



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:04 PM UTC

PDB ID : 7EZT / pdb_00007ezt
Title : The structure and functional mechanism of nucleotide regulated acetylhexosaminidase Am2136 from Akkermansia muciniphila
Authors : Bao, R.; Li, C.C.; Tang, X.Y.; Zhu, Y.B.; Song, Y.J.; Zhao, N.L.; Huang, Q.; Mou, X.Y.; Luo, G.H.; Liu, T.G.
Deposited on : 2021-06-02
Resolution : 2.81 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

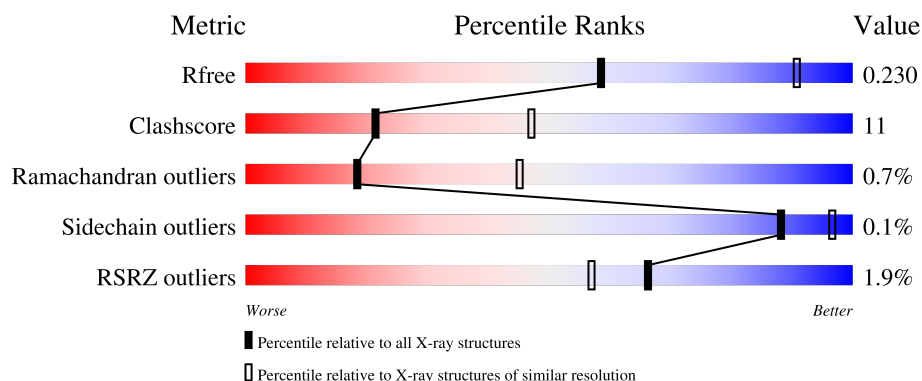
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	737	% 77% 22% .
2	B	727	3% 75% 24% .
3	C	731	3% 71% 27% .
4	D	734	% 81% 18% .

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 23173 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 Beta-N-acetylhexosaminidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	737	Total	C	N	O	S	Se	4	2	0
			5773	3694	995	1061	4	19			

- Molecule 2 is a protein called Beta-N-acetylhexosaminidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	727	Total	C	N	O	S	Se	1	3	0
			5701	3651	982	1045	4	19			

- Molecule 3 is a protein called Beta-N-acetylhexosaminidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	731	Total	C	N	O	S	Se	0	4	0
			5731	3669	986	1053	4	19			

- Molecule 4 is a protein called Beta-N-acetylhexosaminidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	734	Total	C	N	O	S	Se	0	5	0
			5762	3689	991	1059	4	19			

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

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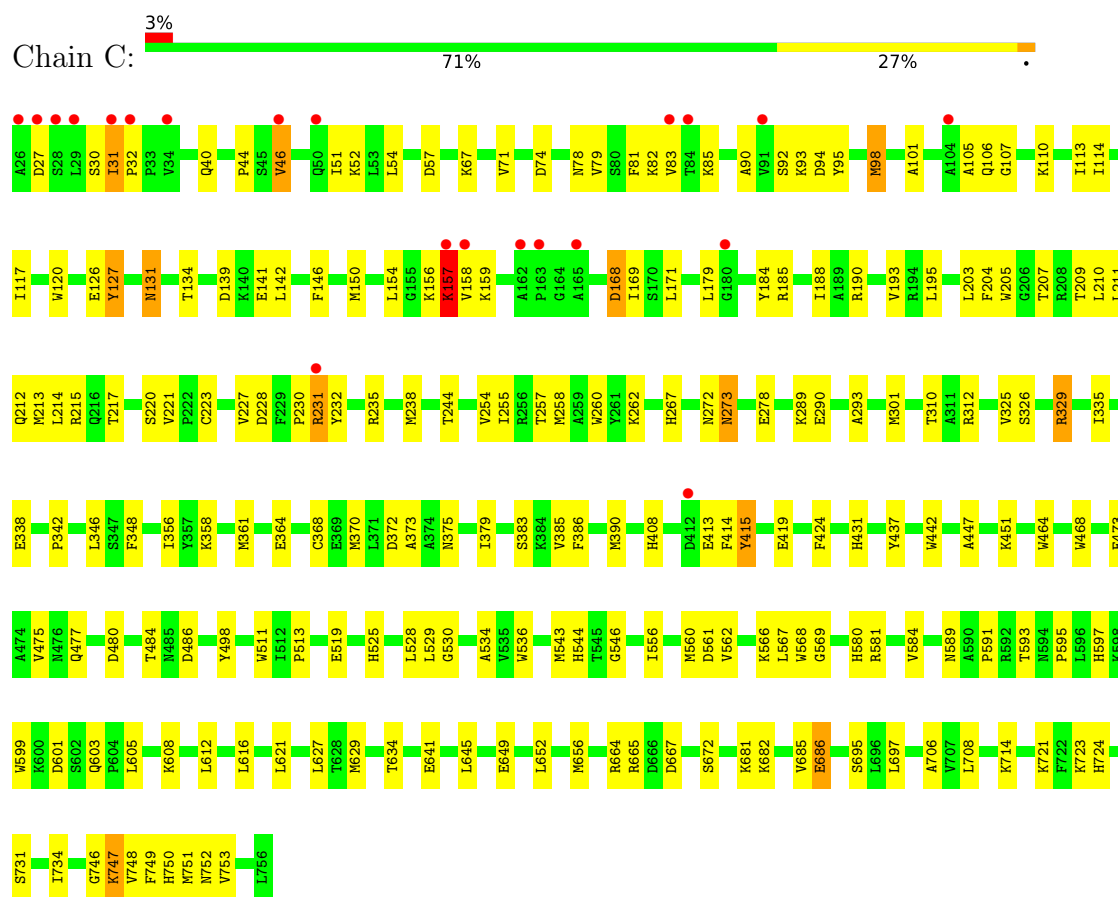
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total 1	Mg 1	0	0

- Molecule 6 is water.

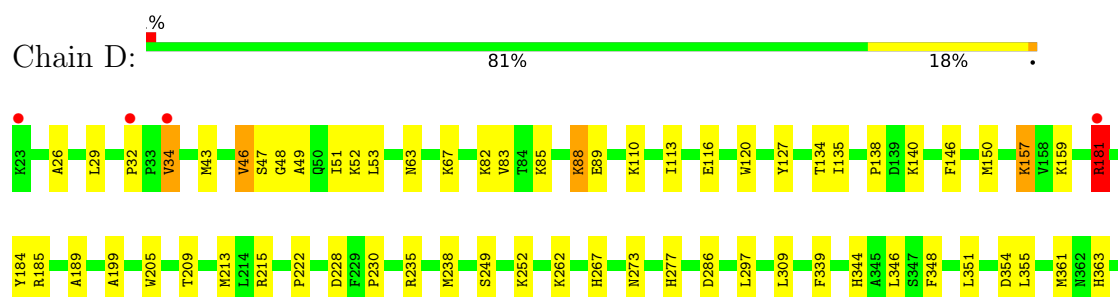
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	48	Total 48	O 48	0	0
6	B	40	Total 40	O 40	0	0
6	C	52	Total 52	O 52	0	0
6	D	62	Total 62	O 62	0	0



• Molecule 3: Beta-N-acetylhexosaminidase



• Molecule 4: Beta-N-acetylhexosaminidase



E369	M370	A373	T378	V385	F386	M390	R398	D403	D412	E413	F414	Y415	K418	F424	P449	A471	W472	E473	Q477	D486	L489	Y490	I491	Y498	R499	M500	K505	Y508	E519	F533	A534	V535	W536	A548	I556	M560	
L567	W568	D575	E578	Q579	H580	R581	V584	T593	M594	P595	D601	P604	P609	L612	M629	E630	T634	E641	M656	V661	R664	R665	E670	F671	S672	F673	K681	K682	E686	K693	L696	L697	A703	A706	S719	D720	K721
S731	E739	S742	Q745	G746	K747	V748	M751	K752	V753	Q754	P755	L756																									

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.20Å 119.50Å 161.93Å 90.00° 103.40° 90.00°	Depositor
Resolution (Å)	26.44 – 2.81 26.44 – 2.81	Depositor EDS
% Data completeness (in resolution range)	98.9 (26.44-2.81) 99.0 (26.44-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.80Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.194 , 0.248 (Not available) , 0.230	Depositor DCC
R_{free} test set	2001 reflections (2.30%)	wwPDB-VP
Wilson B-factor (Å ²)	43.8	Xtriage
Anisotropy	0.736	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	23173	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 19.88 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.8182e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.36	2/5906 (0.0%)	0.69	8/7969 (0.1%)
2	B	0.44	3/5837 (0.1%)	0.76	16/7876 (0.2%)
3	C	0.38	0/5870	0.84	14/7921 (0.2%)
4	D	0.38	0/5904	0.77	14/7966 (0.2%)
All	All	0.39	5/23517 (0.0%)	0.77	52/31732 (0.2%)

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	2
2	B	0	3
3	C	0	5
4	D	0	3
All	All	0	13

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	221	VAL	CA-C	12.31	1.61	1.52
2	B	657	LYS	CG-CD	5.37	1.68	1.52
1	A	88	LYS	CE-NZ	-5.13	1.33	1.49
2	B	126	GLU	CD-OE2	5.05	1.34	1.25
1	A	181	ARG	CZ-NH2	5.04	1.40	1.33

