Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:45 AM GMT

PDB ID	:	2Y73
Title	:	THE NATIVE STRUCTURES OF SOLUBLE HUMAN PRIMARY AMINE OXIDASE AOC3
Authors	:	Elovaara, H.; Kidron, H.; Parkash, V.; Nymalm, Y.; Bligt, E.; Ollikka, P.; Smith, D.J.; Pihlavisto, M.; Salmi, M.; Jalkanen, S.; Salminen, T.A.
Deposited on	:	2011-01-28
Resolution	:	2.60 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

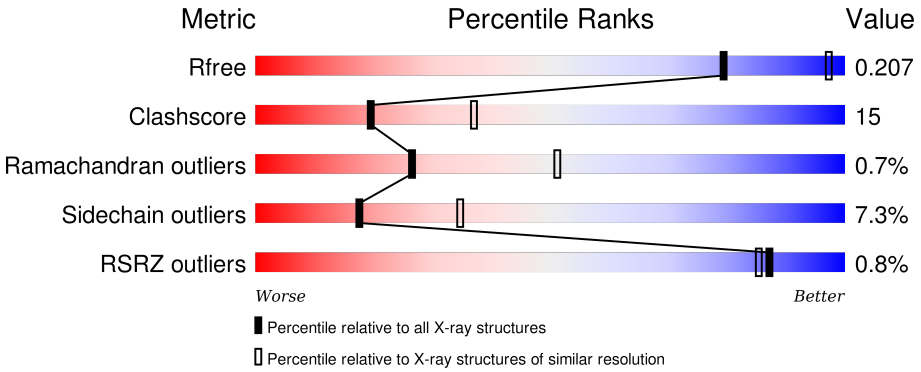
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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 <=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	763	% 66% 23% • 8%
1	B	763	% 66% 22% • • 8%

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
4	IMD	A	1765	-	-	X	-
4	IMD	A	1776	-	-	-	X
4	IMD	B	1766	-	-	-	X
6	NAG	A	1771	-	-	-	X
6	NAG	A	1772	-	-	-	X
6	NAG	B	1771	-	-	-	X
6	NAG	B	1772	-	-	-	X
8	FMT	A	1777	-	-	X	-
8	FMT	A	1778	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11675 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	705	Total	C	N	O	S	0	0	0
			5560	3570	957	1013	20			
1	B	701	Total	C	N	O	S	0	0	0
			5527	3551	950	1007	19			

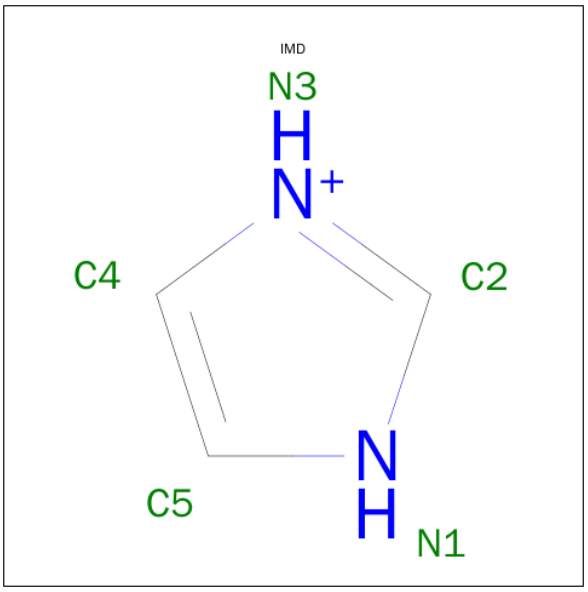
- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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 IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N 5 3 2	0	0
4	A	1	Total C N 5 3 2	0	0
4	A	1	Total C N 5 3 2	0	0
4	A	1	Total C N 5 3 2	0	0
4	B	1	Total C N 5 3 2	0	0
4	B	1	Total C N 5 3 2	0	0
4	B	1	Total C N 5 3 2	0	0
4	B	1	Total C N 5 3 2	0	0

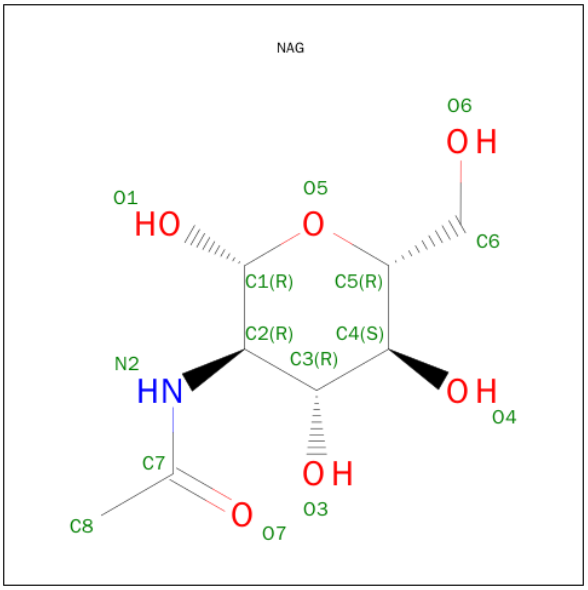
- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

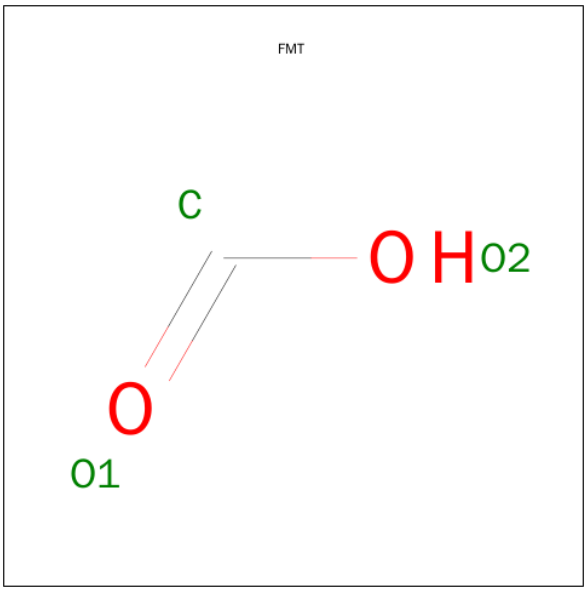
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total C N O 28 16 2 10	0	0
6	B	2	Total C N O 28 16 2 10	0	0

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 8 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 3 1 2	0	0
8	A	1	Total C O 3 1 2	0	0

- Molecule 9 is water.

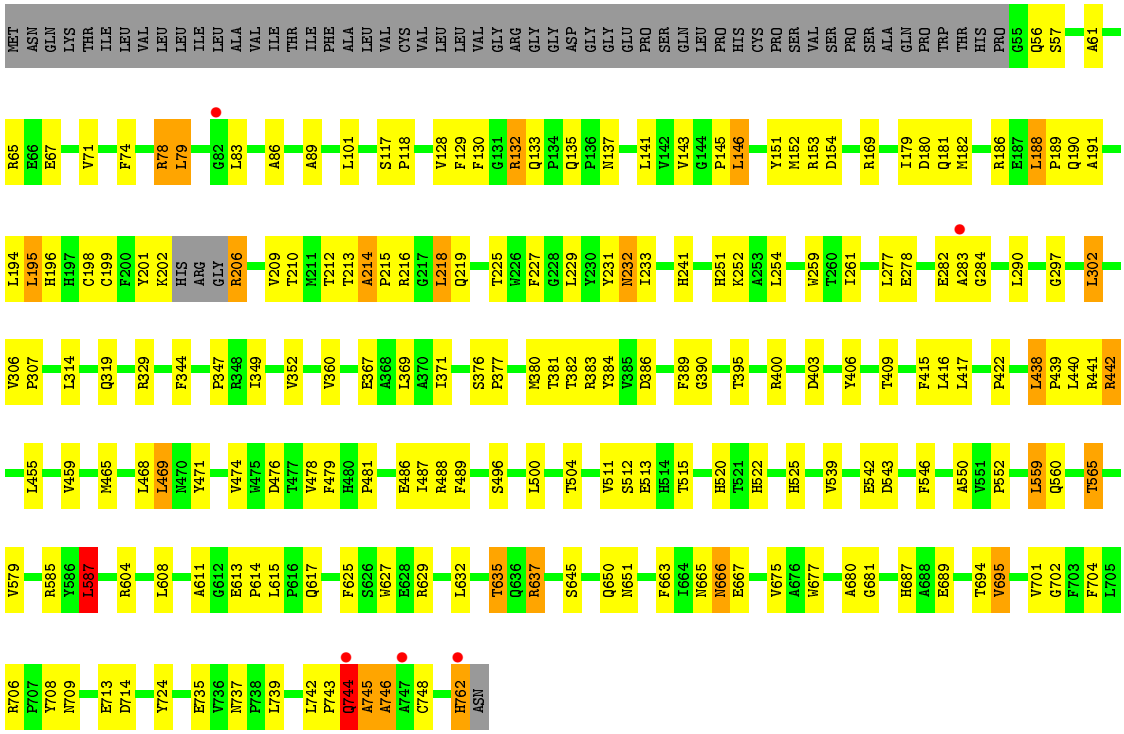
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	191	Total O 191 191	0	0
9	B	155	Total O 155 155	0	0

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 errors 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.

