



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:44 AM UTC

PDB ID : 8Y6B / pdb_00008y6b
Title : Structure of human LGI1-ADAM22 complex in space group P212121
Authors : Liu, H.; Xu, F.
Deposited on : 2024-02-02
Resolution : 3.49 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

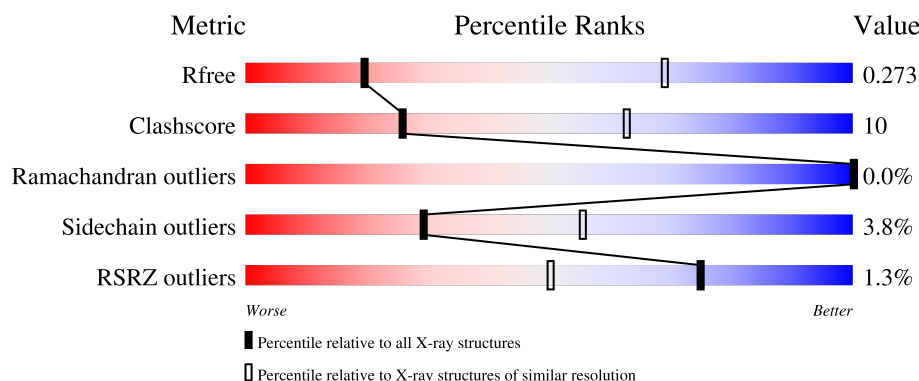
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.49 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	486	2% 80% 20% .
1	B	486	81% 18% .
1	C	486	% 82% 17% .
2	D	526	2% 72% 23% ..
2	E	526	2% 74% 23% ...

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Mol	Chain	Length	Quality of chain
2	F	526	73% 23%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24226 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 Disintegrin and metalloproteinase domain-containing protein 22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	486	Total	C	N	O	S	0	0	0
			3728	2303	643	731	51			
1	B	486	Total	C	N	O	S	0	0	0
			3728	2303	643	731	51			
1	C	486	Total	C	N	O	S	0	0	0
			3728	2303	643	731	51			

- Molecule 2 is a protein called Leucine-rich glioma-inactivated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	517	Total	C	N	O	S	0	0	0
			4194	2700	698	781	15			
2	F	517	Total	C	N	O	S	0	0	0
			4194	2700	698	781	15			
2	E	517	Total	C	N	O	S	0	0	0
			4194	2700	698	781	15			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	32	HIS	-	expression tag	UNP O95970
D	33	HIS	-	expression tag	UNP O95970
D	34	HIS	-	expression tag	UNP O95970
D	35	HIS	-	expression tag	UNP O95970
D	36	HIS	-	expression tag	UNP O95970
D	37	HIS	-	expression tag	UNP O95970
D	38	HIS	-	expression tag	UNP O95970
F	32	HIS	-	expression tag	UNP O95970
F	33	HIS	-	expression tag	UNP O95970
F	34	HIS	-	expression tag	UNP O95970
F	35	HIS	-	expression tag	UNP O95970
F	36	HIS	-	expression tag	UNP O95970

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Chain	Residue	Modelled	Actual	Comment	Reference
F	37	HIS	-	expression tag	UNP O95970
F	38	HIS	-	expression tag	UNP O95970
E	32	HIS	-	expression tag	UNP O95970
E	33	HIS	-	expression tag	UNP O95970
E	34	HIS	-	expression tag	UNP O95970
E	35	HIS	-	expression tag	UNP O95970
E	36	HIS	-	expression tag	UNP O95970
E	37	HIS	-	expression tag	UNP O95970
E	38	HIS	-	expression tag	UNP O95970

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Ca	0	0
			3	3		
4	D	1	Total	Ca	0	0
			1	1		
4	B	3	Total	Ca	0	0
			3	3		
4	C	3	Total	Ca	0	0
			3	3		
4	F	1	Total	Ca	0	0
			1	1		
4	E	1	Total	Ca	0	0
			1	1		

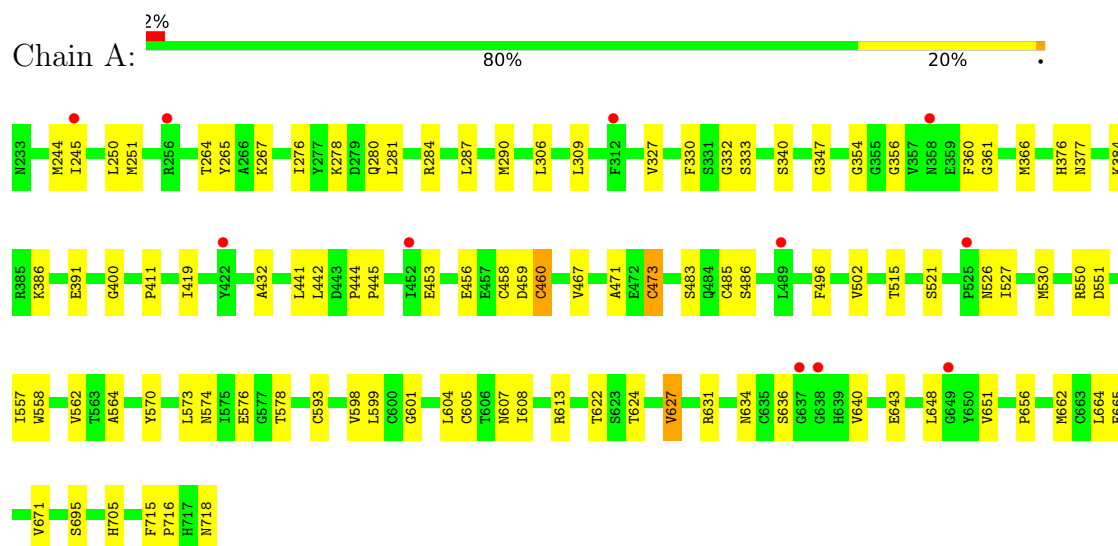
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total 2	O 2	0	0
5	D	13	Total 13	O 13	0	0
5	B	88	Total 88	O 88	0	0
5	C	54	Total 54	O 54	0	0
5	F	13	Total 13	O 13	0	0
5	E	26	Total 26	O 26	0	0