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	181	ARG	CD-NE-CZ	25.40	159.96	124.40
3	C	686	GLU	CG-CD-OE1	19.89	164.14	118.40
3	C	686	GLU	OE1-CD-OE2	-16.79	82.61	122.90
3	C	686	GLU	CG-CD-OE2	-15.01	83.88	118.40
4	D	181	ARG	NE-CZ-NH2	-14.99	105.71	119.20
2	B	340	ASP	CB-CG-OD1	14.41	151.54	118.40
2	B	340	ASP	CB-CG-OD2	-13.44	87.48	118.40
2	B	340	ASP	OD1-CG-OD2	-10.96	96.60	122.90
1	A	710	ASN	CA-C-N	-10.80	102.83	122.50
1	A	710	ASN	C-N-CA	-10.80	102.83	122.50
4	D	181	ARG	NE-CZ-NH1	9.74	131.24	121.50
4	D	181	ARG	CA-C-N	-9.39	107.93	122.49
4	D	181	ARG	C-N-CA	-9.39	107.93	122.49
2	B	413	GLU	CA-CB-CG	9.25	132.59	114.10
3	C	157	LYS	N-CA-CB	9.06	123.32	110.36
3	C	157	LYS	CD-CE-NZ	-9.05	82.94	111.90
3	C	157	LYS	N-CA-C	-8.37	99.48	110.53
3	C	231	ARG	CG-CD-NE	8.19	130.01	112.00
4	D	88	LYS	CG-CD-CE	7.64	128.88	111.30
4	D	181	ARG	CB-CA-C	7.63	125.61	110.42
1	A	32	PRO	O-C-N	7.57	124.79	121.31
2	B	140	LYS	CB-CG-CD	7.38	128.27	111.30
3	C	329	ARG	CG-CD-NE	7.31	128.09	112.00
3	C	98	MSE	CG-SE-CE	-7.14	83.22	98.92
2	B	141	GLU	CA-CB-CG	6.47	127.04	114.10
2	B	363	HIS	CA-C-N	6.33	133.64	121.54
2	B	363	HIS	C-N-CA	6.33	133.64	121.54
4	D	181	ARG	CG-CD-NE	-6.10	98.58	112.00
4	D	157	LYS	CA-CB-CG	-6.08	101.93	114.10
3	C	231	ARG	CB-CG-CD	5.96	125.00	111.30
2	B	40	GLN	CB-CG-CD	5.89	122.61	112.60
2	B	413	GLU	CB-CG-CD	-5.79	102.76	112.60
1	A	32	PRO	N-CA-CB	-5.61	100.05	103.19
4	D	745	GLN	CA-CB-CG	5.60	125.31	114.10
3	C	157	LYS	CB-CA-C	-5.60	98.20	109.68
4	D	181	ARG	O-C-N	-5.51	115.26	122.59
1	A	716	LYS	CA-C-N	5.46	131.97	121.54
1	A	716	LYS	C-N-CA	5.46	131.97	121.54
4	D	88	LYS	CB-CG-CD	-5.43	98.82	111.30
4	D	181	ARG	N-CA-C	5.38	122.26	110.80
2	B	39	LYS	CA-C-N	-5.31	113.33	123.32
2	B	39	LYS	C-N-CA	-5.31	113.33	123.32
1	A	725	ARG	CG-CD-NE	-5.31	100.33	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	39	LYS	CA-CB-CG	5.31	124.71	114.10
3	C	329	ARG	CD-NE-CZ	5.30	131.82	124.40
3	C	747	LYS	CB-CG-CD	5.28	123.44	111.30
1	A	50	GLN	N-CA-C	-5.24	101.16	109.59
2	B	238	MSE	N-CA-C	-5.18	101.83	110.17
3	C	415	TYR	CA-CB-CG	5.09	123.06	113.90
2	B	340	ASP	N-CA-CB	5.05	117.37	109.85
4	D	745	GLN	N-CA-CB	5.04	117.84	110.58
2	B	221	VAL	O-C-N	5.02	126.18	121.11

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	23	LYS	Peptide
1	A	711	PHE	Sidechain
2	B	340	ASP	Sidechain
2	B	614	GLN	Sidechain
2	B	724	HIS	Peptide
3	C	127	TYR	Sidechain
3	C	131	ASN	Peptide
3	C	141	GLU	Sidechain
3	C	273	ASN	Sidechain
3	C	519	GLU	Sidechain
4	D	181	ARG	Mainchain,Sidechain
4	D	601	ASP	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5773	0	5798	113	0
2	B	5701	0	5729	130	1
3	C	5731	0	5759	161	0
4	D	5762	0	5795	106	1
5	A	1	0	0	0	0
5	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	48	0	0	3	0
6	B	40	0	0	0	0
6	C	52	0	0	6	0
6	D	62	0	0	3	0
All	All	23173	0	23081	503	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 11.