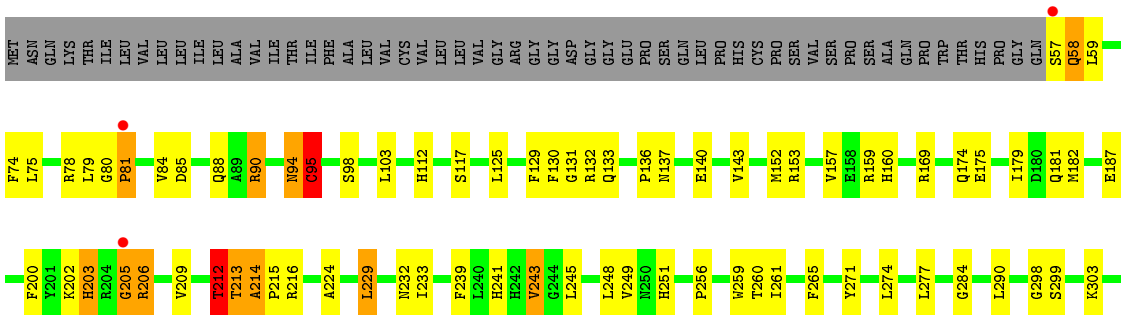
• Molecule 1: MEMBRANE PRIMARY AMINE OXIDASE

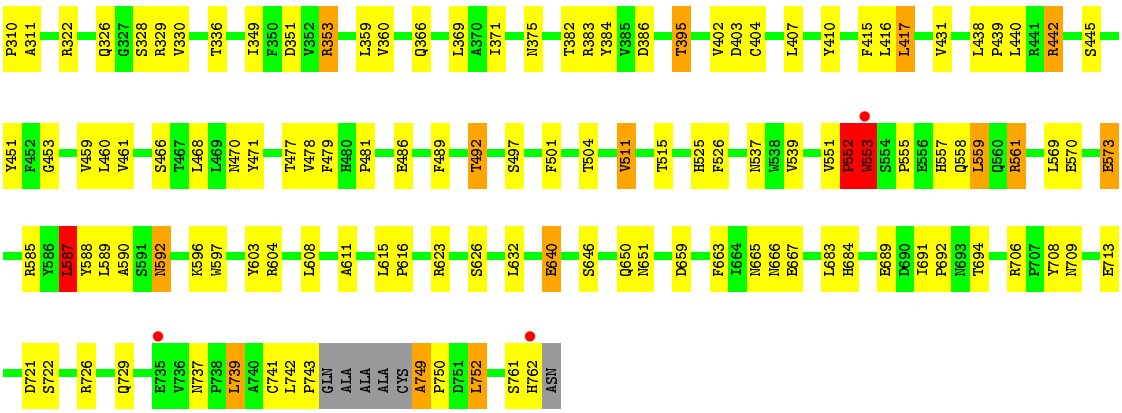
Chain A:



• Molecule 1: MEMBRANE PRIMARY AMINE OXIDASE

Chain B:




P310 A311 R322 Q326 G327 S328 R329 V330 T336 I349 F350 D351 V352 R353 L359 V360 Q366 L369 A370 I371 N375 T382 R383 Y384 V385 D386 T395 V402 D403 C404 L407 Y410 F415 L416 L417 V431 L438 P439 L440 R441 R442 S445
Y451 F452 G453 V459 L460 V461 S466 T467 L468 L469 N470 Y471 T477 V478 F479 H480 P481 E486 F489 T492 S497 F501 T504 V511 T515 H525 F526 N537 W538 V539 V551 P552 W553 S554 P555 E556 H557 Q558 L559 Q560 R561 L569 E570 E573
R585 Y586 L587 Y588 L589 A590 S591 N592 K596 W597 Y603 R604 L608 A611 L615 P616 R623 S626 L632 E640 S646 Q650 M651 D659 F663 I664 N665 N666 E667 L683 H684 E689 D690 I691 P692 N693 T694 R706 P707 Y708 N709 E713
D721 S722 R726 Q729 E735 V736 N737 P738 L739 A740 C741 L742 P743 GLN ALA ALA ALA CYS A749 P750 D751 L752 S761 H762 ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	225.75Å 225.75Å 216.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.93 – 2.60 19.93 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.93-2.60) 100.0 (19.93-2.60)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.56 (at 2.59Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.175 , 0.213 0.165 , 0.207	Depositor DCC
R_{free} test set	4977 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	36.1	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 36.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 99554 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11675	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, IMD, CA, TPQ, FMT, 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	0.76	4/5721 (0.1%)	0.87	9/7800 (0.1%)
1	B	0.80	7/5688 (0.1%)	0.82	5/7757 (0.1%)
All	All	0.78	11/11409 (0.1%)	0.85	14/15557 (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	1
1	B	0	7
All	All	0	8

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	552	PRO	C-N	-19.80	0.88	1.34
1	B	553	TRP	C-N	-11.17	1.08	1.34
1	B	741	CYS	CA-CB	-10.79	1.30	1.53
1	B	95	CYS	CB-SG	-7.89	1.68	1.82
1	A	137	ASN	CG-ND2	7.80	1.52	1.32
1	B	137	ASN	CG-ND2	7.35	1.51	1.32
1	B	232	ASN	CG-ND2	7.09	1.50	1.32
1	A	232	ASN	CG-ND2	6.91	1.50	1.32
1	A	666	ASN	CG-ND2	6.24	1.48	1.32
1	B	592	ASN	CG-ND2	5.96	1.47	1.32
1	A	748	CYS	CB-SG	5.48	1.91	1.82

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	57	SER	N-CA-CB	-14.32	89.03	110.50
1	A	329	ARG	NE-CZ-NH2	-9.39	115.61	120.30
1	B	229	LEU	CA-CB-CG	-9.35	93.80	115.30
1	A	56	GLN	N-CA-C	7.77	131.98	111.00
1	A	587	LEU	CA-CB-CG	-7.31	98.49	115.30
1	B	468	LEU	CA-CB-CG	-6.50	100.35	115.30
1	A	329	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	706	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	B	552	PRO	O-C-N	-6.21	112.77	122.70
1	B	212	THR	CB-CA-C	-5.94	95.56	111.60
1	A	56	GLN	CB-CA-C	-5.73	98.94	110.40
1	A	438	LEU	CA-CB-CG	5.56	128.08	115.30
1	B	587	LEU	CA-CB-CG	-5.51	102.62	115.30
1	A	637	ARG	NE-CZ-NH1	5.38	122.99	120.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	213	THR	Peptide
1	B	203	HIS	Peptide
1	B	205	GLY	Peptide
1	B	213	THR	Peptide
1	B	552	PRO	Mainchain
1	B	553	TRP	Mainchain
1	B	749	ALA	Peptide
1	B	94	ASN	Peptide