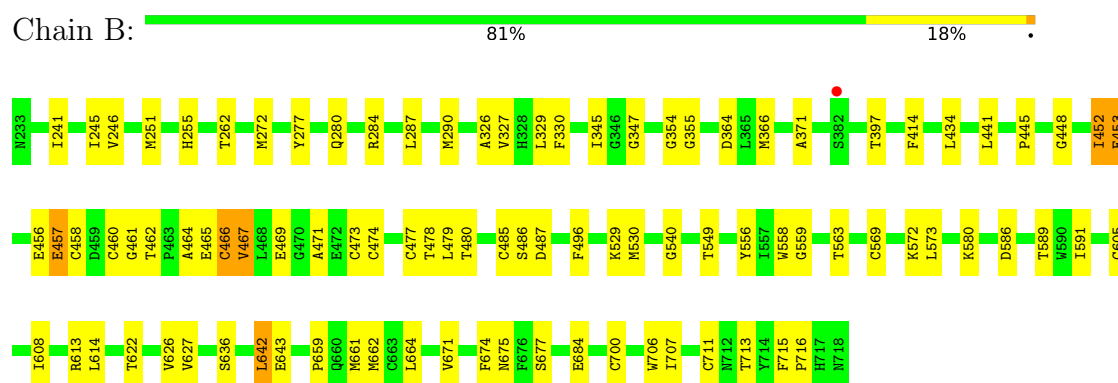
3 Residue-property plots [i](#)

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

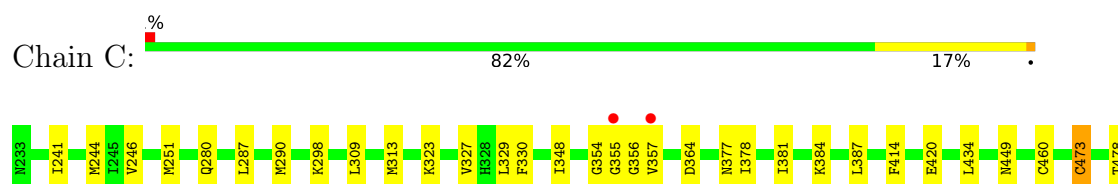
- Molecule 1: Disintegrin and metalloproteinase domain-containing protein 22