All (503) 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:386:PHE:HB3	1:A:390:MSE:HE2	1.37	1.06
3:C:46:VAL:HG12	3:C:51:ILE:HD11	1.46	0.96
2:B:386:PHE:HB3	2:B:390:MSE:HE2	1.50	0.94
3:C:214:LEU:HD12	6:C:901:HOH:O	1.70	0.90
2:B:609:PRO:HG3	2:B:748:VAL:HG23	1.53	0.89
1:A:576:THR:H	1:A:579:GLN:HE21	1.19	0.89
3:C:154:LEU:HD21	3:C:214:LEU:HD23	1.55	0.88
3:C:210:LEU:O	6:C:901:HOH:O	1.92	0.86
1:A:22:ALA:O	6:A:901:HOH:O	1.96	0.82
1:A:128:LYS:NZ	6:A:902:HOH:O	2.12	0.81
3:C:413:GLU:OE1	3:C:468:TRP:HH2	1.64	0.81
2:B:238:MSE:HE2	2:B:534:ALA:HB1	1.63	0.80
2:B:660:THR:HA	2:B:676:LYS:HG2	1.65	0.79
2:B:727:LYS:HE2	2:B:727:LYS:HA	1.63	0.79
3:C:682:LYS:NZ	6:C:902:HOH:O	2.16	0.78
3:C:413:GLU:OE2	3:C:415:TYR:N	2.15	0.78
1:A:124:GLN:OE1	1:A:190:ARG:NH1	2.17	0.77
3:C:289:LYS:NZ	6:C:903:HOH:O	2.19	0.76
1:A:601:ASP:OD2	1:A:603:GLN:HG2	1.85	0.76
3:C:413:GLU:HG2	3:C:415:TYR:HD1	1.51	0.76
2:B:642:GLN:HE21	2:B:745:GLN:HG3	1.50	0.76
3:C:31:ILE:HB	3:C:32:PRO:HD3	1.68	0.75
3:C:213:MSE:HB2	6:C:901:HOH:O	1.85	0.75
1:A:139:ASP:HB3	1:A:142:LEU:HB3	1.69	0.75
4:D:113:ILE:HD11	4:D:213:MSE:HG3	1.70	0.73
3:C:214:LEU:N	6:C:901:HOH:O	2.21	0.72
1:A:33:PRO:O	1:A:34:VAL:HG12	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:505:LYS:NZ	4:D:578:GLU:OE2	2.22	0.72
2:B:629:MSE:HE1	2:B:740:LEU:HD11	1.70	0.71
3:C:231:ARG:HD2	3:C:569:GLY:O	1.91	0.71
3:C:235:ARG:HA	3:C:567:LEU:HD13	1.73	0.71
1:A:23:LYS:HZ2	1:A:88:LYS:HB2	1.55	0.70
4:D:46:VAL:HG23	4:D:47:SER:H	1.57	0.70
4:D:593:THR:HG22	4:D:595:PRO:HD3	1.74	0.70
2:B:593:THR:HG22	2:B:595:PRO:HD3	1.72	0.70
4:D:181:ARG:NH2	4:D:181:ARG:HB2	2.07	0.70
1:A:273:ASN:HD22	1:A:346:LEU:H	1.39	0.69
3:C:528:LEU:HD22	3:C:530:GLY:H	1.57	0.69
2:B:697:LEU:HD23	2:B:702:PRO:HA	1.73	0.69
1:A:445:LEU:HB2	1:A:469:MSE:SE	2.43	0.69
3:C:634:THR:HG23	3:C:746:GLY:HA2	1.75	0.69
3:C:413:GLU:CG	3:C:415:TYR:HD1	2.05	0.68
2:B:169:ILE:HG12	2:B:193:VAL:HB	1.75	0.68
1:A:238:MSE:HE1	1:A:536:TRP:CE2	2.28	0.68
3:C:310:THR:HB	3:C:312:ARG:HH21	1.59	0.68
4:D:413:GLU:HG2	4:D:414:PHE:N	2.09	0.67
3:C:605:LEU:HB3	3:C:753:VAL:HB	1.76	0.67
2:B:309:LEU:HB2	2:B:351:LEU:HD11	1.77	0.67
2:B:633:LEU:HD21	2:B:636:ALA:HB2	1.76	0.67
4:D:32:PRO:O	4:D:34:VAL:HG13	1.94	0.67
2:B:147:ALA:HB2	2:B:160:LEU:HD21	1.77	0.67
1:A:273:ASN:HD21	1:A:369:GLU:HB2	1.59	0.67
4:D:43:MSE:HE1	4:D:53:LEU:HB2	1.77	0.67
3:C:686:GLU:HG3	3:C:697:LEU:HB2	1.77	0.66
3:C:127:TYR:HB2	3:C:190:ARG:HA	1.75	0.66
1:A:113:ILE:HD11	1:A:213:MSE:HG3	1.77	0.66
1:A:31:ILE:HD13	1:A:44:PRO:HG3	1.76	0.66
3:C:361:MSE:SE	3:C:364:GLU:HA	2.45	0.66
2:B:238:MSE:HE1	2:B:536:TRP:CE2	2.30	0.65
4:D:185:ARG:NH2	6:D:901:HOH:O	2.28	0.65
4:D:418:LYS:HD3	4:D:449:PRO:HD2	1.78	0.65
3:C:370:MSE:HE2	3:C:414:PHE:HD1	1.61	0.65
2:B:634:THR:HG23	2:B:746:GLY:HA2	1.77	0.65
1:A:23:LYS:NZ	1:A:88:LYS:HB2	2.10	0.65
4:D:49:ALA:HB2	4:D:85:LYS:HB2	1.77	0.65
2:B:352:ARG:NH2	2:B:354:ASP:OD2	2.21	0.65
2:B:656:MSE:HE2	2:B:660:THR:OG1	1.96	0.64
1:A:276:PHE:CD2	1:A:543:MSE:HE1	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:78:ASN:HB3	3:C:94:ASP:OD1	1.98	0.64
4:D:51:ILE:HG12	4:D:83:VAL:HG12	1.79	0.64
2:B:722:PHE:CD2	2:B:725:ARG:HG2	2.32	0.64
4:D:634:THR:HG23	4:D:746:GLY:HA2	1.80	0.64
2:B:556:ILE:O	2:B:560:MSE:HG3	1.98	0.63
4:D:348:PHE:HE1	4:D:385:VAL:HG21	1.62	0.63
1:A:43:MSE:HE1	1:A:53:LEU:HB2	1.81	0.63
3:C:612:LEU:HD11	3:C:748:VAL:HG23	1.79	0.63
2:B:642:GLN:HB2	2:B:655:VAL:HG12	1.79	0.63
2:B:642:GLN:HE21	2:B:745:GLN:CG	2.12	0.63
4:D:249:SER:HA	4:D:252:LYS:HE3	1.80	0.63
1:A:390:MSE:HE1	1:A:431:HIS:CD2	2.34	0.62
2:B:41:LEU:HD12	2:B:42:PRO:HD2	1.80	0.62
4:D:63:ASN:HD21	4:D:67:LYS:HE3	1.63	0.62
1:A:431:HIS:HA	1:A:434:LYS:HE3	1.81	0.62
3:C:52:LYS:O	3:C:82:LYS:N	2.31	0.62
3:C:544:HIS:CD2	3:C:546:GLY:H	2.18	0.62
3:C:593:THR:HG22	3:C:595:PRO:HD3	1.80	0.62
3:C:81:PHE:H	3:C:92:SER:HB3	1.64	0.62
1:A:161:VAL:HG21	1:A:167:ALA:HB2	1.81	0.62
3:C:158:VAL:O	3:C:159:LYS:HG3	2.01	0.61
2:B:111:PRO:HG2	2:B:213:MSE:HE2	1.82	0.61
2:B:445:LEU:HB2	2:B:469:MSE:SE	2.51	0.61
3:C:231:ARG:HD3	3:C:232:TYR:CE2	2.34	0.61
1:A:479:TYR:O	1:A:527:GLN:NE2	2.30	0.61
4:D:63:ASN:HD21	4:D:67:LYS:CE	2.13	0.61
4:D:88:LYS:HA	4:D:88:LYS:HE2	1.83	0.61
3:C:348:PHE:HE1	3:C:385:VAL:HG21	1.64	0.61
1:A:215:ARG:NH1	1:A:587:ILE:O	2.33	0.61
1:A:716:LYS:HD3	1:A:716:LYS:C	2.26	0.60
3:C:627:LEU:O	3:C:686:GLU:HA	2.01	0.60
1:A:576:THR:H	1:A:579:GLN:NE2	1.95	0.60
1:A:238:MSE:HE1	1:A:536:TRP:CZ2	2.37	0.60
3:C:185:ARG:HG2	3:C:227:VAL:HG22	1.84	0.60
4:D:46:VAL:HG21	4:D:49:ALA:HB3	1.83	0.60
4:D:113:ILE:HG13	4:D:209:THR:HG23	1.84	0.59
3:C:370:MSE:HE2	3:C:414:PHE:HA	1.84	0.59
4:D:230:PRO:HB3	4:D:568:TRP:CE3	2.38	0.59
3:C:210:LEU:HA	3:C:213:MSE:HE3	1.85	0.59
2:B:386:PHE:HB3	2:B:390:MSE:CE	2.30	0.58
3:C:413:GLU:HG3	3:C:414:PHE:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:413:GLU:OE1	3:C:468:TRP:CH2	2.52	0.58
2:B:126:GLU:HB3	2:B:220:SER:HB2	1.86	0.58
1:A:348:PHE:HE1	1:A:385:VAL:HG21	1.69	0.57
1:A:22:ALA:C	1:A:24:GLN:H	2.12	0.57
3:C:238:MSE:HE1	3:C:536:TRP:CE2	2.39	0.57
3:C:413:GLU:HG2	3:C:415:TYR:CD1	2.37	0.57
1:A:359:GLY:O	1:A:367:ARG:NH2	2.38	0.57
3:C:113:ILE:HD11	3:C:213:MSE:HG3	1.87	0.57
2:B:633:LEU:HD13	2:B:744:PHE:HE1	1.70	0.56
1:A:205:TRP:CZ3	1:A:262:LYS:HA	2.40	0.56
1:A:550:TYR:CD1	1:A:732:THR:HG21	2.41	0.56
3:C:205:TRP:CZ3	3:C:262:LYS:HA	2.41	0.56
1:A:267:HIS:NE2	1:A:338:GLU:OE1	2.30	0.56
3:C:83:VAL:HG13	3:C:90:ALA:HB3	1.86	0.56
4:D:508:TYR:OH	4:D:575:ASP:OD1	2.16	0.56
2:B:348:PHE:HE1	2:B:385:VAL:HG21	1.70	0.56
2:B:273:ASN:HD21	2:B:369:GLU:HB2	1.70	0.56
2:B:231:ARG:HH12	2:B:571:ALA:HB2	1.71	0.55
3:C:134:THR:O	3:C:168:ASP:HB2	2.06	0.55
4:D:491:ILE:HG13	4:D:500:MSE:HE3	1.89	0.55
1:A:145:LEU:HD12	1:A:330:LYS:CD	2.36	0.55
1:A:150:MSE:HB3	1:A:158:VAL:HG21	1.88	0.55
3:C:681:LYS:NZ	3:C:682:LYS:O	2.30	0.55
1:A:71:VAL:HG23	1:A:101:ALA:HB2	1.89	0.55
3:C:656:MSE:HE1	3:C:672:SER:HB2	1.89	0.55
4:D:181:ARG:CZ	4:D:181:ARG:CB	2.83	0.55
4:D:706:ALA:HB3	4:D:731:SER:HB3	1.87	0.55
4:D:361:MSE:HE2	4:D:363:HIS:O	2.07	0.55
4:D:719:SER:OG	4:D:721:LYS:HG2	2.08	0.55
3:C:30:SER:HB3	3:C:95:TYR:CE1	2.42	0.54
2:B:431:HIS:HA	2:B:434:LYS:HE3	1.89	0.54
2:B:285:HIS:HE1	2:B:717:ASP:OD1	1.90	0.54
3:C:217:THR:OG1	3:C:220:SER:O	2.24	0.54
4:D:181:ARG:HG3	4:D:199:ALA:CB	2.38	0.54
2:B:181:ARG:N	2:B:181:ARG:HD3	2.23	0.54
3:C:544:HIS:HD2	3:C:546:GLY:H	1.54	0.54
2:B:305:ASP:HB2	2:B:307:THR:HG23	1.91	0.53
2:B:605:LEU:HD21	2:B:618:LYS:HG3	1.89	0.53
3:C:204:PHE:O	3:C:207:THR:OG1	2.22	0.53
2:B:318:LYS:HG2	2:B:400:VAL:HG21	1.91	0.53
3:C:169:ILE:HG13	3:C:193:VAL:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:238:MSE:HG2	2:B:239:LEU:N	2.21	0.53
3:C:528:LEU:HD22	3:C:529:LEU:N	2.23	0.53
4:D:46:VAL:HG23	4:D:47:SER:N	2.22	0.53
1:A:197:ALA:HB3	1:A:203:LEU:HG	1.91	0.53
1:A:273:ASN:ND2	1:A:346:LEU:H	2.05	0.53
4:D:238:MSE:HE1	4:D:536:TRP:CE2	2.43	0.53
1:A:708:LEU:HD11	1:A:710:ASN:HB2	1.91	0.53
2:B:57:ASP:HB3	2:B:523:SER:HB3	1.91	0.53
2:B:641:GLU:CD	2:B:664:ARG:HH22	2.16	0.53
2:B:113:ILE:HG13	2:B:209:THR:HG23	1.90	0.53
2:B:147:ALA:CB	2:B:160:LEU:HD21	2.39	0.53
4:D:681:LYS:HD3	4:D:682:LYS:H	1.74	0.53
1:A:471:ALA:N	1:A:519:GLU:OE1	2.35	0.52
2:B:200:PRO:HA	2:B:203:LEU:HD12	1.91	0.52
3:C:580:HIS:O	3:C:584:VAL:HG23	2.09	0.52
1:A:499:ARG:HB3	1:A:502:ARG:HD2	1.90	0.52
2:B:312:ARG:C	2:B:312:ARG:HD2	2.34	0.52