5.2 Too-close contacts (i)

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	5560	0	5307	179	0
1	B	5527	0	5264	174	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	20	0	20	6	0
4	B	20	0	20	5	0
5	A	39	0	33	2	0
5	B	39	0	34	2	0
6	A	28	0	25	1	0
6	B	28	0	25	0	0
7	A	28	0	26	3	0
7	B	28	0	26	2	0
8	A	6	0	2	4	0
9	A	191	0	0	5	0
9	B	155	0	0	2	0
All	All	11675	0	10782	331	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (331) 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:206:ARG:N	1:A:206:ARG:HD2	1.52	1.13
1:B:58:GLN:HG3	1:B:59:LEU:H	1.15	1.11
1:A:201:TYR:O	1:A:202:LYS:HG2	1.50	1.09
1:B:214:ALA:CB	1:B:215:PRO:HD2	1.90	1.01
1:B:212:THR:HG21	1:B:216:ARG:NH2	1.76	1.01
1:A:314:LEU:HD12	8:A:1778:FMT:H	1.44	1.00
1:B:214:ALA:HB1	1:B:383:ARG:H	1.26	0.99
1:A:214:ALA:HB1	1:A:215:PRO:HD3	1.45	0.95
1:A:78:ARG:HG3	1:A:78:ARG:HH11	1.29	0.93
1:B:57:SER:O	1:B:58:GLN:HB3	1.67	0.93
1:A:206:ARG:N	1:A:206:ARG:CD	2.30	0.93
1:B:214:ALA:CB	1:B:215:PRO:CD	2.48	0.90
1:B:214:ALA:HB1	1:B:215:PRO:CD	2.02	0.90
1:B:214:ALA:HB2	1:B:382:THR:HA	1.50	0.90
1:B:214:ALA:HB3	1:B:215:PRO:HD2	1.55	0.87
1:B:214:ALA:CB	1:B:383:ARG:H	1.86	0.87
1:B:561:ARG:HH11	1:B:561:ARG:HG3	1.37	0.87
1:B:726:ARG:HB2	1:B:729:GLN:HE21	1.40	0.87
1:B:615:LEU:HD12	1:B:616:PRO:HD2	1.56	0.87
1:A:441:ARG:HA	1:B:492:THR:HG21	1.56	0.86
1:A:209:VAL:HG13	1:A:232:ASN:HB2	1.55	0.86
1:B:95:CYS:HB3	1:B:129:PHE:HB2	1.58	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ALA:CB	1:A:215:PRO:CD	2.54	0.85
1:A:743:PRO:O	1:A:744:GLN:HB3	1.73	0.85
1:B:214:ALA:HB1	1:B:215:PRO:HD2	1.59	0.84
1:B:58:GLN:HG3	1:B:59:LEU:N	1.94	0.83
1:A:201:TYR:O	1:A:202:LYS:CG	2.27	0.83
1:A:762:HIS:CD2	1:A:762:HIS:N	2.46	0.83
1:A:666:ASN:HD22	7:A:1774:NAG:H83	1.43	0.83
1:B:57:SER:HB3	1:B:328:SER:H	1.44	0.82
1:B:212:THR:HG21	1:B:216:ARG:HH22	1.43	0.82
1:A:680:ALA:HB1	1:A:701:VAL:HG13	1.63	0.81
1:B:57:SER:HA	1:B:329:ARG:HG3	1.62	0.80
1:B:214:ALA:CB	1:B:382:THR:HA	2.11	0.80
1:B:212:THR:CG2	1:B:216:ARG:NH2	2.44	0.80
1:B:561:ARG:HH11	1:B:561:ARG:CG	1.95	0.79
1:B:57:SER:O	1:B:58:GLN:CB	2.30	0.79
1:A:214:ALA:CB	1:A:383:ARG:H	1.95	0.79
1:B:94:ASN:ND2	1:B:130:PHE:HA	1.98	0.79
1:A:214:ALA:CB	1:A:215:PRO:HD3	2.14	0.78
1:B:587:LEU:HD22	1:B:632:LEU:CD2	2.14	0.78
1:B:561:ARG:NH1	1:B:561:ARG:HG3	1.99	0.76
1:B:587:LEU:HD22	1:B:632:LEU:HD21	1.67	0.76
1:A:214:ALA:HB1	1:A:215:PRO:CD	2.13	0.75
1:A:214:ALA:CB	1:A:382:THR:HA	2.18	0.74
1:A:214:ALA:HB1	1:A:383:ARG:H	1.53	0.73
1:A:500:LEU:HD12	1:A:504:THR:HG21	1.68	0.73
1:A:319:GLN:NE2	1:B:311:ALA:H	1.88	0.72
1:B:552:PRO:HB2	1:B:553:TRP:HE3	1.55	0.72
1:A:319:GLN:HE21	1:B:311:ALA:H	1.37	0.71
1:A:762:HIS:CD2	1:A:762:HIS:H	2.09	0.71
1:A:415:PHE:CD2	1:A:417:LEU:HD12	2.28	0.69
1:B:216:ARG:HD2	1:B:651:ASN:OD1	1.93	0.69
1:B:739:LEU:O	1:B:742:LEU:HD12	1.93	0.69
1:B:573:GLU:OE2	1:B:666:ASN:N	2.27	0.68
1:B:88:GLN:HA	1:B:174:GLN:HE21	1.58	0.67
1:A:214:ALA:HB2	1:A:382:THR:HA	1.74	0.67
1:B:592:ASN:HD22	7:B:1773:NAG:H83	1.59	0.67
1:A:442:ARG:HD3	1:B:403:ASP:OD1	1.95	0.67
1:B:214:ALA:HB2	1:B:382:THR:HG23	1.76	0.66
1:A:180:ASP:OD1	1:A:210:THR:HG21	1.95	0.66
1:B:214:ALA:HB2	1:B:382:THR:CA	2.22	0.66
1:A:383:ARG:HH21	8:A:1777:FMT:H	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ALA:HB2	1:A:382:THR:HG23	1.77	0.66
1:B:726:ARG:H	1:B:729:GLN:HE21	1.42	0.66
1:A:278:GLU:HA	1:A:278:GLU:OE1	1.96	0.66
1:A:512:SER:HB3	1:A:515:THR:HB	1.76	0.66
1:B:749:ALA:N	1:B:750:PRO:O	2.29	0.66
1:B:140:GLU:OE2	1:B:160:HIS:NE2	2.28	0.66
1:B:131:GLY:HA2	1:B:136:PRO:HB3	1.78	0.65
1:A:744:GLN:O	1:A:744:GLN:HG3	1.96	0.65
1:B:551:VAL:CG1	1:B:553:TRP:CE2	2.80	0.65
1:A:438:LEU:HD22	1:A:439:PRO:HD2	1.77	0.65
1:B:706:ARG:HD2	9:B:2146:HOH:O	1.96	0.65
1:B:588:TYR:HB3	1:B:604:ARG:HA	1.79	0.64
1:A:440:LEU:HD23	1:A:455:LEU:HD23	1.79	0.64
1:A:282:GLU:C	1:A:284:GLY:H	2.01	0.64
1:A:201:TYR:C	1:A:202:LYS:CG	2.66	0.64
1:A:78:ARG:CG	1:A:78:ARG:HH11	2.06	0.64
1:B:407:LEU:HD21	1:B:752:LEU:HD12	1.80	0.64
1:A:695:VAL:HG22	1:B:440:LEU:HG	1.80	0.64
1:B:726:ARG:H	1:B:729:GLN:NE2	1.96	0.63
1:A:762:HIS:HD2	1:A:762:HIS:H	1.45	0.63
1:A:666:ASN:HD22	7:A:1774:NAG:C8	2.10	0.63
1:B:737:ASN:OD1	1:B:739:LEU:HB2	1.97	0.63
1:A:214:ALA:HB3	1:A:215:PRO:CD	2.27	0.63
1:A:744:GLN:HE21	1:A:744:GLN:CA	2.11	0.63
1:A:347:PRO:HB3	4:A:1766:IMD:C4	2.28	0.63
1:A:744:GLN:C	1:A:744:GLN:HE21	2.02	0.63
1:A:214:ALA:CB	1:A:383:ARG:N	2.64	0.61
1:A:560:GLN:HG3	1:B:616:PRO:HG2	1.82	0.61
1:A:441:ARG:HA	1:B:492:THR:CG2	2.28	0.61
1:B:587:LEU:CD2	1:B:632:LEU:HD21	2.30	0.61
1:B:551:VAL:HG13	1:B:553:TRP:CZ2	2.36	0.60
1:B:551:VAL:CG1	1:B:553:TRP:CZ2	2.84	0.60
1:A:565:THR:HG22	1:A:565:THR:O	2.00	0.60
1:B:214:ALA:CB	1:B:383:ARG:N	2.63	0.60
1:A:302:LEU:HD13	1:B:453:GLY:HA3	1.82	0.60
1:B:552:PRO:HB2	1:B:553:TRP:CE3	2.36	0.60
1:A:476:ASP:HB2	1:A:488:ARG:HB2	1.84	0.60
1:A:216:ARG:HD2	1:A:651:ASN:OD1	2.02	0.59
1:B:125:LEU:CD1	1:B:159:ARG:HH12	2.15	0.59
1:B:129:PHE:CZ	1:B:169:ARG:HB2	2.37	0.59