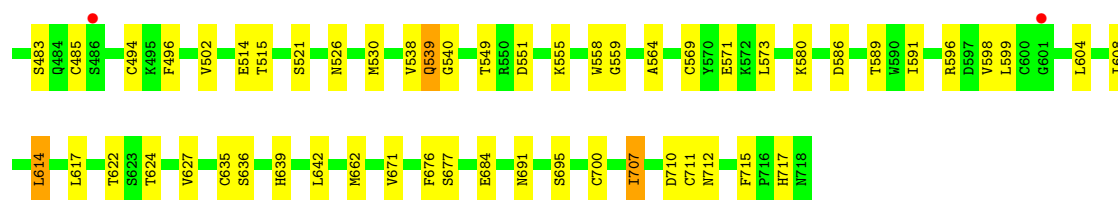


- Molecule 1: Disintegrin and metalloproteinase domain-containing protein 22

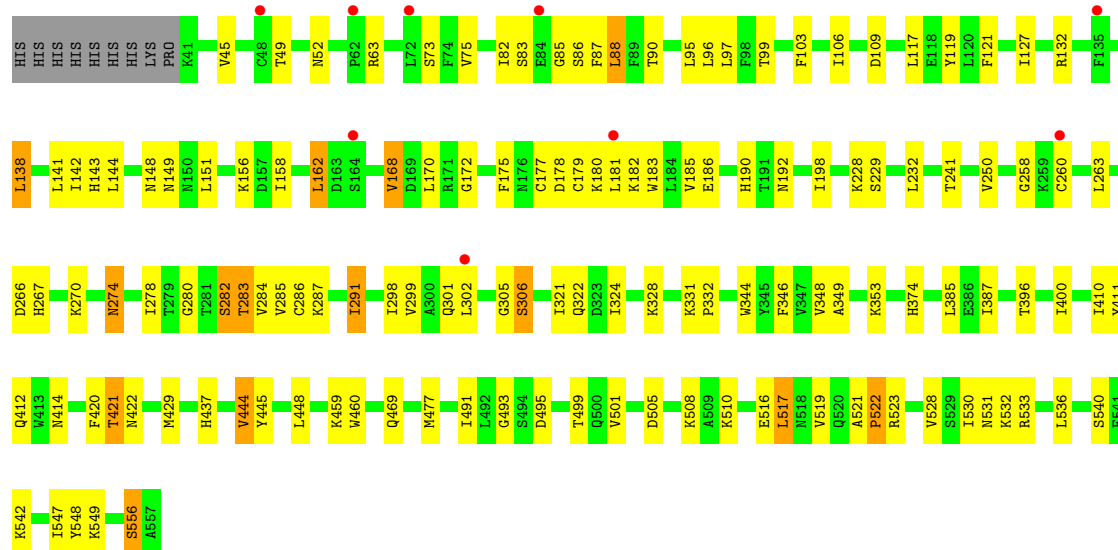


- Molecule 1: Disintegrin and metalloproteinase domain-containing protein 22

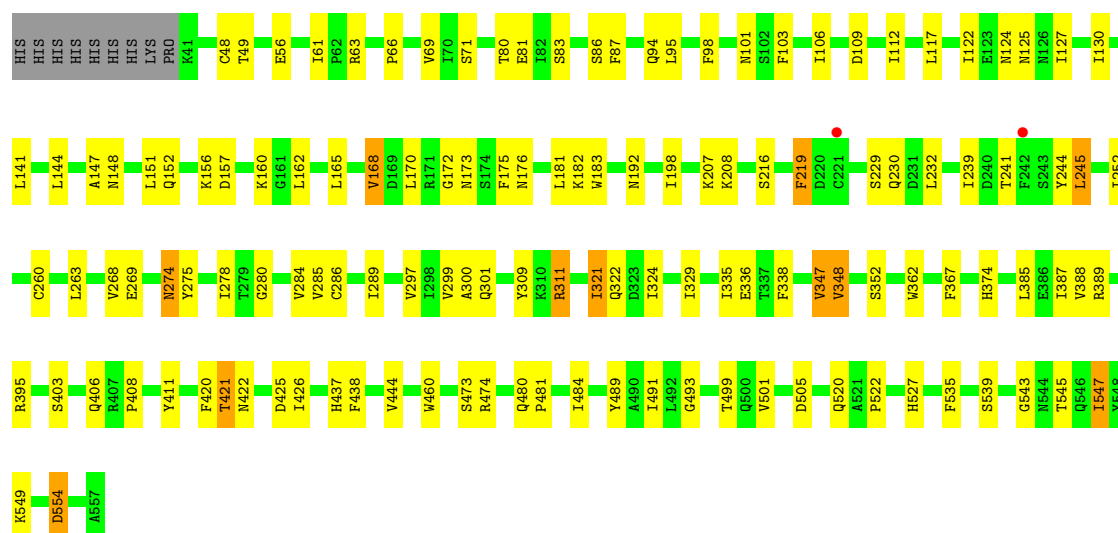




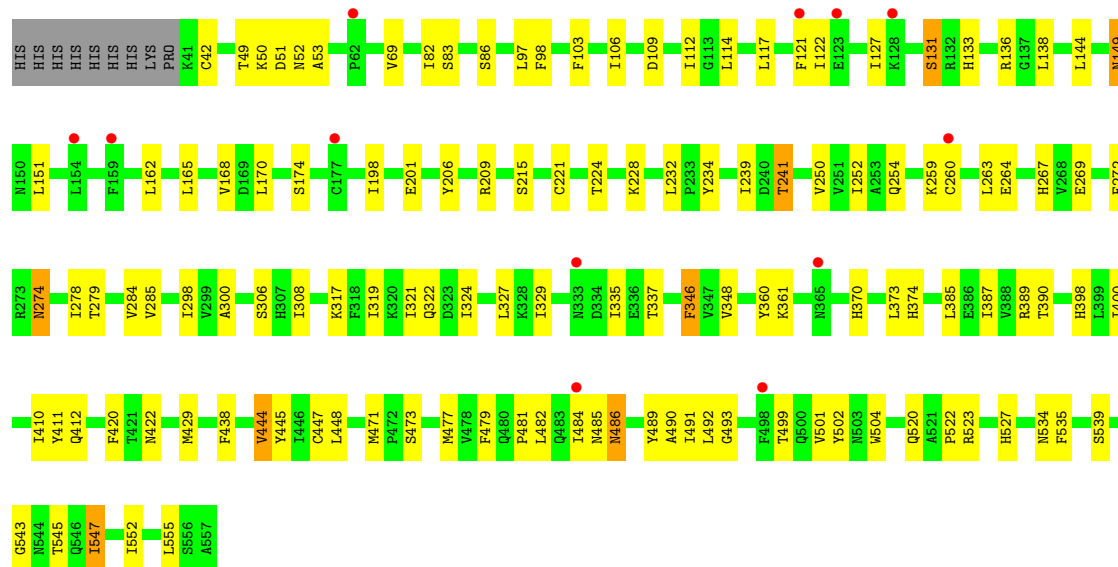
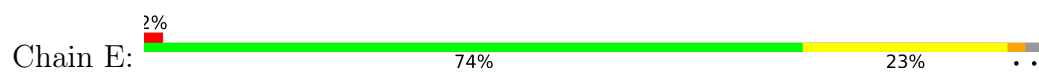
• Molecule 2: Leucine-rich glioma-inactivated protein 1



• Molecule 2: Leucine-rich glioma-inactivated protein 1



• Molecule 2: Leucine-rich glioma-inactivated protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.45Å 196.08Å 420.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.46 – 3.49 42.46 – 3.49	Depositor EDS
% Data completeness (in resolution range)	96.8 (42.46-3.49) 97.0 (42.46-3.49)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.29 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.236 , 0.277 0.235 , 0.273	Depositor DCC
R_{free} test set	2894 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	81.9	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 57.4	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	0.91	EDS
Total number of atoms	24226	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: CA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.17	0/3792	0.41	0/5105
1	B	0.29	0/3792	0.54	0/5105
1	C	0.25	0/3792	0.48	1/5105 (0.0%)
2	D	0.23	0/4301	0.46	0/5836
2	E	0.17	0/4301	0.39	0/5836
2	F	0.14	0/4301	0.36	0/5836
All	All	0.21	0/24279	0.44	1/32823 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	539	GLN	N-CA-C	-7.86	103.19	114.12

There are no chirality outliers.

There are no planarity outliers.

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	3728	0	3579	76	0
1	B	3728	0	3580	63	0
1	C	3728	0	3579	54	0
2	D	4194	0	4110	98	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	4194	0	4111	76	0
2	F	4194	0	4110	74	0
3	A	42	0	39	3	0
3	B	42	0	39	7	0
3	C	42	0	39	0	0
3	D	42	0	39	4	0
3	E	42	0	39	7	0
3	F	42	0	39	2	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	2	0	0	2	0
5	B	88	0	0	3	0
5	C	54	0	0	2	0
5	D	13	0	0	0	0
5	E	26	0	0	1	0
5	F	13	0	0	0	0
All	All	24226	0	23303	451	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 10.