3:C:113:ILE:HD11	3:C:213:MSE:CG	2.40	0.52
3:C:721:LYS:HA	3:C:723:LYS:HE2	1.92	0.52
4:D:578:GLU:N	4:D:578:GLU:OE1	2.43	0.52
2:B:447:ALA:O	2:B:448:LYS:HD3	2.09	0.52
4:D:386:PHE:CD1	4:D:390:MSE:HE3	2.45	0.52
3:C:232:TYR:CE2	3:C:513:PRO:HG2	2.45	0.52
3:C:706:ALA:HB3	3:C:731:SER:HB2	1.92	0.52
4:D:630:GLU:OE2	4:D:682:LYS:HE3	2.09	0.52
2:B:412:ASP:O	2:B:413:GLU:HB3	2.09	0.52
4:D:26:ALA:HA	4:D:29:LEU:HD13	1.91	0.52
1:A:145:LEU:HD12	1:A:330:LYS:HD2	1.92	0.51
3:C:342:PRO:HB2	3:C:370:MSE:HE3	1.92	0.51
4:D:238:MSE:HG3	4:D:267:HIS:CG	2.45	0.51
4:D:604:PRO:HG3	4:D:754:GLN:HE22	1.75	0.51
1:A:556:ILE:HG22	1:A:560:MSE:HE3	1.93	0.51
4:D:609:PRO:HG2	4:D:748:VAL:O	2.10	0.51
2:B:278:GLU:OE1	2:B:278:GLU:N	2.32	0.51
1:A:370:MSE:HE3	1:A:415:TYR:CE2	2.44	0.51
1:A:412:ASP:OD1	1:A:413:GLU:N	2.44	0.51
2:B:434:LYS:NZ	4:D:286:ASP:OD2	2.40	0.51
3:C:325:VAL:O	3:C:329:ARG:HG2	2.11	0.51
3:C:641:GLU:OE2	3:C:664:ARG:NH2	2.43	0.51
1:A:693:LYS:HE2	6:A:913:HOH:O	2.10	0.51
2:B:501:ASP:N	2:B:501:ASP:OD1	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:326:SER:HA	3:C:329:ARG:HG2	1.92	0.51
4:D:46:VAL:CG2	4:D:49:ALA:HB3	2.41	0.51
4:D:48:GLY:H	4:D:85:LYS:HZ1	1.57	0.51
1:A:392:LYS:HG3	3:C:364:GLU:OE2	2.11	0.50
2:B:614:GLN:OE1	2:B:616:LEU:HD23	2.11	0.50
3:C:171:LEU:HD22	3:C:195:LEU:HB3	1.91	0.50
3:C:656:MSE:HE1	3:C:672:SER:CB	2.41	0.50
4:D:656:MSE:HE1	4:D:672:SER:HB2	1.92	0.50
4:D:693:LYS:HA	4:D:731:SER:HB2	1.92	0.50
1:A:469:MSE:HE2	1:A:474:ALA:HA	1.92	0.50
1:A:670:GLU:N	1:A:710:ASN:OD1	2.38	0.50
3:C:57:ASP:OD2	3:C:78:ASN:HB2	2.12	0.50
4:D:184:TYR:CE1	4:D:228:ASP:HB3	2.47	0.50
2:B:625:TYR:CZ	2:B:689:GLY:HA3	2.46	0.50
2:B:693:LYS:C	2:B:693:LYS:HD3	2.37	0.50
4:D:110:LYS:NZ	4:D:116:GLU:OE2	2.43	0.50
3:C:747:LYS:HD2	3:C:749:PHE:CZ	2.47	0.50
4:D:751:MSE:HE3	4:D:753:VAL:HG23	1.94	0.50
2:B:505:LYS:HG3	2:B:577:PHE:CE2	2.46	0.50
3:C:71:VAL:HG12	3:C:101:ALA:HB2	1.94	0.50
2:B:44:PRO:HG2	2:B:51:ILE:HG21	1.94	0.50
3:C:325:VAL:HA	3:C:335:ILE:HD12	1.92	0.50
3:C:301:MSE:HE3	3:C:385:VAL:HG22	1.94	0.49
4:D:309:LEU:HB2	4:D:351:LEU:HD11	1.93	0.49
4:D:556:ILE:O	4:D:560:MSE:HG3	2.12	0.49
1:A:230:PRO:HB3	1:A:568:TRP:CE3	2.47	0.49
4:D:205:TRP:CZ3	4:D:262:LYS:HA	2.47	0.49
1:A:436:GLY:C	3:C:358:LYS:HD3	2.37	0.49
3:C:93:LYS:HD3	3:C:93:LYS:N	2.28	0.49
4:D:641:GLU:CD	4:D:664:ARG:HH22	2.20	0.49
1:A:238:MSE:HE2	1:A:534:ALA:HB1	1.94	0.49
1:A:556:ILE:CG2	1:A:560:MSE:HE3	2.43	0.49
2:B:273:ASN:HD21	2:B:369:GLU:CB	2.25	0.49
2:B:656:MSE:HE2	2:B:660:THR:HG1	1.77	0.49
4:D:127:TYR:HB2	4:D:189:ALA:O	2.13	0.49
2:B:370:MSE:HE3	2:B:415:TYR:H	1.77	0.49
3:C:386:PHE:CD1	3:C:390:MSE:HE3	2.47	0.49
4:D:273:ASN:HD22	4:D:346:LEU:H	1.61	0.49
1:A:318:LYS:HG2	1:A:400:VAL:HG21	1.94	0.49
3:C:212:GLN:NE2	3:C:260:TRP:O	2.46	0.49
4:D:656:MSE:HE1	4:D:672:SER:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:PRO:HB2	1:A:42:PRO:HB2	1.95	0.48
4:D:373:ALA:HB1	4:D:424:PHE:HB2	1.94	0.48
4:D:601:ASP:OD1	4:D:601:ASP:N	2.40	0.48
3:C:629:MSE:N	3:C:685:VAL:O	2.44	0.48
4:D:146:PHE:O	4:D:150:MSE:HG2	2.12	0.48
2:B:35:LYS:HG2	2:B:42:PRO:HG3	1.95	0.48
3:C:98:MSE:O	3:C:98:MSE:HG3	2.13	0.48
2:B:358:LYS:HA	2:B:367:ARG:HH11	1.79	0.48
3:C:110:LYS:HD2	3:C:117:ILE:HB	1.96	0.48
4:D:696:LEU:HD23	4:D:703:ALA:HB3	1.95	0.48
4:D:370:MSE:HE3	4:D:415:TYR:CD2	2.48	0.48
4:D:661:VAL:HG12	4:D:673:PHE:HD2	1.79	0.48
2:B:370:MSE:HE3	2:B:415:TYR:N	2.29	0.48
4:D:48:GLY:H	4:D:85:LYS:NZ	2.11	0.48
4:D:473:GLU:HG2	6:D:949:HOH:O	2.13	0.48
1:A:413:GLU:OE2	1:A:448:LYS:NZ	2.29	0.48
2:B:489:LEU:HB3	2:B:533:PHE:HA	1.95	0.48
2:B:655:VAL:HA	2:B:660:THR:O	2.13	0.48
4:D:63:ASN:ND2	4:D:67:LYS:HE3	2.28	0.48
3:C:74:ASP:HB3	3:C:98:MSE:HE1	1.96	0.48
3:C:486:ASP:HB2	3:C:498:TYR:CE1	2.49	0.48
1:A:627:LEU:O	1:A:686:GLU:HA	2.14	0.48
3:C:40:GLN:OE1	3:C:67:LYS:HD3	2.14	0.48
3:C:188:ILE:HG21	3:C:221:VAL:HG23	1.96	0.48
2:B:629:MSE:HE3	2:B:751:MSE:SE	2.64	0.47
1:A:417:ASP:OD2	1:A:418:LYS:N	2.46	0.47
3:C:238:MSE:HG3	3:C:267:HIS:CG	2.49	0.47
3:C:480:ASP:HB3	3:C:529:LEU:HD11	1.95	0.47
1:A:491:ILE:HG13	1:A:500:MSE:HE3	1.95	0.47
2:B:601:ASP:HB3	2:B:603:GLN:OE1	2.13	0.47
2:B:624:ASN:HA	2:B:689:GLY:O	2.15	0.47
3:C:31:ILE:CB	3:C:32:PRO:HD3	2.42	0.47
3:C:217:THR:OG1	3:C:217:THR:O	2.32	0.47
1:A:159:LYS:HE3	2:B:613:PRO:HD2	1.96	0.47
2:B:300:LYS:HG2	2:B:388:GLU:OE2	2.13	0.47
2:B:722:PHE:CE1	2:B:724:HIS:HB2	2.48	0.47
3:C:31:ILE:HG13	3:C:44:PRO:HB3	1.97	0.47
3:C:188:ILE:HG22	3:C:223:CYS:HA	1.95	0.47
2:B:112:ARG:O	2:B:113:ILE:HD13	2.14	0.47
2:B:154:LEU:HD21	2:B:214:LEU:HD13	1.96	0.47
2:B:159:LYS:NZ	2:B:161:VAL:HG12	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:440:ARG:HA	2:B:460:GLN:O	2.14	0.47
3:C:215:ARG:NH1	3:C:589:ASN:O	2.34	0.47
1:A:151:GLU:HG2	1:A:158:VAL:HG23	1.96	0.47
3:C:131:ASN:HB2	3:C:156:LYS:HG2	1.97	0.47
3:C:608:LYS:HE2	3:C:750:HIS:ND1	2.30	0.47
4:D:43:MSE:HE3	4:D:52:LYS:HD2	1.97	0.47
1:A:338:GLU:HG3	1:A:408:HIS:ND1	2.29	0.47
3:C:601:ASP:CG	3:C:603:GLN:H	2.22	0.47
1:A:696:LEU:HG	1:A:703:ALA:HB3	1.96	0.47
3:C:146:PHE:CZ	3:C:150:MSE:HE3	2.50	0.47
1:A:271:ASN:HB3	1:A:295:PHE:HD1	1.80	0.46
2:B:205:TRP:CZ3	2:B:262:LYS:HA	2.49	0.46
2:B:600:LYS:HD2	2:B:600:LYS:N	2.29	0.46
2:B:722:PHE:C	2:B:724:HIS:H	2.23	0.46
1:A:469:MSE:HE2	1:A:474:ALA:CA	2.46	0.46
2:B:112:ARG:CZ	2:B:583:LEU:HD13	2.46	0.46
2:B:212:GLN:HG2	2:B:260:TRP:CZ2	2.50	0.46
2:B:642:GLN:HB2	2:B:655:VAL:CG1	2.44	0.46
3:C:254:VAL:HG13	3:C:560:MSE:HE1	1.98	0.46
3:C:258:MSE:HG3	3:C:560:MSE:SE	2.65	0.46
3:C:447:ALA:HB2	3:C:468:TRP:HA	1.97	0.46
4:D:134:THR:HG22	4:D:159:LYS:HB3	1.96	0.46
1:A:63:ASN:OD1	1:A:67:LYS:N	2.42	0.46
3:C:156:LYS:HA	3:C:156:LYS:HD3	1.59	0.46
3:C:267:HIS:HE2	3:C:338:GLU:HB2	1.80	0.46
4:D:581:ARG:HA	4:D:581:ARG:HD3	1.75	0.46
2:B:433:LEU:HD22	4:D:354:ASP:HA	1.97	0.46
3:C:486:ASP:N	3:C:486:ASP:OD1	2.44	0.46
3:C:599:TRP:CD2	3:C:621:LEU:HD13	2.50	0.46
1:A:556:ILE:O	1:A:560:MSE:HG3	2.16	0.46
3:C:543:MSE:HG2	3:C:724:HIS:O	2.15	0.46
4:D:664:ARG:HH11	4:D:670:GLU:CD	2.24	0.46
4:D:629:MSE:HE3	4:D:751:MSE:SE	2.65	0.46
2:B:697:LEU:HD23	2:B:702:PRO:CA	2.43	0.46
3:C:179:LEU:HD21	3:C:185:ARG:HG3	1.97	0.46
4:D:363:HIS:HD2	6:D:922:HOH:O	1.98	0.46
2:B:173:LEU:HD23	2:B:173:LEU:HA	1.82	0.46
4:D:473:GLU:O	4:D:477:GLN:HG3	2.16	0.46
1:A:26:ALA:HB1	1:A:92:SER:HA	1.98	0.45
3:C:419:GLU:CD	3:C:451:LYS:H	2.24	0.45
4:D:235:ARG:HG2	4:D:567:LEU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:446:SER:OG	2:B:473:GLU:OE1	2.26	0.45
3:C:601:ASP:OD2	3:C:603:GLN:HB2	2.16	0.45
1:A:250:TYR:O	1:A:254:VAL:HG23	2.15	0.45
3:C:171:LEU:HA	3:C:195:LEU:O	2.17	0.45
3:C:686:GLU:CG	3:C:697:LEU:HB2	2.44	0.45
2:B:112:ARG:C	2:B:113:ILE:HD13	2.41	0.45
3:C:390:MSE:HG2	3:C:437:TYR:CE2	2.51	0.45
4:D:661:VAL:HG12	4:D:673:PHE:CD2	2.51	0.45
1:A:271:ASN:HB3	1:A:295:PHE:CD1	2.51	0.45
2:B:656:MSE:HE1	2:B:672:SER:HB2	1.99	0.45
3:C:54:LEU:H	3:C:81:PHE:HA	1.81	0.45
3:C:203:LEU:HD23	3:C:203:LEU:HA	1.84	0.45
3:C:230:PRO:HD3	3:C:568:TRP:CH2	2.52	0.45
3:C:616:LEU:HD13	3:C:751:MSE:HE1	1.98	0.45
4:D:238:MSE:HE1	4:D:536:TRP:CD2	2.51	0.45
1:A:26:ALA:O	1:A:95:TYR:OH	2.23	0.45
3:C:126:GLU:HB2	3:C:220:SER:OG	2.17	0.45
3:C:370:MSE:HE2	3:C:414:PHE:CD1	2.48	0.45
3:C:597:HIS:ND1	3:C:734:ILE:HD13	2.32	0.45
4:D:486:ASP:HB2	4:D:498:TYR:CE1	2.52	0.45
1:A:274:TYR:OH	1:A:543:MSE:HE2	2.17	0.45
1:A:543:MSE:HG2	1:A:724:HIS:O	2.17	0.45