1:B:169:ARG:HG2	1:B:169:ARG:HH11	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:LEU:HD22	1:B:481:PRO:HG2	1.84	0.59
1:B:95:CYS:CB	1:B:129:PHE:HB2	2.32	0.59
1:B:133:GLN:NE2	5:B:1768:NAG:O6	2.35	0.58
1:A:306:VAL:HG13	1:A:307:PRO:HD2	1.85	0.58
1:A:194:LEU:CD2	1:A:277:LEU:HD21	2.33	0.58
1:A:403:ASP:OD1	1:B:442:ARG:HD3	2.03	0.58
1:A:201:TYR:C	1:A:202:LYS:HG2	2.23	0.58
1:B:214:ALA:HB1	1:B:383:ARG:N	2.09	0.58
1:A:78:ARG:NH1	1:A:78:ARG:HG3	2.07	0.58
1:A:744:GLN:O	1:A:745:ALA:CB	2.52	0.57
1:B:359:LEU:HD13	1:B:603:TYR:CZ	2.39	0.57
1:A:78:ARG:CG	1:A:78:ARG:NH1	2.66	0.57
1:A:442:ARG:H	1:B:492:THR:HG21	1.68	0.57
1:A:608:LEU:HD11	1:A:704:PHE:CE1	2.39	0.57
1:B:553:TRP:C	1:B:555:PRO:HD3	2.25	0.57
1:B:79:LEU:O	1:B:81:PRO:HD3	2.05	0.57
1:B:79:LEU:HD21	1:B:152:MET:HE1	1.87	0.57
1:A:471:TPQ:O2	4:A:1765:IMD:N3	2.36	0.57
1:A:252:LYS:HG3	1:A:252:LYS:O	2.05	0.57
1:B:478:VAL:HB	1:B:486:GLU:HB3	1.86	0.56
1:B:80:GLY:O	1:B:81:PRO:C	2.43	0.56
1:B:125:LEU:HD11	1:B:159:ARG:NH1	2.20	0.56
5:B:1768:NAG:H61	5:B:1769:NAG:C1	2.36	0.56
1:B:739:LEU:HD12	1:B:742:LEU:HD11	1.87	0.56
1:A:665:ASN:OD1	1:A:667:GLU:HG3	2.07	0.55
1:A:478:VAL:HB	1:A:486:GLU:HB3	1.89	0.54
1:A:559:LEU:O	1:A:559:LEU:HD12	2.07	0.54
1:A:145:PRO:HD3	1:A:151:TYR:CE2	2.41	0.54
1:B:749:ALA:N	1:B:750:PRO:C	2.60	0.54
1:A:383:ARG:HH21	8:A:1777:FMT:C	2.20	0.54
1:A:743:PRO:O	1:A:744:GLN:CB	2.52	0.54
1:A:233:ILE:HG13	1:A:241:HIS:CD2	2.42	0.54
1:A:214:ALA:HB3	1:A:382:THR:HA	1.88	0.54
1:B:349:ILE:HD11	4:B:1765:IMD:H5	1.89	0.54
1:B:623:ARG:HD3	1:B:659:ASP:OD2	2.07	0.53
1:B:205:GLY:N	1:B:206:ARG:HA	2.22	0.53
1:B:726:ARG:HB2	1:B:729:GLN:NE2	2.17	0.53
1:A:352:VAL:HB	1:A:360:VAL:CG2	2.39	0.53
1:B:551:VAL:HG12	1:B:553:TRP:CE2	2.42	0.53
1:B:552:PRO:HD2	1:B:553:TRP:CZ3	2.44	0.53
1:A:395:THR:HG23	9:A:2097:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:GLN:CG	1:B:59:LEU:H	1.99	0.52
1:B:251:HIS:HA	1:B:259:TRP:CD1	2.44	0.52
1:A:587:LEU:HD22	1:A:632:LEU:HD21	1.92	0.52
1:B:592:ASN:ND2	7:B:1773:NAG:H83	2.24	0.52
1:B:395:THR:HA	1:B:466:SER:HA	1.91	0.52
1:B:200:PHE:CZ	1:B:290:LEU:HD21	2.45	0.52
1:A:500:LEU:CD1	1:A:504:THR:HG21	2.40	0.52
1:A:441:ARG:CA	1:B:492:THR:HG21	2.34	0.52
1:B:125:LEU:HD11	1:B:159:ARG:HH12	1.73	0.51
1:A:377:PRO:HA	1:A:380:MET:HE3	1.92	0.51
1:B:726:ARG:N	1:B:729:GLN:HE21	2.07	0.51
1:A:133:GLN:HE22	5:A:1768:NAG:H61	1.75	0.51
1:B:94:ASN:HA	1:B:129:PHE:O	2.11	0.51
1:B:369:LEU:HD12	1:B:384:TYR:O	2.10	0.51
1:A:744:GLN:O	1:A:744:GLN:CG	2.58	0.51
1:A:637:ARG:HD2	9:A:2080:HOH:O	2.10	0.51
1:A:739:LEU:HD11	1:B:402:VAL:HG23	1.93	0.51
1:B:182:MET:CE	1:B:261:ILE:HG12	2.40	0.51
1:A:61:ALA:O	1:A:101:LEU:HD22	2.11	0.51
1:B:438:LEU:HD12	1:B:439:PRO:HD2	1.93	0.51
1:A:465:MET:SD	1:B:442:ARG:HD3	2.52	0.50
1:A:195:LEU:HB3	1:A:201:TYR:HB2	1.93	0.50
1:A:635:THR:HG22	1:A:675:VAL:CG1	2.40	0.50
1:A:635:THR:CG2	1:A:677:TRP:HE1	2.24	0.50
1:B:415:PHE:CD2	1:B:417:LEU:HD12	2.46	0.50
1:A:71:VAL:HG13	1:A:143:VAL:HG11	1.94	0.50
1:A:469:LEU:CD2	4:A:1765:IMD:H5	2.42	0.50
1:A:611:ALA:O	1:B:585:ARG:NH1	2.44	0.50
1:B:202:LYS:O	1:B:203:HIS:C	2.51	0.49
1:A:615:LEU:HD11	8:A:1777:FMT:H	1.94	0.49
1:B:386:ASP:OD2	4:B:1767:IMD:H2	2.12	0.49
1:A:587:LEU:HD22	1:A:632:LEU:CD2	2.43	0.49
1:A:251:HIS:HA	1:A:259:TRP:CD1	2.47	0.49
1:B:526:PHE:HE1	4:B:1776:IMD:H5	1.77	0.49
1:A:744:GLN:O	1:A:745:ALA:HB3	2.13	0.49
1:B:233:ILE:HG13	1:B:241:HIS:HD2	1.76	0.49
1:A:469:LEU:HD23	4:A:1765:IMD:H5	1.95	0.49
1:A:349:ILE:HD12	1:A:352:VAL:CG2	2.42	0.49
1:B:551:VAL:HG12	1:B:553:TRP:CD2	2.48	0.49
1:B:349:ILE:HG13	1:B:477:THR:HG21	1.95	0.49
1:A:212:THR:OG1	1:A:216:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ALA:HB2	1:A:382:THR:CA	2.43	0.48
1:A:133:GLN:HE22	5:A:1768:NAG:C6	2.26	0.48
1:A:182:MET:HB2	1:A:186:ARG:NH2	2.29	0.48
1:A:585:ARG:NH1	1:B:611:ALA:O	2.47	0.48
1:A:542:GLU:HA	1:A:565:THR:O	2.13	0.48
1:A:742:LEU:HD23	1:A:742:LEU:HA	1.68	0.48
1:A:442:ARG:CD	1:B:403:ASP:OD1	2.61	0.48
1:A:382:THR:C	1:A:383:ARG:HD2	2.35	0.48
1:A:442:ARG:HG3	1:A:442:ARG:O	2.11	0.48
1:B:175:GLU:O	1:B:179:ILE:HG13	2.14	0.47
1:B:187:GLU:HB3	1:B:274:LEU:CD1	2.43	0.47
1:A:744:GLN:HA	1:A:744:GLN:HE21	1.78	0.47
1:B:371:ILE:HD13	1:B:615:LEU:HB2	1.96	0.47
1:A:560:GLN:CG	1:B:616:PRO:HG2	2.44	0.47
1:B:471:TPQ:O2	4:B:1767:IMD:N1	2.39	0.47
1:B:588:TYR:CB	1:B:604:ARG:HA	2.45	0.47
1:A:714:ASP:HB2	1:B:689:GLU:O	2.15	0.47
1:A:129:PHE:CZ	1:A:169:ARG:HB2	2.50	0.47
1:A:319:GLN:NE2	1:B:310:PRO:HA	2.29	0.47
1:A:416:LEU:HD12	1:A:422:PRO:N	2.31	0.46
1:B:471:TPQ:H6	1:B:492:THR:O	2.16	0.46
1:B:665:ASN:OD1	1:B:667:GLU:HG3	2.15	0.46
1:B:239:PHE:CD1	1:B:470:ASN:HB3	2.50	0.46
1:A:666:ASN:ND2	7:A:1774:NAG:H83	2.22	0.46
1:A:403:ASP:OD1	1:B:442:ARG:CD	2.63	0.46
1:A:386:ASP:OD2	4:A:1765:IMD:H2	2.16	0.46
1:A:381:THR:HG22	1:B:559:LEU:HD12	1.96	0.46
1:A:694:THR:HG21	9:A:2109:HOH:O	2.14	0.46
1:B:214:ALA:HB2	1:B:382:THR:CG2	2.43	0.46
1:B:386:ASP:OD1	4:B:1767:IMD:H2	2.16	0.46