All (451) 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:715:PHE:CD2	1:A:716:PRO:HD2	1.74	1.21
1:A:664:LEU:HD23	1:A:665:GLU:CG	1.84	1.07
1:A:664:LEU:CD2	1:A:665:GLU:HG2	1.90	1.02
1:A:664:LEU:HD23	1:A:665:GLU:HG2	1.05	1.01
2:D:477:MET:HG3	2:D:523:ARG:NH1	1.78	0.97
2:D:148:ASN:ND2	2:D:172:GLY:HA3	1.82	0.94
2:E:389:ARG:NH2	3:E:603:NAG:H82	1.81	0.93
3:B:803:NAG:H83	3:B:803:NAG:H3	1.53	0.90
1:B:458:CYS:SG	1:B:486:SER:HB3	2.11	0.90
2:E:52:ASN:HD22	2:E:53:ALA:N	1.70	0.90
1:A:705:HIS:CE1	1:A:718:ASN:O	2.25	0.88
3:D:601:NAG:H82	3:D:601:NAG:C1	2.03	0.88
1:A:718:ASN:O	1:A:718:ASN:ND2	2.08	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:501:VAL:HG23	2:D:517:LEU:HD13	1.57	0.85
1:A:441:LEU:HD23	1:A:453:GLU:OE2	1.77	0.85
1:A:715:PHE:CG	1:A:716:PRO:HD2	2.13	0.84
2:E:228:LYS:HG3	5:E:708:HOH:O	1.78	0.83
2:E:398:HIS:CD2	2:E:412:GLN:HG2	2.14	0.83
2:E:389:ARG:CZ	3:E:603:NAG:H82	2.08	0.83
2:D:521:ALA:O	2:D:540:SER:HA	1.81	0.81
1:B:706:TRP:CE3	1:B:713:THR:O	2.34	0.80
2:E:484:ILE:CG2	2:E:489:TYR:HE2	1.94	0.80
1:B:467:VAL:HA	1:B:471:ALA:HB2	1.63	0.80
2:F:101:ASN:H	2:F:125:ASN:HD22	1.28	0.79
1:C:580:LYS:HA	1:C:622:THR:HG21	1.64	0.78
3:D:601:NAG:C1	3:D:601:NAG:C8	2.61	0.77
1:A:715:PHE:CD2	1:A:716:PRO:CD	2.64	0.77
1:A:715:PHE:CE2	1:A:716:PRO:HD2	2.20	0.77
2:F:321:ILE:HG22	2:F:322:GLN:HG3	1.67	0.76
2:E:52:ASN:HD22	2:E:53:ALA:H	1.33	0.75
1:A:715:PHE:CG	1:A:716:PRO:CD	2.70	0.75
2:D:228:LYS:HA	2:D:548:TYR:HA	1.67	0.75
2:D:412:GLN:HB3	2:D:422:ASN:HB3	1.68	0.74
2:D:517:LEU:N	2:D:517:LEU:HD12	2.04	0.73
2:E:520:GLN:HG3	2:E:543:GLY:HA3	1.71	0.73
1:B:605:CYS:HB2	1:B:608:ILE:HD11	1.71	0.72
1:C:280:GLN:HE22	1:C:414:PHE:H	1.37	0.72
1:A:605:CYS:HB2	1:A:608:ILE:HD11	1.71	0.72
1:B:706:TRP:HE3	1:B:713:THR:O	1.72	0.72
2:F:192:ASN:HB3	3:F:601:NAG:N2	2.04	0.72
1:C:251:MET:HE3	1:C:330:PHE:HB3	1.70	0.72
1:C:280:GLN:NE2	1:C:414:PHE:H	1.89	0.71
2:F:520:GLN:HG3	2:F:543:GLY:HA3	1.71	0.71
2:E:174:SER:HA	2:E:201:GLU:HG3	1.74	0.70
1:B:251:MET:HE3	1:B:330:PHE:HB3	1.74	0.69
2:F:535:PHE:HB3	2:F:547:ILE:HD11	1.73	0.69
2:D:148:ASN:HD22	2:D:172:GLY:HA3	1.59	0.68
2:D:477:MET:CG	2:D:523:ARG:NH1	2.56	0.68
1:C:280:GLN:HE22	1:C:414:PHE:N	1.92	0.68
1:A:306:LEU:HD13	1:A:643:GLU:HG2	1.76	0.67
2:D:280:GLY:HA3	2:D:301:GLN:NE2	2.10	0.67
2:E:321:ILE:HG22	2:E:322:GLN:HG3	1.75	0.66
2:D:321:ILE:HG22	2:D:322:GLN:HG3	1.76	0.66
2:E:535:PHE:HB3	2:E:547:ILE:HD11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:259:LYS:HG2	2:E:279:THR:HG22	1.76	0.66
2:E:260:CYS:HB3	2:E:278:ILE:HB	1.78	0.66
2:E:284:VAL:HG12	2:E:285:VAL:HG23	1.78	0.66
1:C:715:PHE:HE2	1:C:717:HIS:HB3	1.60	0.66
1:B:458:CYS:SG	1:B:486:SER:CB	2.83	0.65
2:E:484:ILE:CG2	2:E:489:TYR:CE2	2.78	0.65
2:F:232:LEU:HB2	2:F:545:THR:HG23	1.78	0.65
2:E:473:SER:HB3	2:E:492:LEU:HD21	1.79	0.64
1:B:662:MET:HE2	1:B:671:VAL:HG12	1.78	0.64
1:B:675:ASN:OD1	3:B:803:NAG:H82	1.98	0.64
1:C:313:MET:HE2	1:C:354:GLY:H	1.61	0.64
1:C:710:ASP:OD1	1:C:712:ASN:HB2	1.98	0.64
2:D:501:VAL:HG23	2:D:517:LEU:CD1	2.28	0.64
2:D:477:MET:HG3	2:D:523:ARG:CZ	2.27	0.63
2:F:147:ALA:HA	2:F:173:ASN:HD21	1.63	0.63
3:B:803:NAG:H82	3:B:803:NAG:C1	2.29	0.63
1:C:323:LYS:HA	5:C:932:HOH:O	1.98	0.63
1:A:640:VAL:HB	1:A:648:LEU:HB2	1.80	0.63
2:F:207:LYS:HG2	2:F:208:LYS:HG2	1.79	0.62
2:D:536:LEU:HG	2:D:548:TYR:HB2	1.80	0.62
2:E:103:PHE:HB2	2:E:127:ILE:HG12	1.81	0.62
2:D:501:VAL:CG2	2:D:517:LEU:CD1	2.78	0.62
2:E:263:LEU:HA	2:E:274:ASN:HA	1.82	0.62
1:A:278:LYS:HB2	1:A:284:ARG:HH11	1.65	0.62
2:D:148:ASN:HD21	2:D:172:GLY:HA3	1.63	0.61
2:E:232:LEU:HB2	2:E:545:THR:HG23	1.82	0.61
2:E:83:SER:HB3	2:E:86:SER:HB2	1.83	0.61
2:E:387:ILE:HG22	2:E:444:VAL:HG11	1.81	0.61
1:A:622:THR:O	1:A:636:SER:HA	2.00	0.61
1:C:569:CYS:O	1:C:573:LEU:HB2	2.00	0.61
3:E:602:NAG:H3	3:E:602:NAG:H83	1.83	0.60
