	744	GLN	2.5
1	A	80	GLY	2.4
1	A	204	ARG	2.3
1	B	743	PRO	2.1

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

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
1	TPQ	B	471	14/15	0.98	0.26	-	44,53,56,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	TPQ	A	471	14/15	0.98	0.19	-	43,48,52,54	0

6.3 Carbohydrates [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(\AA^2)	Q<0.9
5	NAG	A	1769	14/15	0.88	0.18	0.52	91,112,124,126	0
4	NAG	A	1765	14/15	0.97	0.13	-0.28	65,71,75,77	0
5	NAG	B	1770	14/15	0.95	0.11	-0.74	70,86,93,104	0
5	NAG	A	1768	14/15	0.98	0.10	-0.96	72,83,99,101	0
8	NAG	B	1765	14/15	0.98	0.09	-1.62	49,56,59,66	0
8	MAN	B	1769	11/12	0.89	0.31	-	112,126,141,142	0
5	NAG	B	1771	14/15	0.91	0.17	-	105,119,128,130	0
4	NAG	A	1766	14/15	0.94	0.18	-	63,76,95,112	0
8	BMA	B	1767	11/12	0.89	0.19	-	116,126,135,160	0
4	BMA	A	1767	11/12	0.76	0.30	-	110,116,124,128	0
8	BMA	B	1768	11/12	0.72	0.26	-	116,140,161,163	0
8	NAG	B	1766	14/15	0.91	0.18	-	67,101,115,119	0

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(\AA^2)	Q<0.9
7	JW7	A	2000	25/25	0.91	0.29	4.57	65,90,143,148	0
7	JW7	B	2000	25/25	0.96	0.19	1.00	46,54,97,99	0
3	CA	A	1763	1/1	0.96	0.06	-1.26	51,51,51,51	0
3	CA	B	1763	1/1	0.98	0.06	-1.41	51,51,51,51	0
3	CA	B	1764	1/1	0.98	0.03	-3.40	60,60,60,60	0
3	CA	A	1764	1/1	0.93	0.04	-4.32	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CU	A	1762	1/1	1.00	0.20	-	54,54,54,54	0
6	NAG	B	1775	14/15	0.84	0.28	-	72,97,107,109	0
6	NAG	A	1770	14/15	0.84	0.31	-	74,93,115,115	0
6	NAG	B	1773	14/15	0.79	0.23	-	87,129,136,136	0
2	CU	B	1762	1/1	1.00	0.18	-	54,54,54,54	0
6	NAG	A	1771	14/15	0.82	0.24	-	77,97,104,105	0
6	NAG	B	1772	14/15	0.73	0.31	-	103,132,140,141	0
6	NAG	B	1774	14/15	0.55	0.40	-	94,121,135,136	0

6.5 Other polymers [i](#)

There are no such residues in this entry.