1:A:86:ALA:HA	1:A:89:ALA:HB2	1.98	0.46
1:B:492:THR:HG23	1:B:694:THR:O	2.16	0.45
1:B:460:LEU:HB3	1:B:479:PHE:HB2	1.97	0.45
1:A:737:ASN:OD1	1:A:739:LEU:HB2	2.17	0.45
1:A:132:ARG:HH11	1:A:132:ARG:HG2	1.81	0.45
1:B:551:VAL:HG13	1:B:553:TRP:CH2	2.51	0.45
1:A:344:PHE:HA	1:A:390:GLY:HA2	1.99	0.45
1:A:608:LEU:HD11	1:A:704:PHE:HE1	1.78	0.45
1:A:680:ALA:CB	1:A:701:VAL:HG13	2.40	0.45
1:B:284:GLY:HA2	9:B:2033:HOH:O	2.17	0.45
1:A:465:MET:HG2	1:A:474:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:LEU:HD13	1:B:557:HIS:ND1	2.32	0.45
1:B:573:GLU:H	1:B:573:GLU:HG2	1.58	0.45
1:A:349:ILE:HD13	1:A:479:PHE:HZ	1.81	0.45
1:A:635:THR:HG21	1:A:677:TRP:HE1	1.82	0.45
1:A:282:GLU:C	1:A:284:GLY:N	2.65	0.44
1:B:243:VAL:O	1:B:243:VAL:HG13	2.16	0.44
1:A:225:THR:HB	1:A:227:PHE:CE1	2.53	0.44
1:B:431:VAL:HA	1:B:461:VAL:O	2.17	0.44
1:B:322:ARG:NH1	1:B:721:ASP:OD2	2.46	0.44
1:A:117:SER:HB3	1:A:118:PRO:CD	2.48	0.44
1:B:663:PHE:N	1:B:663:PHE:CD1	2.85	0.44
1:B:683:LEU:HD12	1:B:684:HIS:H	1.82	0.44
1:B:537:ASN:HA	1:B:590:ALA:O	2.17	0.44
1:A:188:LEU:HA	1:A:188:LEU:HD12	1.72	0.44
1:A:546:PHE:CD2	1:B:616:PRO:HD3	2.53	0.44
1:B:169:ARG:HG2	1:B:169:ARG:NH1	2.31	0.44
1:A:744:GLN:C	1:A:744:GLN:NE2	2.70	0.44
1:A:67:GLU:O	1:A:71:VAL:HG23	2.16	0.44
1:B:511:VAL:CG1	1:B:691:ILE:HD11	2.47	0.44
1:A:141:LEU:HD23	1:A:154:ASP:HA	2.00	0.44
1:B:375:ASN:ND2	1:B:504:THR:HG22	2.33	0.44
1:A:708:TYR:O	1:A:709:ASN:HB2	2.18	0.44
1:B:588:TYR:HB2	1:B:603:TYR:O	2.18	0.44
1:A:635:THR:HG22	1:A:675:VAL:HG13	1.99	0.44
1:B:245:LEU:HD12	1:B:265:PHE:O	2.18	0.44
1:B:130:PHE:O	1:B:136:PRO:HA	2.18	0.44
1:B:125:LEU:CD1	1:B:159:ARG:NH1	2.80	0.44
1:B:57:SER:HB3	1:B:328:SER:N	2.23	0.43
1:A:65:ARG:HG3	9:A:2006:HOH:O	2.18	0.43
1:A:386:ASP:OD1	4:A:1765:IMD:H2	2.18	0.43
1:A:233:ILE:HG13	1:A:241:HIS:HD2	1.83	0.43
1:A:74:PHE:HE1	1:A:152:MET:HB3	1.83	0.43
1:A:488:ARG:HD3	1:A:488:ARG:HA	1.57	0.43
1:B:351:ASP:OD2	1:B:353:ARG:NH1	2.52	0.43
1:B:382:THR:C	1:B:383:ARG:HD2	2.39	0.43
1:A:179:ILE:HD11	1:A:251:HIS:CG	2.53	0.43
1:A:400:ARG:HG2	1:A:406:TYR:CD1	2.53	0.43
1:A:579:VAL:HG11	1:A:614:PRO:HD3	2.01	0.43
1:B:366:GLN:HB2	1:B:525:HIS:HB3	1.99	0.43
1:A:145:PRO:HD3	1:A:151:TYR:HE2	1.83	0.43
1:B:375:ASN:ND2	1:B:501:PHE:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:GLU:O	1:A:284:GLY:N	2.51	0.43
1:A:386:ASP:HB3	1:A:468:LEU:HD22	2.01	0.43
1:B:179:ILE:HG23	1:B:249:VAL:HG11	2.00	0.43
1:B:112:HIS:HA	1:B:117:SER:O	2.19	0.43
1:A:471:TPQ:HA	1:A:471:TPQ:H6	1.85	0.43
1:B:256:PRO:HA	1:B:259:TRP:CE2	2.54	0.43
1:A:371:ILE:O	1:A:520:HIS:HA	2.19	0.42
1:A:383:ARG:HD2	1:A:383:ARG:N	2.33	0.42
1:B:351:ASP:CG	1:B:353:ARG:HH11	2.23	0.42
1:A:254:LEU:HD23	1:A:254:LEU:HA	1.53	0.42
1:B:497:SER:HB2	1:B:515:THR:HG23	2.01	0.42
1:A:525:HIS:HB2	1:A:627:TRP:CE3	2.54	0.42
1:A:188:LEU:N	1:A:189:PRO:CD	2.83	0.42
1:B:75:LEU:HD21	1:B:143:VAL:HG21	2.01	0.42
1:A:487:ILE:O	1:A:702:GLY:HA3	2.19	0.42
1:B:596:LYS:HD3	1:B:597:TRP:CH2	2.55	0.42
1:B:404:CYS:HB2	1:B:410:TYR:OH	2.19	0.42
1:A:389:PHE:HE1	1:A:650:GLN:OE1	2.02	0.42
1:A:232:ASN:ND2	6:A:1771:NAG:O7	2.52	0.42
1:B:132:ARG:O	1:B:133:GLN:HB3	2.20	0.42
1:B:98:SER:HB2	1:B:417:LEU:HD23	2.01	0.42
1:A:663:PHE:N	1:A:663:PHE:CD1	2.86	0.42
1:A:369:LEU:HD12	1:A:384:TYR:O	2.20	0.41
1:B:90:ARG:HD2	1:B:90:ARG:HA	1.81	0.41
1:B:640:GLU:H	1:B:640:GLU:HG3	1.47	0.41
1:B:271:TYR:CE1	1:B:277:LEU:HD13	2.55	0.41
1:A:231:TYR:O	1:A:233:ILE:HG12	2.20	0.41
1:A:352:VAL:HB	1:A:360:VAL:HG23	2.02	0.41
1:A:189:PRO:C	1:A:191:ALA:H	2.23	0.41
1:B:84:VAL:HG12	1:B:85:ASP:N	2.35	0.41
1:B:330:VAL:O	1:B:336:THR:HA	2.20	0.41
1:A:214:ALA:HB2	1:A:382:THR:CG2	2.47	0.41
1:B:74:PHE:HE1	1:B:152:MET:HB2	1.86	0.41
1:A:559:LEU:C	1:A:559:LEU:HD12	2.40	0.41
1:A:744:GLN:NE2	1:A:744:GLN:CA	2.82	0.41
1:A:352:VAL:HB	1:A:360:VAL:HG22	2.03	0.41
1:A:687:HIS:HD2	1:A:689:GLU:OE1	2.03	0.41
1:A:128:VAL:HG11	1:A:130:PHE:CZ	2.55	0.41
1:A:195:LEU:HB3	1:A:201:TYR:CB	2.50	0.41
1:B:762:HIS:N	1:B:762:HIS:CD2	2.89	0.41
1:A:67:GLU:HB3	1:A:146:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:HIS:O	1:A:681:GLY:HA3	2.21	0.41
1:B:742:LEU:HA	1:B:743:PRO:HA	1.55	0.41
1:A:742:LEU:O	1:A:746:ALA:HB3	2.21	0.41
1:A:79:LEU:HA	1:A:79:LEU:HD12	1.52	0.41
1:B:416:LEU:C	1:B:417:LEU:HG	2.41	0.41
1:A:481:PRO:HG3	9:A:2106:HOH:O	2.20	0.41
1:B:94:ASN:HD22	1:B:130:PHE:HA	1.82	0.40
1:A:194:LEU:HD23	1:A:277:LEU:HD21	2.01	0.40
1:A:543:ASP:O	1:A:565:THR:HB	2.22	0.40
1:A:132:ARG:CG	1:A:132:ARG:HH11	2.35	0.40
1:A:550:ALA:O	1:A:552:PRO:HD3	2.21	0.40
1:B:212:THR:HG22	1:B:213:THR:N	2.35	0.40
1:B:182:MET:HE1	1:B:261:ILE:HG12	2.04	0.40
1:A:724:TYR:C	1:A:724:TYR:CD1	2.94	0.40
1:B:224:ALA:HB1	1:B:248:LEU:HD11	2.03	0.40
1:B:589:LEU:HD23	1:B:589:LEU:N	2.36	0.40
1:B:298:GLY:O	1:B:692:PRO:HB3	2.21	0.40
1:A:367:GLU:OE1	1:A:645:SER:OG	2.33	0.40
1:B:445:SER:CB	1:B:451:TYR:CE1	3.04	0.40
1:A:201:TYR:CG	1:A:202:LYS:N	2.90	0.40
1:B:708:TYR:O	1:B:709:ASN:HB2	2.20	0.40
1:B:539:VAL:HG22	1:B:569:LEU:HB2	2.02	0.40