1:B:280:GLN:HE22	1:B:414:PHE:H	1.50	0.60
1:C:280:GLN:CD	1:C:414:PHE:H	2.09	0.60
1:C:244:MET:HB3	1:C:327:VAL:HG12	1.83	0.60
2:F:156:LYS:HA	2:F:183:TRP:CD1	2.36	0.60
2:F:61:ILE:HG21	2:F:87:PHE:HE1	1.67	0.60
1:B:715:PHE:CD1	1:B:716:PRO:HD2	2.37	0.60
1:C:538:VAL:HG12	1:C:538:VAL:O	2.02	0.60
1:C:662:MET:HE2	1:C:671:VAL:HG12	1.84	0.60
1:C:715:PHE:CE2	1:C:717:HIS:HB3	2.36	0.60
1:A:361:GLY:H	1:A:366:MET:HE2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:485:ASN:C	2:E:486:ASN:CG	2.69	0.59
3:B:803:NAG:H3	3:B:803:NAG:C8	2.29	0.59
1:B:441:LEU:HB2	1:B:453:GLU:OE2	2.02	0.59
1:A:453:GLU:O	1:A:456:GLU:HG2	2.03	0.59
1:B:675:ASN:CG	3:B:803:NAG:H82	2.28	0.59
1:C:573:LEU:HD21	1:C:624:THR:HB	1.85	0.59
2:E:206:TYR:HB3	2:E:209:ARG:HG3	1.83	0.59
2:E:482:LEU:HD23	2:E:527:HIS:HB2	1.85	0.58
2:E:398:HIS:HD2	2:E:412:GLN:HG2	1.65	0.58
2:D:177:CYS:HA	2:D:181:LEU:HD12	1.85	0.58
2:F:324:ILE:HG21	2:F:329:ILE:HD12	1.86	0.58
3:A:803:NAG:H3	3:A:803:NAG:H83	1.85	0.58
2:F:148:ASN:ND2	2:F:172:GLY:HA3	2.19	0.58
2:D:179:CYS:HB3	2:D:556:SER:HA	1.86	0.57
1:C:287:LEU:HD21	1:C:290:MET:HE3	1.85	0.57
1:B:280:GLN:NE2	1:B:414:PHE:H	2.02	0.57
2:D:291:ILE:HD13	2:D:344:TRP:CD1	2.40	0.57
3:A:802:NAG:H83	3:A:802:NAG:H3	1.87	0.56
1:C:558:TRP:CE2	1:C:608:ILE:HD11	2.40	0.56
1:A:557:ILE:HG12	1:A:648:LEU:HD13	1.85	0.56
1:B:457:GLU:OE1	1:B:478:THR:HG23	2.06	0.56
1:B:347:GLY:O	1:B:354:GLY:HA2	2.05	0.56
1:C:502:VAL:HG22	1:C:515:THR:HG22	1.88	0.56
3:B:801:NAG:H83	3:B:801:NAG:H3	1.87	0.56
1:A:502:VAL:HG22	1:A:515:THR:HG22	1.88	0.56
2:F:151:LEU:HB2	2:F:175:PHE:HE1	1.70	0.55
2:F:336:GLU:HB3	2:F:347:VAL:HG23	1.87	0.55
1:B:586:ASP:HB2	1:B:591:ILE:HD11	1.86	0.55
2:D:266:ASP:HB3	2:D:270:LYS:HB2	1.88	0.55
2:E:400:ILE:HG12	2:E:410:ILE:HG12	1.88	0.55
2:D:241:THR:HG21	2:D:528:VAL:HG22	1.89	0.55
2:D:516:GLU:C	2:D:517:LEU:HD12	2.31	0.55
1:B:707:ILE:HG22	1:B:707:ILE:O	2.07	0.55
2:F:83:SER:HB3	2:F:86:SER:HB2	1.87	0.55
2:E:484:ILE:HD11	2:E:534:ASN:CB	2.37	0.55
2:F:493:GLY:HA2	2:F:499:THR:HG23	1.88	0.55
2:E:109:ASP:HB3	2:E:112:ILE:HD13	1.89	0.55
2:E:300:ALA:HB2	2:E:335:ILE:HD11	1.88	0.55
1:C:313:MET:HE2	1:C:354:GLY:N	2.20	0.55
1:A:287:LEU:HD21	1:A:290:MET:HE3	1.88	0.55
2:D:95:LEU:HD13	2:D:119:TYR:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:284:VAL:HG12	2:D:285:VAL:HG23	1.89	0.55
2:F:109:ASP:HB3	2:F:112:ILE:HD13	1.88	0.55
2:E:239:ILE:HG12	2:E:252:ILE:HG12	1.89	0.54
2:E:493:GLY:HA2	2:E:499:THR:HG23	1.88	0.54
2:D:282:SER:O	2:D:301:GLN:HA	2.08	0.54
2:F:98:PHE:HD2	2:F:122:ILE:HG12	1.71	0.54
2:E:114:LEU:HB3	2:E:117:LEU:HB2	1.89	0.54
3:E:601:NAG:H83	3:E:601:NAG:H3	1.88	0.54
2:F:263:LEU:HA	2:F:274:ASN:HA	1.89	0.54
2:E:484:ILE:HD11	2:E:534:ASN:HB3	1.90	0.54
2:F:141:LEU:HD21	2:F:144:LEU:HB2	1.89	0.54
1:A:453:GLU:HB2	5:A:901:HOH:O	2.07	0.54
2:D:49:THR:HG22	2:D:52:ASN:HB2	1.89	0.54
1:C:614:LEU:HD21	1:C:642:LEU:HD11	1.90	0.54
2:E:82:ILE:HG21	2:E:106:ILE:HG23	1.90	0.54
2:F:232:LEU:HD11	2:F:547:ILE:HG22	1.90	0.53
1:A:656:PRO:HA	1:A:662:MET:HA	1.90	0.53
2:F:297:VAL:HG22	2:F:309:TYR:HB2	1.90	0.53
1:A:245:ILE:HB	1:A:290:MET:HE2	1.89	0.53
1:C:381:ILE:HD12	1:C:614:LEU:HB2	1.91	0.53
2:D:332:PRO:HA	2:D:349:ALA:O	2.09	0.53
1:A:664:LEU:CD2	1:A:665:GLU:CG	2.67	0.53
1:C:700:CYS:HB3	1:C:711:CYS:SG	2.48	0.53
2:E:491:ILE:HG23	2:E:501:VAL:HG22	1.91	0.53
1:C:586:ASP:HB2	1:C:591:ILE:HD11	1.89	0.53
1:A:244:MET:HB3	1:A:327:VAL:HG22	1.91	0.53
2:F:157:ASP:HB3	2:F:160:LYS:HB3	1.90	0.53
2:F:480:GLN:HE21	2:F:481:PRO:HD2	1.74	0.53
2:E:221:CYS:HB3	2:E:555:LEU:HB2	1.91	0.53
1:C:710:ASP:OD1	1:C:712:ASN:CB	2.57	0.52
2:D:83:SER:HB3	2:D:86:SER:HB2	1.90	0.52
2:D:501:VAL:CG2	2:D:517:LEU:HD11	2.39	0.52
2:F:411:TYR:HB3	2:F:420:PHE:HB3	1.91	0.52
2:F:522:PRO:HA	2:F:539:SER:O	2.09	0.52
1:A:550:ARG:NH2	1:A:599:LEU:HD23	2.23	0.52