2:B:664:ARG:HB2	2:B:670:GLU:HG2	1.99	0.45
2:B:722:PHE:HD2	2:B:725:ARG:HG2	1.78	0.45
2:B:40:GLN:O	2:B:68:ILE:HD12	2.17	0.45
1:A:189:ALA:HB3	1:A:191:ASP:OD1	2.17	0.45
1:A:489:LEU:HB3	1:A:533:PHE:HA	1.99	0.45
1:A:645:LEU:HB2	1:A:652:LEU:HB3	1.99	0.45
2:B:43:MSE:HE1	2:B:53:LEU:HB2	1.98	0.45
2:B:693:LYS:HE2	2:B:695:SER:HB3	1.99	0.45
3:C:267:HIS:NE2	3:C:338:GLU:OE1	2.51	0.44
3:C:408:HIS:HE1	3:C:442:TRP:CD1	2.35	0.44
4:D:82:LYS:HD3	4:D:89:GLU:OE2	2.17	0.44
1:A:260:TRP:CE3	1:A:591:PRO:HD3	2.52	0.44
2:B:665:ARG:NH2	2:B:667:ASP:OD2	2.45	0.44
4:D:580:HIS:O	4:D:584:VAL:HG23	2.17	0.44
1:A:429:LEU:HD21	1:A:441:ILE:HB	1.99	0.44
2:B:81:PHE:HE2	2:B:95:TYR:HD2	1.65	0.44
3:C:278:GLU:H	3:C:278:GLU:CD	2.25	0.44
1:A:297:LEU:HD23	1:A:297:LEU:HA	1.75	0.44
1:A:413:GLU:OE2	1:A:414:PHE:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:238:MSE:HE2	3:C:534:ALA:HB1	1.99	0.44
3:C:272:ASN:OD1	3:C:273:ASN:N	2.47	0.44
4:D:370:MSE:HE3	4:D:415:TYR:CG	2.52	0.44
4:D:641:GLU:CD	4:D:664:ARG:NH2	2.75	0.44
2:B:627:LEU:O	2:B:686:GLU:HA	2.18	0.44
2:B:716:LYS:HB2	2:B:716:LYS:HE2	1.70	0.44
4:D:277:HIS:HE1	4:D:369:GLU:HB3	1.82	0.44
3:C:110:LYS:HA	3:C:120:TRP:CD1	2.52	0.44
3:C:293:ALA:HB2	3:C:346:LEU:HD23	2.00	0.44
1:A:118:LEU:N	1:A:228:ASP:OD1	2.40	0.44
1:A:613:PRO:HD3	2:B:159:LYS:HD2	1.99	0.44
2:B:655:VAL:HG23	2:B:659:GLY:C	2.42	0.44
1:A:186:LEU:HB3	1:A:226:ALA:HB3	2.00	0.44
1:A:370:MSE:HE3	1:A:415:TYR:CZ	2.53	0.44
3:C:473:GLU:O	3:C:477:GLN:HG3	2.18	0.44
1:A:291:SER:O	1:A:350:ARG:NH2	2.48	0.43
1:A:576:THR:HG23	1:A:579:GLN:NE2	2.33	0.43
1:A:608:LYS:HD3	1:A:749:PHE:O	2.17	0.43
2:B:338:GLU:OE2	2:B:340:ASP:OD1	2.36	0.43
2:B:503:ASN:C	2:B:505:LYS:H	2.25	0.43
4:D:471:ALA:N	4:D:519:GLU:OE1	2.35	0.43
1:A:629:MSE:HE2	1:A:631:LEU:HD23	2.00	0.43
3:C:105:ALA:O	3:C:107:GLY:N	2.51	0.43
4:D:48:GLY:C	4:D:85:LYS:HZ3	2.26	0.43
4:D:344:HIS:NE2	4:D:412:ASP:OD2	2.45	0.43
1:A:581:ARG:HD3	1:A:581:ARG:HA	1.78	0.43
2:B:713:ASP:O	2:B:716:LYS:NZ	2.51	0.43
3:C:210:LEU:HD23	3:C:213:MSE:CE	2.49	0.43
3:C:235:ARG:HG2	3:C:567:LEU:HB3	2.01	0.43
4:D:181:ARG:CZ	4:D:181:ARG:HB3	2.48	0.43
2:B:57:ASP:HB2	2:B:231:ARG:HD2	2.00	0.43
2:B:629:MSE:HG2	2:B:751:MSE:HG3	1.99	0.43
1:A:598:LYS:HA	1:A:598:LYS:HD2	1.80	0.43
1:A:609:PRO:HG2	1:A:748:VAL:HG12	1.99	0.43
3:C:79:VAL:O	3:C:95:TYR:N	2.51	0.43
3:C:156:LYS:HD3	3:C:157:LYS:N	2.33	0.43
4:D:262:LYS:HD3	4:D:568:TRP:CH2	2.53	0.43
4:D:751:MSE:HE3	4:D:753:VAL:CG2	2.48	0.43
2:B:50:GLN:O	2:B:83:VAL:HA	2.19	0.43
4:D:681:LYS:HD3	4:D:682:LYS:N	2.34	0.43
1:A:273:ASN:HD22	1:A:346:LEU:CB	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:297:LEU:HD23	2:B:297:LEU:HA	1.86	0.43
2:B:598:LYS:NZ	2:B:623:PRO:O	2.52	0.43
4:D:110:LYS:HD3	4:D:120:TRP:HB3	2.01	0.43
1:A:576:THR:OG1	1:A:579:GLN:HG3	2.19	0.43
2:B:61:LEU:HA	2:B:69:ALA:HB3	2.01	0.43
2:B:273:ASN:HD22	2:B:346:LEU:HB2	1.83	0.43
2:B:499:ARG:HB3	2:B:502:ARG:HD2	2.00	0.43
3:C:649:GLU:OE1	3:C:649:GLU:N	2.52	0.43
4:D:686:GLU:HB2	4:D:697:LEU:HB2	2.00	0.43
3:C:114:ILE:HD13	3:C:580:HIS:CE1	2.54	0.43
3:C:290:GLU:O	3:C:714:LYS:NZ	2.41	0.43
1:A:124:GLN:H	1:A:124:GLN:HG3	1.58	0.42
1:A:321:PHE:O	1:A:325:VAL:HG23	2.19	0.42
3:C:110:LYS:HD3	3:C:120:TRP:HB2	2.01	0.42
3:C:171:LEU:CD2	3:C:195:LEU:HB3	2.49	0.42
3:C:379:ILE:HD12	3:C:379:ILE:HA	1.94	0.42
4:D:215:ARG:HD3	4:D:215:ARG:HA	1.88	0.42
1:A:665:ARG:HB2	1:A:667:ASP:OD1	2.19	0.42
2:B:623:PRO:HA	2:B:624:ASN:HA	1.72	0.42
3:C:581:ARG:HD3	3:C:581:ARG:HA	1.64	0.42
4:D:181:ARG:HB2	4:D:181:ARG:CZ	2.47	0.42
4:D:398:ARG:NH2	4:D:403:ASP:OD1	2.52	0.42
1:A:22:ALA:C	1:A:24:GLN:N	2.76	0.42
3:C:475:VAL:HG11	3:C:525:HIS:NE2	2.34	0.42
4:D:339:PHE:HB2	4:D:386:PHE:CZ	2.54	0.42
1:A:715:SER:O	1:A:718:PHE:HB2	2.20	0.42
2:B:475:VAL:HG11	2:B:525:HIS:NE2	2.34	0.42
3:C:665:ARG:HB2	3:C:667:ASP:OD1	2.20	0.42
1:A:734:ILE:O	1:A:736:PRO:HD3	2.19	0.42
3:C:257:THR:O	3:C:260:TRP:HB3	2.18	0.42
1:A:522:PRO:HG2	1:A:525:HIS:HB2	2.02	0.42
1:A:651:GLU:OE2	1:A:664:ARG:NH1	2.53	0.42
2:B:212:GLN:HG2	2:B:260:TRP:CH2	2.54	0.42
2:B:313:ASP:OD1	2:B:314:LEU:N	2.53	0.42
3:C:78:ASN:HB3	3:C:94:ASP:CG	2.45	0.42
1:A:276:PHE:CE2	1:A:543:MSE:HE1	2.55	0.42
2:B:200:PRO:O	2:B:203:LEU:HB2	2.20	0.42
2:B:638:GLU:OE1	2:B:638:GLU:N	2.48	0.42
3:C:85:LYS:HD2	3:C:85:LYS:HA	1.69	0.42
3:C:260:TRP:CE3	3:C:591:PRO:HD3	2.54	0.42
4:D:138:PRO:O	4:D:140:LYS:NZ	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:641:GLU:OE2	4:D:664:ARG:NH2	2.43	0.42
2:B:464:TRP:CE3	2:B:465:SER:HB2	2.55	0.42
3:C:146:PHE:CE2	3:C:211:LEU:HD21	2.55	0.42
3:C:171:LEU:HD13	3:C:203:LEU:HD22	2.00	0.42
3:C:561:ASP:OD1	3:C:562:VAL:N	2.52	0.42
4:D:181:ARG:HB2	4:D:181:ARG:HH21	1.84	0.42
4:D:489:LEU:HB3	4:D:533:PHE:HA	2.01	0.42
2:B:52:LYS:HG2	2:B:53:LEU:N	2.35	0.41
3:C:383[A]:SER:HB2	3:C:431:HIS:CE1	2.54	0.41
4:D:297:LEU:HD23	4:D:297:LEU:HA	1.87	0.41
2:B:645:LEU:HB2	2:B:652:LEU:HB3	2.02	0.41
3:C:184:TYR:CE1	3:C:228:ASP:HB3	2.55	0.41
4:D:135:ILE:HD11	4:D:150:MSE:HG3	2.02	0.41
1:A:238:MSE:HG2	1:A:239:LEU:N	2.34	0.41
1:A:431:HIS:O	1:A:434:LYS:HG2	2.20	0.41
2:B:145:LEU:CD2	2:B:330:LYS:HG2	2.50	0.41
2:B:709:LYS:HA	2:B:709:LYS:HD2	1.78	0.41
3:C:156:LYS:O	3:C:157:LYS:C	2.61	0.41
1:A:76:PRO:HB3	1:A:98:MSE:HE2	2.02	0.41
3:C:232:TYR:CE1	3:C:528:LEU:HD13	2.56	0.41
3:C:255:ILE:HD11	3:C:335:ILE:HD11	2.02	0.41
3:C:370:MSE:CE	3:C:414:PHE:HA	2.47	0.41
1:A:505:LYS:HG3	1:A:577:PHE:CD2	2.55	0.41
1:A:613:PRO:CD	2:B:159:LYS:HD2	2.51	0.41
2:B:115:PRO:HD2	2:B:262:LYS:HD2	2.02	0.41
2:B:348:PHE:CE1	2:B:385:VAL:HG21	2.54	0.41
3:C:139:ASP:HB3	3:C:142:LEU:HB3	2.01	0.41
1:A:599:TRP:CG	1:A:621:LEU:HD13	2.56	0.41
2:B:655:VAL:HG23	2:B:659:GLY:O	2.20	0.41
3:C:372:ASP:HB3	3:C:375:ASN:HB2	2.01	0.41
3:C:645:LEU:HB2	3:C:652:LEU:HB3	2.03	0.41
3:C:556:ILE:O	3:C:560:MSE:HG3	2.21	0.41
4:D:548:ALA:HB2	4:D:665:ARG:CZ	2.50	0.41
1:A:313:ASP:OD1	1:A:314:LEU:N	2.52	0.41
2:B:57:ASP:OD1	2:B:57:ASP:N	2.53	0.41
2:B:607:VAL:CG2	2:B:751:MSE:HB3	2.51	0.41
3:C:373:ALA:HB1	3:C:424:PHE:HB2	2.03	0.41
3:C:546:GLY:HA2	3:C:708:LEU:HD22	2.03	0.41
4:D:213:MSE:HE3	4:D:222:PRO:HD2	2.03	0.41
2:B:238:MSE:CE	2:B:534:ALA:HB1	2.43	0.41
2:B:341:THR:HG21	2:B:382:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:209:THR:HG22	3:C:213:MSE:HE2	2.03	0.41
3:C:511:TRP:O	3:C:566:LYS:HE3	2.21	0.41
3:C:605:LEU:O	3:C:752:ASN:HA	2.21	0.41
4:D:355:LEU:HD13	4:D:378:THR:HA	2.03	0.41
1:A:623:PRO:HA	1:A:624:ASN:HA	1.80	0.40
1:A:654:ALA:O	1:A:661:VAL:HG22	2.21	0.40
2:B:317:THR:HG23	2:B:320:GLU:OE1	2.21	0.40
2:B:503:ASN:C	2:B:505:LYS:N	2.80	0.40
3:C:528:LEU:HD22	3:C:530:GLY:N	2.31	0.40
2:B:159:LYS:HZ2	2:B:161:VAL:HG12	1.85	0.40
2:B:599:TRP:CD2	2:B:621:LEU:HD13	2.57	0.40
2:B:629:MSE:HE1	2:B:644:LEU:HD21	2.02	0.40
3:C:244:THR:OG1	3:C:544:HIS:HE1	2.05	0.40
4:D:238:MSE:HE2	4:D:534:ALA:HB1	2.03	0.40
4:D:238:MSE:HA	4:D:267:HIS:HB3	2.02	0.40
4:D:664:ARG:NH1	4:D:670:GLU:CD	2.79	0.40
1:A:525:HIS:HA	1:A:526:PRO:HD3	1.93	0.40
1:A:114:ILE:HA	1:A:115:PRO:HA	1.82	0.40
1:A:271:ASN:HA	1:A:294:ALA:O	2.22	0.40
2:B:134:THR:OG1	2:B:167:ALA:HA	2.22	0.40
3:C:156:LYS:HD3	3:C:157:LYS:H	1.86	0.40
3:C:356:ILE:HD13	3:C:368:CYS:HA	2.03	0.40
3:C:464:TRP:HA	3:C:484:THR:O	2.22	0.40
4:D:157:LYS:HA	4:D:157:LYS:HD3	1.86	0.40
4:D:739:GLU:OE1	4:D:742:SER:OG	2.34	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:362:ASN:OD1	4:D:612:LEU:N[2_555]	2.16	0.04