There are no symmetry-related clashes.

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	700/763 (92%)	656 (94%)	37 (5%)	7 (1%)	19	39
1	B	696/763 (91%)	653 (94%)	40 (6%)	3 (0%)	39	65
All	All	1396/1526 (92%)	1309 (94%)	77 (6%)	10 (1%)	26	51

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	ALA
1	A	744	GLN
1	A	745	ALA
1	A	746	ALA
1	B	58	GLN
1	B	214	ALA
1	A	190	GLN
1	A	283	ALA
1	A	297	GLY
1	B	81	PRO

5.3.2 Protein sidechains (i)

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	585/634 (92%)	541 (92%)	44 (8%)	17	33
1	B	581/634 (92%)	540 (93%)	41 (7%)	18	36
All	All	1166/1268 (92%)	1081 (93%)	85 (7%)	17	35

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	ARG
1	A	79	LEU
1	A	83	LEU
1	A	132	ARG
1	A	135	GLN
1	A	146	LEU
1	A	153	ARG
1	A	181	GLN
1	A	188	LEU
1	A	195	LEU
1	A	196	HIS
1	A	198	CYS
1	A	199	CYS

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Mol	Chain	Res	Type
1	A	206	ARG
1	A	218	LEU
1	A	219	GLN
1	A	229	LEU
1	A	261	ILE
1	A	290	LEU
1	A	302	LEU
1	A	376	SER
1	A	409	THR
1	A	442	ARG
1	A	459	VAL
1	A	469	LEU
1	A	489	PHE
1	A	496	SER
1	A	511	VAL
1	A	513	GLU
1	A	539	VAL
1	A	559	LEU
1	A	565	THR
1	A	587	LEU
1	A	604	ARG
1	A	613	GLU
1	A	617	GLN
1	A	625	PHE
1	A	629	ARG
1	A	635	THR
1	A	695	VAL
1	A	713	GLU
1	A	735	GLU
1	A	744	GLN
1	A	762	HIS
1	B	78	ARG
1	B	90	ARG
1	B	95	CYS
1	B	103	LEU
1	B	153	ARG
1	B	157	VAL
1	B	181	GLN
1	B	206	ARG
1	B	209	VAL
1	B	212	THR
1	B	229	LEU

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Mol	Chain	Res	Type
1	B	243	VAL
1	B	260	THR
1	B	299	SER
1	B	303	LYS
1	B	326	GLN
1	B	353	ARG
1	B	360	VAL
1	B	395	THR
1	B	417	LEU
1	B	442	ARG
1	B	459	VAL
1	B	489	PHE
1	B	492	THR
1	B	511	VAL
1	B	558	GLN
1	B	559	LEU
1	B	561	ARG
1	B	570	GLU
1	B	573	GLU
1	B	587	LEU
1	B	608	LEU
1	B	626	SER
1	B	640	GLU
1	B	646	SER
1	B	650	GLN
1	B	713	GLU
1	B	722	SER
1	B	739	LEU
1	B	752	LEU
1	B	761	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	A	135	GLN
1	A	174	GLN
1	A	197	HIS
1	A	276	GLN
1	A	319	GLN
1	A	355	GLN
1	A	450	HIS

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Mol	Chain	Res	Type
1	A	618	ASN
1	A	744	GLN
1	A	762	HIS
1	B	58	GLN
1	B	77	GLN
1	B	94	ASN
1	B	112	HIS
1	B	174	GLN
1	B	185	ASN
1	B	241	HIS
1	B	262	GLN
1	B	267	GLN
1	B	276	GLN
1	B	287	ASN
1	B	650	GLN
1	B	693	ASN
1	B	699	ASN
1	B	729	GLN
1	B	762	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	1,2	13,14,15	3.76	7 (53%)	15,19,21	1.35	2 (13%)
1	TPQ	B	471	1,2	13,14,15	3.62	7 (53%)	15,19,21	1.77	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
1	TPQ	A	471	1,2	-	0/4/22/24	0/1/1/1
1	TPQ	B	471	1,2	-	0/4/22/24	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	471	TPQ	C1-C2	-8.49	1.37	1.49
1	B	471	TPQ	C1-C2	-7.39	1.39	1.49
1	A	471	TPQ	C4-C5	-2.34	1.40	1.47
1	B	471	TPQ	C4-C5	-2.26	1.40	1.47
1	A	471	TPQ	O4-C4	3.04	1.42	1.34
1	B	471	TPQ	O4-C4	3.26	1.42	1.34
1	B	471	TPQ	C6-C1	3.82	1.44	1.34
1	A	471	TPQ	C6-C1	3.86	1.44	1.34
1	A	471	TPQ	C3-C4	4.30	1.42	1.35
1	B	471	TPQ	C3-C4	4.48	1.43	1.35
1	A	471	TPQ	O2-C2	5.31	1.39	1.24
1	B	471	TPQ	O2-C2	5.49	1.39	1.24
1	B	471	TPQ	O5-C5	5.52	1.39	1.24
1	A	471	TPQ	O5-C5	5.59	1.40	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	471	TPQ	C3-C4-C5	-2.28	118.79	121.18
1	A	471	TPQ	O2-C2-C1	2.02	122.61	120.85
1	B	471	TPQ	CB-C1-C2	2.90	122.86	118.33
1	A	471	TPQ	CB-C1-C2	3.07	123.12	118.33
1	B	471	TPQ	O2-C2-C1	3.96	124.31	120.85

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	471	TPQ	2	0
1	B	471	TPQ	2	0