2:F:192:ASN:HB3	3:F:601:NAG:C7	2.39	0.52
2:D:422:ASN:HB2	3:D:601:NAG:N2	2.25	0.52
3:B:803:NAG:C1	3:B:803:NAG:C8	2.88	0.52
1:C:662:MET:HE1	1:C:676:PHE:HE2	1.75	0.52
2:E:144:LEU:O	2:E:168:VAL:HA	2.09	0.52
2:D:469:GLN:HG3	2:D:510:LYS:HE3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:490:ALA:HB3	2:E:502:TYR:HB2	1.91	0.52
1:A:467:VAL:HA	1:A:471:ALA:HB2	1.91	0.51
2:D:400:ILE:HG12	2:D:410:ILE:HG12	1.92	0.51
2:F:385:LEU:HD11	2:F:444:VAL:HG11	1.93	0.51
2:D:517:LEU:N	2:D:517:LEU:CD1	2.73	0.51
1:C:614:LEU:HG	1:C:642:LEU:HD21	1.91	0.51
2:F:106:ILE:HB	2:F:130:ILE:HG13	1.92	0.51
1:A:384:LYS:HG3	1:A:613:ARG:HG3	1.92	0.51
2:F:300:ALA:HB2	2:F:335:ILE:HD11	1.93	0.51
2:D:142:ILE:HG13	2:D:143:HIS:H	1.75	0.51
2:F:182:LYS:HG2	2:F:219:PHE:CE1	2.46	0.51
2:F:260:CYS:HB3	2:F:278:ILE:HB	1.93	0.51
1:B:287:LEU:HD21	1:B:290:MET:HE3	1.92	0.51
2:F:170:LEU:HB2	2:F:198:ILE:HG21	1.92	0.51
2:E:485:ASN:O	2:E:486:ASN:CG	2.54	0.50
2:D:156:LYS:HA	2:D:183:TRP:CE2	2.45	0.50
1:B:485:CYS:HB3	1:B:496:PHE:CE1	2.46	0.50
2:D:283:THR:HA	2:D:301:GLN:HG2	1.94	0.50
2:D:493:GLY:HA2	2:D:499:THR:HG23	1.94	0.50
2:E:484:ILE:HG22	2:E:489:TYR:CE2	2.46	0.50
1:B:241:ILE:HG12	1:B:434:LEU:HD22	1.93	0.50
1:C:348:ILE:HG12	1:C:434:LEU:HD11	1.92	0.50
1:C:691:ASN:HB2	1:C:711:CYS:O	2.11	0.50
2:E:385:LEU:HD21	2:E:400:ILE:HD12	1.92	0.50
1:A:276:ILE:HG23	1:A:280:GLN:OE1	2.11	0.50
2:D:117:LEU:HD23	2:D:138:LEU:HD13	1.94	0.50
2:D:414:ASN:HB2	2:D:421:THR:HG22	1.93	0.50
1:B:589:THR:HA	5:B:943:HOH:O	2.11	0.50
2:E:484:ILE:HG23	2:E:484:ILE:O	2.11	0.50
1:A:570:TYR:OH	1:A:604:LEU:O	2.22	0.50
2:D:103:PHE:HB2	2:D:127:ILE:HG12	1.94	0.50
2:F:152:GLN:HA	2:F:175:PHE:HA	1.94	0.50
2:F:338:PHE:HE1	2:F:347:VAL:HG22	1.76	0.49
2:E:324:ILE:HG21	2:E:329:ILE:HD12	1.93	0.49
2:D:180:LYS:O	2:D:183:TRP:CD1	2.65	0.49
2:F:165:LEU:HD21	2:F:168:VAL:HG23	1.95	0.49
1:A:453:GLU:O	1:A:456:GLU:CG	2.60	0.49
1:B:580:LYS:HA	1:B:622:THR:HG21	1.95	0.49
2:F:491:ILE:HG23	2:F:501:VAL:HG22	1.94	0.49
2:D:306:SER:HB3	2:D:324:ILE:HB	1.94	0.49
2:E:224:THR:HG22	2:E:552:ILE:HG12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:ALA:O	1:A:526:ASN:HB3	2.12	0.49
2:D:530:ILE:HB	2:D:533:ARG:HB2	1.94	0.49
2:F:144:LEU:O	2:F:168:VAL:HA	2.12	0.49
2:F:480:GLN:NE2	2:F:481:PRO:HD2	2.28	0.49
1:A:485:CYS:HB3	1:A:496:PHE:CE1	2.48	0.49
1:A:551:ASP:HA	1:A:564:ALA:HB2	1.94	0.49
1:B:462:THR:HB	1:B:465:GLU:HB3	1.93	0.49
1:A:332:GLY:HA2	1:A:360:PHE:HB2	1.95	0.49
3:D:601:NAG:H3	3:D:601:NAG:H83	1.94	0.49
1:B:280:GLN:CD	1:B:414:PHE:H	2.20	0.49
2:E:522:PRO:HA	2:E:539:SER:O	2.13	0.49
1:B:462:THR:HG22	1:B:464:ALA:N	2.28	0.48
2:F:103:PHE:HB2	2:F:127:ILE:HG12	1.94	0.48
2:D:141:LEU:HD21	2:D:144:LEU:HB2	1.95	0.48
2:D:181:LEU:O	2:D:185:VAL:HG23	2.14	0.48
1:B:530:MET:HE3	1:B:530:MET:HB2	1.69	0.48
1:B:700:CYS:HB3	1:B:711:CYS:SG	2.53	0.48
1:A:473:CYS:HB3	1:A:483:SER:HB2	1.96	0.48
1:A:598:VAL:HG12	1:A:599:LEU:HD12	1.95	0.48
1:B:466:CYS:O	1:B:469:GLU:O	2.30	0.48
1:B:572:LYS:HD3	1:B:626:VAL:HG13	1.95	0.48
2:D:82:ILE:HG21	2:D:106:ILE:HG23	1.95	0.48
2:D:501:VAL:HG21	2:D:517:LEU:HD11	1.95	0.48
2:D:170:LEU:HB2	2:D:198:ILE:HG21	1.96	0.48
2:E:149:ASN:OD1	2:E:151:LEU:HG	2.14	0.48
2:D:149:ASN:OD1	2:D:151:LEU:HG	2.14	0.48
2:E:51:ASP:HA	2:E:69:VAL:HA	1.95	0.48
2:D:429:MET:HE1	2:D:448:LEU:HD13	1.96	0.48
1:B:452:ILE:O	1:B:452:ILE:HG13	2.11	0.47
2:E:373:LEU:HD22	2:E:411:TYR:CE2	2.49	0.47
2:F:335:ILE:HG12	2:F:348:VAL:HG13	1.97	0.47
2:E:274:ASN:OD1	3:E:602:NAG:H82	2.14	0.47
1:A:485:CYS:HB2	1:A:521:SER:HB3	1.96	0.47
2:D:421:THR:HG23	2:D:422:ASN:H	1.80	0.47
1:B:280:GLN:HE22	1:B:414:PHE:N	2.09	0.47
1:C:384:LYS:HA	1:C:387:LEU:HG	1.97	0.47
1:A:573:LEU:HD11	1:A:624:THR:HG21	1.96	0.47
2:D:229:SER:HB3	2:D:549:LYS:HB2	1.96	0.47
1:B:559:GLY:HA2	1:B:613:ARG:HD2	1.96	0.47