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	737/737 (100%)	711 (96%)	20 (3%)	6 (1%)	16	41
2	B	728/727 (100%)	687 (94%)	35 (5%)	6 (1%)	16	41
3	C	733/731 (100%)	693 (94%)	35 (5%)	5 (1%)	18	45
4	D	737/734 (100%)	706 (96%)	29 (4%)	2 (0%)	36	64
All	All	2935/2929 (100%)	2797 (95%)	119 (4%)	19 (1%)	18	48

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
2	B	31	ILE
3	C	27	ASP
3	C	46	VAL
3	C	168	ASP
1	A	33	PRO
1	A	34	VAL
1	A	717	ASP
3	C	31	ILE
3	C	106	GLN
2	B	140	LYS
4	D	46	VAL
1	A	713	ASP
2	B	33	PRO
2	B	106	GLN
2	B	47	SER
2	B	725	ARG
1	A	163	PRO
4	D	34	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	619/598 (104%)	619 (100%)	0	100	100
2	B	612/590 (104%)	612 (100%)	0	100	100
3	C	616/593 (104%)	613 (100%)	3 (0%)	81	93
4	D	620/596 (104%)	619 (100%)	1 (0%)	87	96
All	All	2467/2377 (104%)	2463 (100%)	4 (0%)	88	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	157	LYS
3	C	695[A]	SER
3	C	695[B]	SER
4	D	181	ARG