5.5 Carbohydrates (i)

10 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	$\#\|Z\| > 2$
5	NAG	A	1768	1,5	14,14,15	1.89	4 (28%)	15,19,21	1.88	5 (33%)
5	NAG	A	1769	5	14,14,15	2.17	5 (35%)	15,19,21	1.71	3 (20%)
5	MAN	A	1770	5	11,11,12	1.80	3 (27%)	14,15,17	2.11	6 (42%)
6	NAG	A	1771	1,6	14,14,15	2.09	5 (35%)	15,19,21	1.47	3 (20%)
6	NAG	A	1772	6	14,14,15	1.97	4 (28%)	15,19,21	1.43	2 (13%)
5	NAG	B	1768	1,5	14,14,15	1.91	5 (35%)	15,19,21	1.52	3 (20%)
5	NAG	B	1769	5	14,14,15	1.95	5 (35%)	15,19,21	2.58	4 (26%)
5	MAN	B	1770	5	11,11,12	1.68	3 (27%)	14,15,17	2.37	5 (35%)
6	NAG	B	1771	1,6	14,14,15	1.88	4 (28%)	15,19,21	2.09	4 (26%)
6	NAG	B	1772	6	14,14,15	2.07	5 (35%)	15,19,21	2.15	4 (26%)

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	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
5	MAN	A	1770	5	-	0/2/19/22	1/1/1/1
6	NAG	A	1771	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1772	6	-	0/6/23/26	0/1/1/1
5	NAG	B	1768	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	1769	5	-	0/6/23/26	0/1/1/1
5	MAN	B	1770	5	-	0/2/19/22	1/1/1/1
6	NAG	B	1771	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	1772	6	-	0/6/23/26	0/1/1/1

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1768	NAG	C3-C2	-4.19	1.42	1.52
5	A	1768	NAG	C3-C2	-3.73	1.43	1.52
6	A	1771	NAG	C3-C2	-3.47	1.44	1.52
5	B	1770	MAN	C4-C3	-3.39	1.43	1.52
6	B	1771	NAG	C3-C2	-3.33	1.44	1.52
5	A	1770	MAN	C4-C3	-3.20	1.44	1.52
5	B	1769	NAG	C4-C5	-2.94	1.46	1.53
5	B	1768	NAG	C1-C2	-2.94	1.48	1.52
5	A	1769	NAG	C1-C2	-2.85	1.48	1.52
6	A	1771	NAG	C1-C2	-2.83	1.48	1.52
5	A	1770	MAN	C2-C3	-2.60	1.48	1.52
6	B	1772	NAG	C4-C5	-2.57	1.47	1.53
6	A	1772	NAG	C4-C5	-2.47	1.47	1.53
5	A	1768	NAG	C4-C3	-2.40	1.46	1.52
5	B	1768	NAG	C4-C3	-2.38	1.46	1.52
5	A	1769	NAG	C3-C2	-2.28	1.47	1.52
5	B	1769	NAG	O5-C1	-2.04	1.40	1.43
5	B	1769	NAG	C6-C5	-2.02	1.44	1.51
5	A	1769	NAG	C4-C5	-2.01	1.48	1.53
5	B	1770	MAN	C2-C3	-2.00	1.49	1.52
6	B	1772	NAG	C2-N2	2.06	1.50	1.46
5	B	1768	NAG	O5-C1	2.15	1.47	1.43
6	A	1772	NAG	C8-C7	2.15	1.54	1.50
6	B	1771	NAG	O4-C4	2.21	1.48	1.43
6	A	1771	NAG	O5-C1	2.46	1.47	1.43
6	B	1772	NAG	C8-C7	2.55	1.55	1.50
5	A	1768	NAG	C7-N2	2.68	1.44	1.34
5	B	1769	NAG	C7-N2	2.74	1.44	1.34
5	A	1768	NAG	O5-C1	2.78	1.48	1.43
5	B	1768	NAG	C7-N2	2.86	1.45	1.34
6	B	1771	NAG	C2-N2	2.98	1.51	1.46
5	A	1769	NAG	C7-N2	3.07	1.46	1.34
5	B	1770	MAN	O5-C5	3.20	1.50	1.43
5	A	1770	MAN	O5-C5	3.40	1.50	1.43
6	B	1771	NAG	C7-N2	3.43	1.47	1.34
6	A	1771	NAG	C2-N2	3.46	1.52	1.46
6	A	1771	NAG	C7-N2	3.54	1.47	1.34
6	A	1772	NAG	C7-N2	3.67	1.48	1.34
6	B	1772	NAG	C7-N2	3.90	1.49	1.34
5	B	1769	NAG	O5-C5	4.11	1.52	1.43
6	A	1772	NAG	O5-C5	4.25	1.52	1.43
6	B	1772	NAG	O5-C5	4.27	1.52	1.43
5	A	1769	NAG	O5-C5	4.97	1.54	1.43

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1769	NAG	C2-N2-C7	-7.56	113.33	123.04
5	B	1770	MAN	C1-C2-C3	-4.67	104.01	109.54
6	B	1772	NAG	C1-O5-C5	-4.28	106.81	112.25
5	A	1769	NAG	O4-C4-C3	-3.87	101.62	110.34
5	B	1768	NAG	C2-N2-C7	-3.70	118.28	123.04
5	A	1768	NAG	C6-C5-C4	-3.43	104.55	113.02
5	A	1770	MAN	C1-C2-C3	-3.29	105.65	109.54
5	A	1770	MAN	C1-O5-C5	-3.22	108.17	112.25
5	A	1768	NAG	C3-C2-N2	-3.21	102.88	110.56
5	A	1770	MAN	O5-C1-C2	-3.15	105.75	110.86
6	B	1772	NAG	O7-C7-C8	-3.13	116.31	122.06
6	B	1771	NAG	C2-N2-C7	-2.94	119.27	123.04
6	B	1771	NAG	C1-O5-C5	-2.81	108.68	112.25
5	A	1769	NAG	O5-C5-C6	-2.64	101.64	107.35
5	A	1769	NAG	C2-N2-C7	-2.63	119.67	123.04
5	B	1769	NAG	O4-C4-C3	-2.55	104.60	110.34
6	A	1771	NAG	C1-O5-C5	-2.55	109.02	112.25
5	B	1769	NAG	O5-C5-C6	-2.13	102.74	107.35
5	A	1768	NAG	O7-C7-N2	-2.06	117.67	121.86
5	B	1768	NAG	C3-C2-N2	-2.01	105.73	110.56
6	A	1772	NAG	C4-C3-C2	2.10	114.50	111.23
5	B	1770	MAN	O5-C5-C6	2.22	112.15	107.35
6	A	1772	NAG	O6-C6-C5	2.28	118.87	111.33
5	A	1770	MAN	O6-C6-C5	2.35	119.08	111.33
6	A	1771	NAG	C3-C4-C5	2.44	114.46	110.20
5	A	1768	NAG	C3-C4-C5	2.45	114.47	110.20
5	B	1770	MAN	O6-C6-C5	2.58	119.87	111.33
5	A	1770	MAN	O5-C5-C6	2.59	112.96	107.35
5	B	1768	NAG	C3-C4-C5	2.68	114.87	110.20
5	A	1770	MAN	O2-C2-C1	2.69	114.60	109.21
5	B	1770	MAN	O2-C2-C3	3.01	116.17	110.12
6	B	1772	NAG	C8-C7-N2	3.18	122.19	116.11
6	A	1771	NAG	C4-C3-C2	3.48	116.64	111.23
5	A	1768	NAG	C1-O5-C5	3.70	116.95	112.25
6	B	1772	NAG	C2-N2-C7	3.91	128.06	123.04
5	B	1769	NAG	C4-C3-C2	3.97	117.40	111.23
6	B	1771	NAG	C3-C4-C5	4.06	117.27	110.20
5	B	1770	MAN	O2-C2-C1	4.38	117.98	109.21
6	B	1771	NAG	C4-C3-C2	4.50	118.23	111.23

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1770	MAN	C1-C2-C3-C4-C5-O5
5	B	1770	MAN	C1-C2-C3-C4-C5-O5

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1768	NAG	2	0
6	A	1771	NAG	1	0
5	B	1768	NAG	2	0
5	B	1769	NAG	1	0