1:B:664:LEU:HB2	1:B:674:PHE:HE1	1.79	0.47
1:A:574:ASN:CG	1:A:598:VAL:HG22	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:MET:HE2	1:A:671:VAL:HG12	1.96	0.47
2:D:385:LEU:HG	2:D:387:ILE:HG23	1.95	0.47
2:D:385:LEU:HD13	2:D:437:HIS:CG	2.49	0.47
1:C:604:LEU:HD23	1:C:635:CYS:HB3	1.96	0.47
2:E:389:ARG:HD2	2:E:412:GLN:OE1	2.14	0.47
1:C:707:ILE:HG13	1:C:715:PHE:HB3	1.96	0.47
1:C:355:GLY:HA2	1:C:377:ASN:OD1	2.15	0.47
2:F:286:CYS:SG	2:F:299:VAL:HG12	2.55	0.47
1:B:558:TRP:CG	1:B:608:ILE:HD12	2.49	0.47
2:F:554:ASP:N	2:F:554:ASP:OD1	2.47	0.47
2:E:361:LYS:H	2:E:370:HIS:HB2	1.80	0.47
1:B:664:LEU:HB2	1:B:674:PHE:CE1	2.50	0.46
1:B:569:CYS:O	1:B:573:LEU:HB2	2.15	0.46
1:A:599:LEU:O	1:A:651:VAL:HG21	2.16	0.46
2:D:298:ILE:HG21	2:D:346:PHE:CZ	2.50	0.46
1:B:458:CYS:C	1:B:474:CYS:SG	2.99	0.46
2:D:97:LEU:HA	2:D:121:PHE:O	2.16	0.46
2:D:444:VAL:HG23	2:D:460:TRP:HB3	1.98	0.46
1:B:448:GLY:C	1:B:461:GLY:HA2	2.41	0.46
1:C:514:GLU:OE1	1:C:526:ASN:HA	2.15	0.46
1:C:598:VAL:HG12	1:C:599:LEU:HD12	1.98	0.46
2:D:258:GLY:HA2	2:D:283:THR:OG1	2.16	0.46
2:F:389:ARG:HH12	2:F:422:ASN:HD22	1.62	0.46
2:E:98:PHE:HD1	2:E:122:ILE:HG12	1.81	0.46
1:C:571:GLU:HA	1:C:598:VAL:HG11	1.98	0.46
2:E:438:PHE:HB3	2:E:481:PRO:HB2	1.97	0.46
2:D:241:THR:HG22	2:D:250:VAL:HG22	1.97	0.45
1:B:245:ILE:HB	1:B:290:MET:HE2	1.98	0.45
1:B:622:THR:O	1:B:636:SER:HA	2.16	0.45
2:F:63:ARG:NH2	2:F:86:SER:HA	2.31	0.45
2:F:362:TRP:HB2	2:F:367:PHE:CE1	2.52	0.45
1:A:264:THR:HA	1:A:267:LYS:HE3	1.99	0.45
1:A:458:CYS:HB2	1:A:486:SER:HB3	1.98	0.45
2:D:232:LEU:HD11	2:D:547:ILE:HD11	1.98	0.45
1:C:473:CYS:HB3	1:C:483:SER:HB2	1.99	0.45
1:C:485:CYS:HB3	1:C:496:PHE:CE1	2.51	0.45
2:D:182:LYS:O	2:D:186:GLU:HG2	2.16	0.45
1:B:462:THR:HB	1:B:465:GLU:CB	2.47	0.45
1:C:241:ILE:HD11	1:C:378:ILE:HD12	1.99	0.45
1:A:444:PRO:HA	1:A:445:PRO:HD3	1.89	0.45
1:C:530:MET:HE1	1:C:677:SER:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:148:ASN:N	2:F:148:ASN:HD22	2.13	0.45
1:A:281:LEU:HD23	1:A:419:ILE:HD13	1.98	0.45
2:F:124:ASN:ND2	2:F:148:ASN:HB2	2.32	0.45
2:D:477:MET:HB2	2:D:523:ARG:HH11	1.82	0.45
1:A:627:VAL:HA	1:A:631:ARG:O	2.17	0.45
2:F:98:PHE:HB2	2:F:122:ILE:HG23	1.99	0.45
2:E:97:LEU:HA	2:E:121:PHE:O	2.16	0.44
1:A:562:VAL:HG22	1:A:607:ASN:O	2.17	0.44
2:D:491:ILE:HG23	2:D:501:VAL:HG22	2.00	0.44
1:A:576:GLU:HB3	1:A:578:THR:HG23	1.99	0.44
1:A:634:ASN:HB2	3:A:802:NAG:N2	2.32	0.44
1:B:458:CYS:HB2	1:B:479:LEU:HG	1.99	0.44
2:F:230:GLN:H	2:F:547:ILE:HG23	1.81	0.44
2:E:49:THR:OG1	2:E:50:LYS:N	2.51	0.44
2:E:317:LYS:HE3	2:E:319:ILE:HD11	1.99	0.44
2:D:87:PHE:CE2	2:D:96:LEU:HD21	2.52	0.44
2:D:411:TYR:HB3	2:D:420:PHE:HB3	1.99	0.44
1:B:572:LYS:HE3	5:B:961:HOH:O	2.18	0.44
1:C:485:CYS:O	1:C:494:CYS:HA	2.17	0.44
2:D:387:ILE:HG22	2:D:444:VAL:HG21	1.99	0.44
1:B:272:MET:HE1	1:B:364:ASP:HB3	1.98	0.44
1:B:467:VAL:HA	1:B:471:ALA:CB	2.42	0.44
2:F:239:ILE:HG12	2:F:252:ILE:HG12	1.99	0.44
2:E:241:THR:HB	2:E:250:VAL:HG12	1.99	0.44
2:D:495:ASP:OD1	2:D:522:PRO:HD2	2.17	0.44
2:E:306:SER:HB2	2:E:324:ILE:HB	1.99	0.44
1:A:278:LYS:HD2	1:A:284:ARG:NH1	2.32	0.44
2:F:80:THR:HG22	2:F:81:GLU:HG2	1.99	0.44
2:E:411:TYR:HB3	2:E:420:PHE:HB3	1.99	0.44
2:F:244:TYR:CD2	2:F:245:LEU:HD23	2.53	0.44
2:E:485:ASN:O	2:E:486:ASN:ND2	2.51	0.43
1:A:309:LEU:HD13	1:A:356:GLY:HA2	2.00	0.43
2:F:66:PRO:HB2	2:F:69:VAL:HG23	2.01	0.43
2:D:258:GLY:HA2	2:D:283:THR:HG1	1.82	0.43
2:D:301:GLN:H	2:D:305:GLY:HA3	1.83	0.43
2:D:306:SER:CB	2:D:324:ILE:HB	2.48	0.43
2:D:521:ALA:HB3	2:D:542:LYS:H	1.83	0.43
2:F:484:ILE:HD11	2:F:489:TYR:HE2	1.82	0.43
1:A:574:ASN:HD22	1:A:593:CYS:CB	2.31	0.43
2:F:388:VAL:HG13	2:F:395:ARG:HG2	1.99	0.43
1:A:340:SER:HA	2:D:353:LYS:HZ1	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:LEU:HD12	1:A:442:LEU:HA	1.91	0.43
1:B:556:TYR:CE2	1:B:614:LEU:HD21	2.53	0.43