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

Mol	Chain	Res	Type
1	A	273	ASN
1	A	283	ASN
1	A	485	ASN
1	A	579	GLN
1	A	603	GLN
2	B	100	GLN
2	B	108	ASN
2	B	273	ASN
2	B	283	ASN
2	B	285	HIS
2	B	431	HIS
2	B	745	GLN
3	C	106	GLN
3	C	108	ASN
3	C	431	HIS
3	C	485	ASN
3	C	544	HIS
3	C	580	HIS
4	D	78	ASN
4	D	273	ASN
4	D	277	HIS
4	D	334	ASN
4	D	363	HIS

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Mol	Chain	Res	Type
4	D	580	HIS
4	D	745	GLN
4	D	750	HIS
4	D	754	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	718/737 (97%)	-0.20	11 (1%) 72 63	28, 46, 78, 141	2 (0%)
2	B	708/727 (97%)	-0.06	19 (2%) 56 46	26, 50, 97, 157	3 (0%)
3	C	712/731 (97%)	-0.01	21 (2%) 53 43	26, 50, 97, 145	4 (0%)
4	D	715/734 (97%)	-0.43	4 (0%) 85 80	21, 37, 69, 123	5 (0%)
All	All	2853/2929 (97%)	-0.17	55 (1%) 66 57	21, 46, 89, 157	14 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	104	ALA	7.2
3	C	26	ALA	5.4
2	B	32	PRO	4.5
2	B	34	VAL	4.2
1	A	105	ALA	3.9
1	A	721	LYS	3.8
3	C	31	ILE	3.7
3	C	162	ALA	3.6
2	B	46	VAL	3.6
3	C	84	THR	3.5
3	C	28	SER	3.4
3	C	163	PRO	3.3
1	A	23	LYS	3.2
2	B	638	GLU	3.2
2	B	162	ALA	3.1
3	C	46	VAL	3.0
2	B	30	SER	3.0
4	D	32	PRO	3.0
2	B	721	LYS	2.9
3	C	412	ASP	2.7
2	B	720	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
3	C	34	VAL	2.6
2	B	33	PRO	2.6
3	C	165	ALA	2.6
2	B	31	ILE	2.5
1	A	162	ALA	2.5
3	C	104	ALA	2.5
4	D	23	LYS	2.5
2	B	163	PRO	2.5
1	A	86	ASP	2.4
1	A	124	GLN	2.4
3	C	29	LEU	2.4
2	B	36	ALA	2.4
3	C	83	VAL	2.3
3	C	180	GLY	2.3
2	B	601	ASP	2.3
3	C	157	LYS	2.3
2	B	105	ALA	2.3
1	A	84	THR	2.2
3	C	158	VAL	2.2
3	C	50	GLN	2.2
3	C	231	ARG	2.1
4	D	34	VAL	2.1
3	C	91	VAL	2.1
2	B	712	SER	2.1
3	C	32	PRO	2.1
1	A	716	LYS	2.1
2	B	722	PHE	2.1
1	A	34	VAL	2.0
1	A	722	PHE	2.0
4	D	181	ARG	2.0
3	C	27	ASP	2.0
2	B	166	LYS	2.0
2	B	47	SER	2.0
2	B	104	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

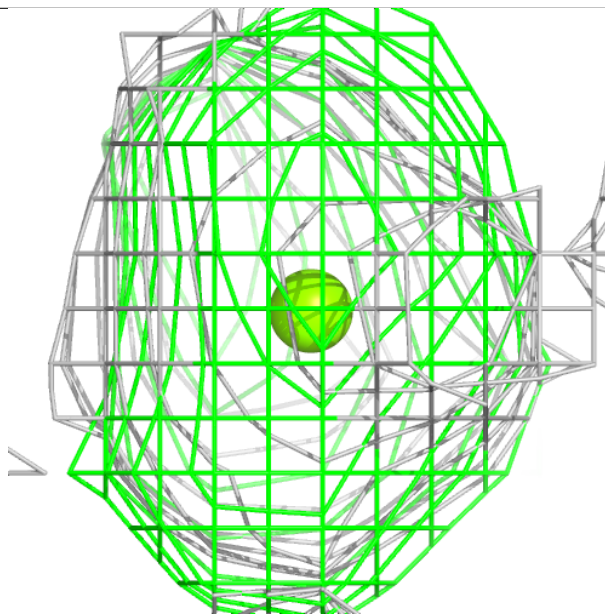
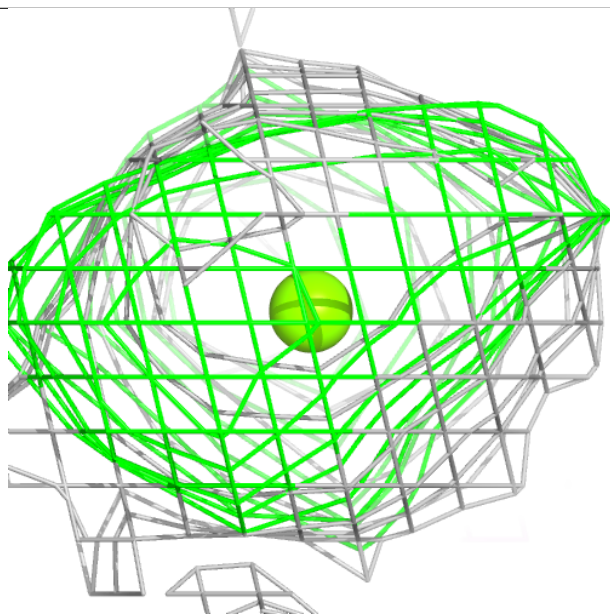
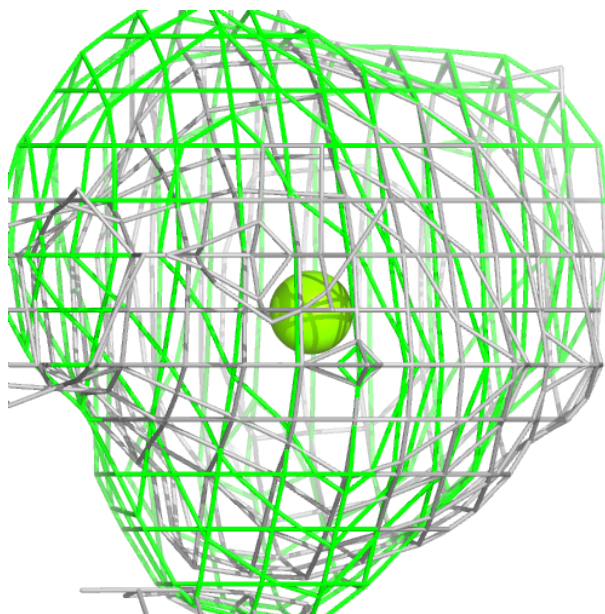
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	A	801	1/1	0.97	0.26	22,22,22,22	0
5	MG	B	801	1/1	0.97	0.24	23,23,23,23	0
5	MG	C	801	1/1	0.98	0.27	29,29,29,29	0
5	MG	D	801	1/1	0.99	0.28	24,24,24,24	0