5.6 Ligand geometry

Of 20 ligands modelled in this entry, 6 are monoatomic - leaving 14 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	$\#\|Z\| > 2$
4	IMD	A	1765	-	3,5,5	0.57	0	4,5,5	0.53	0
4	IMD	A	1766	-	3,5,5	0.56	0	4,5,5	0.81	0
4	IMD	A	1767	-	3,5,5	0.54	0	4,5,5	0.73	0
7	NAG	A	1773	1	14,14,15	0.89	1 (7%)	15,19,21	2.31	3 (20%)
7	NAG	A	1774	1	14,14,15	1.98	5 (35%)	15,19,21	2.90	4 (26%)
4	IMD	A	1776	-	3,5,5	0.61	0	4,5,5	0.51	0
8	FMT	A	1777	-	0,2,2	0.00	-	0,1,1	0.00	-
8	FMT	A	1778	-	0,2,2	0.00	-	0,1,1	0.00	-
4	IMD	B	1765	-	3,5,5	0.60	0	4,5,5	0.65	0
4	IMD	B	1766	-	3,5,5	0.66	0	4,5,5	0.43	0
4	IMD	B	1767	-	3,5,5	0.64	0	4,5,5	0.42	0
7	NAG	B	1773	1	14,14,15	1.96	5 (35%)	15,19,21	2.66	6 (40%)
7	NAG	B	1774	1	14,14,15	0.84	0	15,19,21	2.36	4 (26%)
4	IMD	B	1776	-	3,5,5	0.62	0	4,5,5	0.89	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
4	IMD	A	1765	-	-	0/0/0/0	0/1/1/1
4	IMD	A	1766	-	-	0/0/0/0	0/1/1/1
4	IMD	A	1767	-	-	0/0/0/0	0/1/1/1
7	NAG	A	1773	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1774	1	-	0/6/23/26	0/1/1/1
4	IMD	A	1776	-	-	0/0/0/0	0/1/1/1
8	FMT	A	1777	-	-	0/0/0/0	0/0/0/0
8	FMT	A	1778	-	-	0/0/0/0	0/0/0/0
4	IMD	B	1765	-	-	0/0/0/0	0/1/1/1
4	IMD	B	1766	-	-	0/0/0/0	0/1/1/1
4	IMD	B	1767	-	-	0/0/0/0	0/1/1/1
7	NAG	B	1773	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1774	1	-	0/6/23/26	0/1/1/1
4	IMD	B	1776	-	-	0/0/0/0	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1774	NAG	C4-C3	-2.87	1.44	1.52
7	B	1773	NAG	C3-C2	-2.42	1.46	1.52
7	B	1773	NAG	C4-C3	-2.42	1.46	1.52
7	A	1774	NAG	C3-C2	-2.21	1.47	1.52
7	A	1773	NAG	O5-C1	-2.10	1.40	1.43
7	B	1773	NAG	C1-C2	2.00	1.55	1.52
7	A	1774	NAG	C1-C2	2.30	1.55	1.52
7	B	1773	NAG	O5-C5	3.24	1.50	1.43
7	A	1774	NAG	O5-C5	3.76	1.51	1.43
7	A	1774	NAG	C7-N2	4.26	1.50	1.34
7	B	1773	NAG	C7-N2	4.45	1.51	1.34

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	1774	NAG	C6-C5-C4	-4.76	101.27	113.02
7	A	1773	NAG	C6-C5-C4	-3.85	103.51	113.02
7	B	1774	NAG	C4-C3-C2	-3.22	106.22	111.23
7	B	1773	NAG	O7-C7-C8	-3.07	116.42	122.06
7	A	1773	NAG	C4-C3-C2	-2.82	106.84	111.23
7	B	1773	NAG	O7-C7-N2	-2.67	116.42	121.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1774	NAG	O7-C7-C8	-2.43	117.61	122.06
7	B	1774	NAG	O5-C5-C6	2.02	111.73	107.35
7	B	1773	NAG	C3-C4-C5	2.73	114.96	110.20
7	B	1773	NAG	O6-C6-C5	3.45	122.73	111.33
7	A	1774	NAG	C8-C7-N2	3.56	122.92	116.11
7	A	1774	NAG	O6-C6-C5	3.66	123.44	111.33
7	B	1773	NAG	C1-O5-C5	5.03	118.63	112.25
7	B	1773	NAG	C8-C7-N2	5.55	126.72	116.11
7	B	1774	NAG	C1-O5-C5	6.26	120.19	112.25
7	A	1773	NAG	C1-O5-C5	6.41	120.38	112.25
7	A	1774	NAG	C1-O5-C5	8.89	123.53	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1765	IMD	5	0
4	A	1766	IMD	1	0
7	A	1774	NAG	3	0
8	A	1777	FMT	3	0
8	A	1778	FMT	1	0
4	B	1765	IMD	1	0
4	B	1767	IMD	3	0
7	B	1773	NAG	2	0
4	B	1776	IMD	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	704/763 (92%)	-0.87	5 (0%)	89	87	18, 33, 56, 101	0
1	B	700/763 (91%)	-0.84	6 (0%)	85	83	17, 35, 60, 104	0
All	All	1404/1526 (92%)	-0.85	11 (0%)	87	85	17, 34, 58, 104	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	762	HIS	4.0
1	B	57	SER	4.0
1	B	762	HIS	3.2
1	B	205	GLY	3.1
1	B	735	GLU	2.7
1	A	744	GLN	2.6
1	A	283	ALA	2.3
1	A	747	ALA	2.3
1	B	81	PRO	2.2
1	B	553	TRP	2.1
1	A	82	GLY	2.0

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, 95^{th} 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	0.09	-	27,35,43,45	0
1	TPQ	A	471	14/15	0.97	0.09	-	26,39,44,46	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, 95^{th} 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
6	NAG	B	1772	14/15	0.86	0.43	5.35	66,96,105,105	0
6	NAG	A	1772	14/15	0.86	0.40	4.66	67,92,102,109	0
6	NAG	B	1771	14/15	0.93	0.23	2.41	57,68,81,92	0
6	NAG	A	1771	14/15	0.93	0.22	2.25	59,74,83,87	0
5	NAG	A	1769	14/15	0.92	0.17	1.70	48,65,76,93	0
5	NAG	A	1768	14/15	0.96	0.11	-0.77	32,38,47,53	0
5	NAG	B	1768	14/15	0.96	0.08	-1.27	35,44,56,61	0
5	MAN	B	1770	11/12	0.75	0.33	-	59,84,97,102	0
5	MAN	A	1770	11/12	0.83	0.33	-	80,96,105,111	0
5	NAG	B	1769	14/15	0.88	0.20	-	48,72,82,88	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, 95^{th} 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
4	IMD	A	1776	5/5	0.97	0.18	11.55	58,60,66,69	0
4	IMD	B	1766	5/5	0.94	0.23	11.00	49,55,60,66	0
8	FMT	A	1778	3/3	0.96	0.13	2.51	38,38,43,50	0
4	IMD	A	1765	5/5	0.97	0.10	0.73	49,52,55,58	0
4	IMD	A	1766	5/5	1.00	0.13	0.51	20,22,26,26	0
4	IMD	B	1765	5/5	0.99	0.11	0.20	24,24,28,28	0
4	IMD	A	1767	5/5	0.98	0.10	-0.14	23,27,32,33	0
3	CA	A	1763	1/1	1.00	0.09	-0.52	24,24,24,24	0
3	CA	B	1763	1/1	0.99	0.10	-0.56	29,29,29,29	0
4	IMD	B	1776	5/5	0.99	0.07	-1.51	30,32,32,34	0
4	IMD	B	1767	5/5	0.99	0.08	-1.61	43,43,48,48	0
3	CA	A	1764	1/1	1.00	0.05	-2.15	29,29,29,29	0
8	FMT	A	1777	3/3	0.99	0.07	-2.28	34,34,35,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	CA	B	1764	1/1	0.99	0.06	-3.44	32,32,32,32	0
7	NAG	B	1773	14/15	0.78	0.33	-	52,85,100,105	0
7	NAG	B	1774	14/15	0.75	0.44	-	77,78,78,79	0
2	CU	A	1762	1/1	1.00	0.06	-	32,32,32,32	0
2	CU	B	1762	1/1	1.00	0.07	-	29,29,29,29	0
7	NAG	A	1774	14/15	0.79	0.42	-	72,88,95,98	0
7	NAG	A	1773	14/15	0.86	0.32	-	77,78,78,79	0

6.5 Other polymers

There are no such residues in this entry.