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

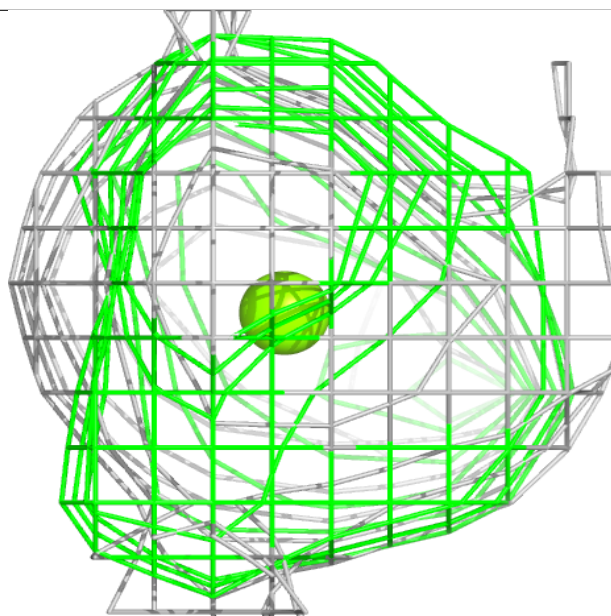
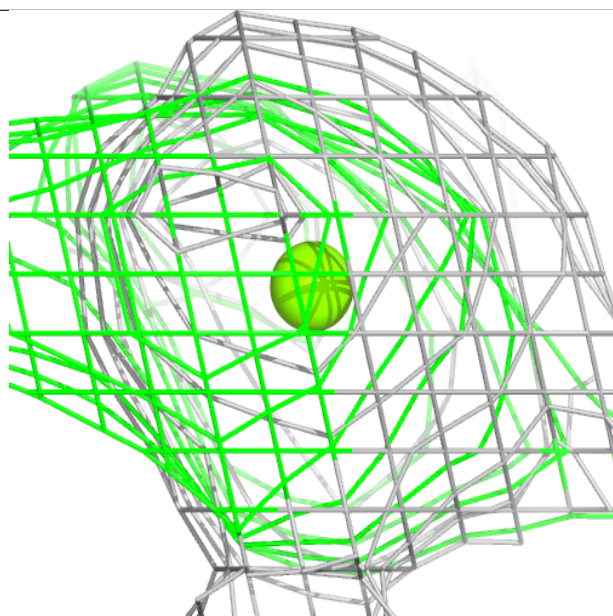
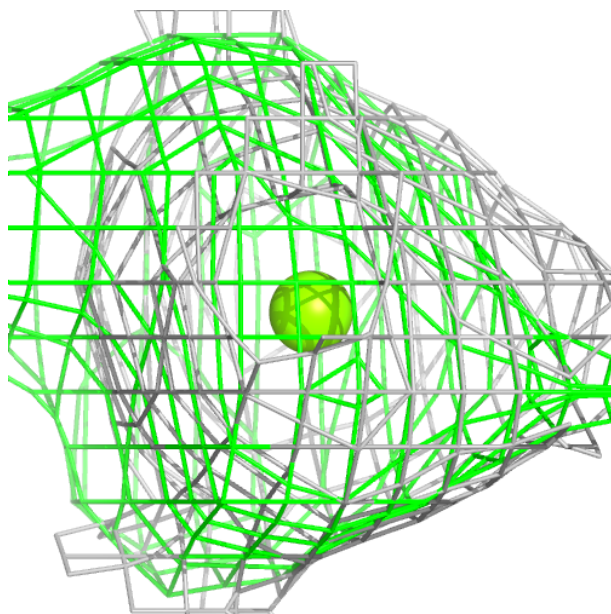
Electron density around MG A 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



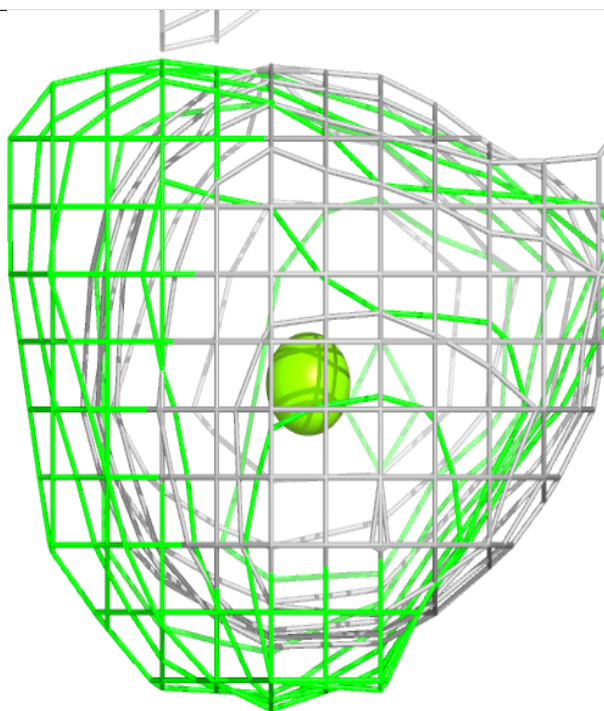
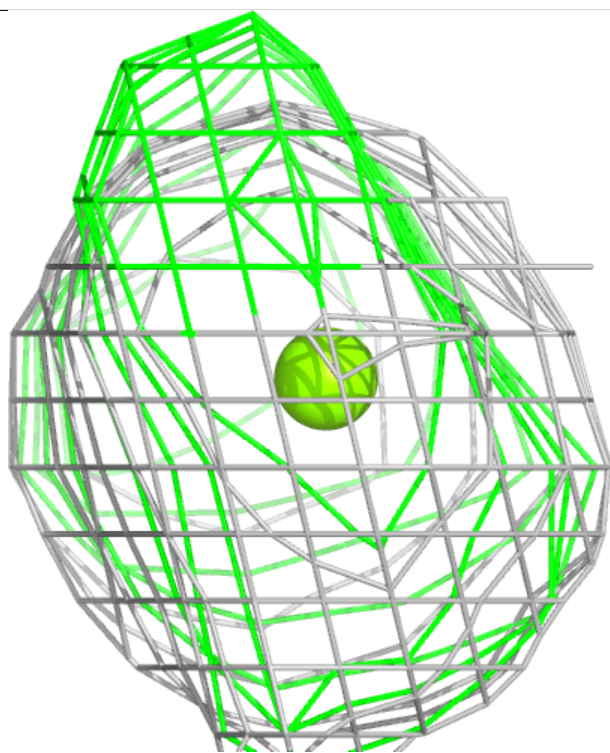
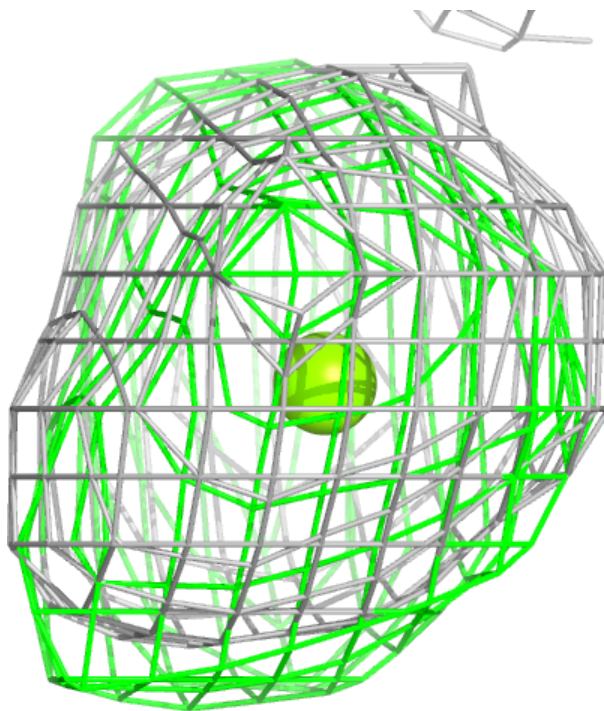
Electron density around MG B 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



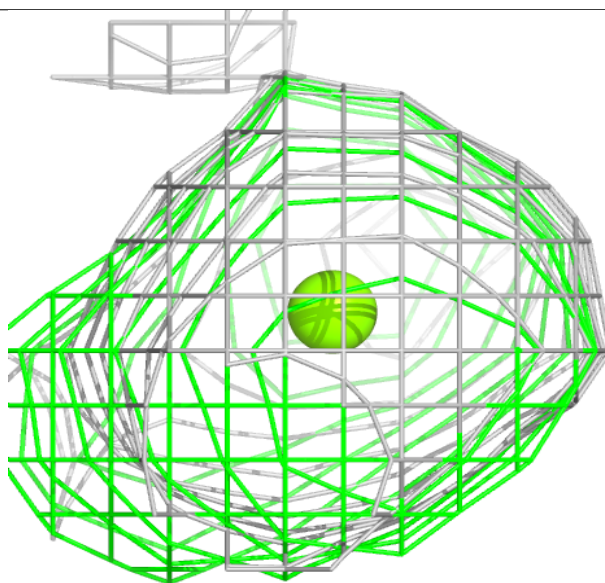
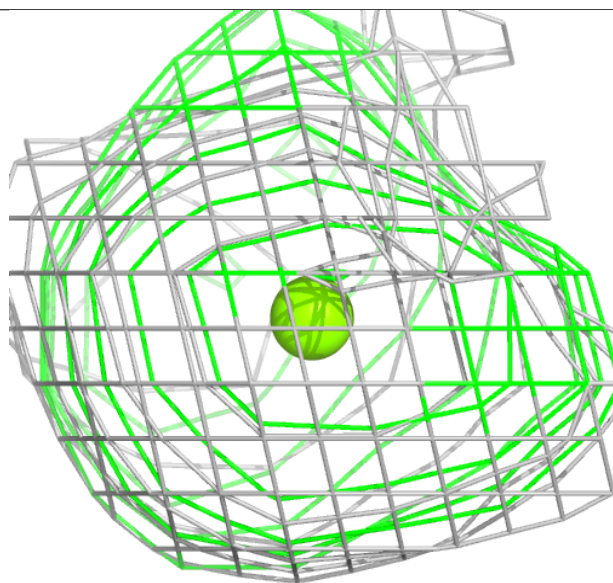
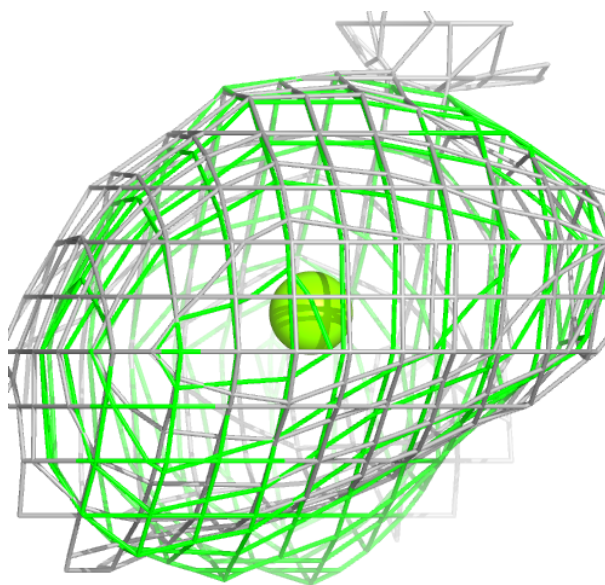
Electron density around MG C 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG D 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.