2:F:421:THR:HG22	2:F:422:ASN:H	1.83	0.43
1:A:386:LYS:O	1:A:391:GLU:N	2.51	0.43
1:A:453:GLU:CG	5:A:901:HOH:O	2.66	0.43
2:D:519:VAL:HG11	2:D:522:PRO:HB3	2.01	0.43
2:D:530:ILE:HG22	2:D:531:ASN:H	1.83	0.43
1:B:462:THR:HG22	1:B:464:ALA:H	1.82	0.43
1:C:555:LYS:HA	1:C:559:GLY:O	2.19	0.43
2:F:61:ILE:HG21	2:F:87:PHE:CE1	2.51	0.43
2:F:216:SER:HA	2:F:219:PHE:HE1	1.83	0.43
2:F:385:LEU:HD13	2:F:437:HIS:CG	2.52	0.43
2:F:438:PHE:HB3	2:F:481:PRO:HB2	2.01	0.43
1:A:347:GLY:O	1:A:354:GLY:HA2	2.19	0.43
2:D:186:GLU:O	2:D:190:HIS:ND1	2.50	0.43
1:B:458:CYS:O	1:B:477:CYS:HA	2.18	0.43
2:F:403:SER:HB2	2:F:406:GLN:HB3	2.01	0.43
2:E:422:ASN:OD1	3:E:603:NAG:C7	2.66	0.43
2:E:422:ASN:OD1	3:E:603:NAG:N2	2.52	0.43
2:D:144:LEU:O	2:D:168:VAL:HA	2.19	0.43
2:D:162:LEU:H	2:D:162:LEU:HG	1.74	0.43
2:D:445:TYR:CD1	2:D:459:LYS:HA	2.54	0.43
2:E:298:ILE:HG21	2:E:346:PHE:CE1	2.54	0.43
1:A:400:GLY:C	1:A:411:PRO:HB3	2.44	0.42
2:E:133:HIS:O	2:E:136:ARG:HB2	2.19	0.42
1:A:557:ILE:HD13	1:A:648:LEU:HB3	2.00	0.42
1:B:540:GLY:HA3	1:B:549:THR:HG22	2.00	0.42
1:C:539:GLN:OE1	1:C:539:GLN:HA	2.19	0.42
2:E:234:TYR:HB2	2:E:254:GLN:NE2	2.34	0.42
1:A:384:LYS:HG3	1:A:613:ARG:CG	2.49	0.42
1:C:364:ASP:OD1	1:C:364:ASP:N	2.52	0.42
1:A:558:TRP:CG	1:A:608:ILE:HD12	2.54	0.42
2:D:396:THR:HG21	2:D:412:GLN:HE22	1.84	0.42
1:B:277:TYR:OH	1:B:371:ALA:O	2.33	0.42
1:B:326:ALA:HA	1:B:354:GLY:O	2.20	0.42
1:B:453:GLU:O	1:B:456:GLU:HB2	2.20	0.42
1:C:530:MET:HB3	1:C:695:SER:O	2.19	0.42
2:F:124:ASN:HD22	2:F:148:ASN:HB2	1.84	0.42
2:F:275:TYR:HE2	2:F:311:ARG:HH11	1.66	0.42
2:E:165:LEU:HD12	2:E:165:LEU:HA	1.91	0.42
2:E:445:TYR:HE2	2:E:504:TRP:CH2	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:63:ARG:NH2	2:D:86:SER:HA	2.34	0.42
1:C:530:MET:HB2	1:C:530:MET:HE3	1.71	0.42
2:D:75:VAL:HG13	2:D:99:THR:HG23	2.00	0.42
2:D:302:LEU:HD23	2:D:331:LYS:NZ	2.35	0.42
2:D:499:THR:HB	2:D:517:LEU:O	2.19	0.42
2:D:385:LEU:HD13	2:D:437:HIS:ND1	2.34	0.42
2:D:505:ASP:HB3	2:D:508:LYS:HB2	2.01	0.42
2:F:284:VAL:HG12	2:F:285:VAL:HG23	2.02	0.42
2:E:346:PHE:CD2	2:E:360:TYR:HB2	2.54	0.42
2:E:114:LEU:HD13	2:E:117:LEU:HD22	2.02	0.42
2:E:429:MET:HE3	2:E:448:LEU:HD22	2.02	0.42
1:A:340:SER:HA	2:D:353:LYS:NZ	2.35	0.42
2:D:178:ASP:OD2	2:D:180:LYS:HG2	2.19	0.42
1:B:445:PRO:HB3	1:B:453:GLU:HB3	2.02	0.42
2:E:477:MET:HG3	2:E:523:ARG:CZ	2.49	0.42
2:F:387:ILE:HD12	2:F:460:TRP:CE2	2.55	0.41
2:E:170:LEU:HB2	2:E:198:ILE:HG21	2.02	0.41
1:B:290:MET:HE3	1:B:290:MET:HB2	1.91	0.41
1:B:530:MET:HE1	1:B:677:SER:O	2.19	0.41
2:E:106:ILE:O	2:E:131:SER:HB2	2.20	0.41
1:C:309:LEU:HD13	1:C:356:GLY:HA2	2.01	0.41
2:F:408:PRO:HB2	2:F:426:ILE:HD12	2.02	0.41
1:B:327:VAL:O	1:B:355:GLY:HA3	2.21	0.41
1:B:529:LYS:NZ	5:B:905:HOH:O	2.52	0.41
2:F:229:SER:HB2	2:F:549:LYS:HG3	2.02	0.41
1:A:485:CYS:HB3	1:A:496:PHE:HE1	1.83	0.41
1:A:530:MET:HE2	1:A:530:MET:HB3	1.96	0.41
1:C:540:GLY:HA3	1:C:549:THR:HG22	2.02	0.41
2:E:447:CYS:HB3	2:E:479:PHE:CD2	2.56	0.41
1:A:251:MET:HE3	1:A:330:PHE:HB3	2.01	0.41
2:D:88:LEU:C	2:D:90:THR:H	2.29	0.41
2:D:328:LYS:HD3	2:D:328:LYS:HA	1.90	0.41
1:C:246:VAL:O	1:C:329:LEU:HD12	2.21	0.41
1:A:265:TYR:HE2	1:A:366:MET:HE3	1.84	0.41
1:A:558:TRP:CB	1:A:562:VAL:HG21	2.50	0.41
1:C:622:THR:O	1:C:636:SER:HA	2.21	0.41
1:A:250:LEU:HD22	1:A:333:SER:HB3	2.03	0.41
1:A:251:MET:HE2	1:A:251:MET:HB2	1.96	0.41
1:A:459:ASP:OD1	1:A:460:CYS:N	2.54	0.41
2:D:285:VAL:HG12	2:D:287:LYS:HG2	2.02	0.41
1:B:246:VAL:O	1:B:329:LEU:HD12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:HIS:ND1	1:B:262:THR:HG22	2.36	0.41
1:C:551:ASP:HA	1:C:564:ALA:HB2	2.03	0.41
1:C:662:MET:HE1	1:C:676:PHE:CE2	2.54	0.41
2:F:182:LYS:HD3	2:F:182:LYS:C	2.46	0.41
1:A:441:LEU:H	1:A:453:GLU:CD	2.29	0.41
2:D:263:LEU:HA	2:D:274:ASN:HA	2.03	0.41
2:D:532:LYS:HD3	2:D:532:LYS:HA	1.91	0.41
2:F:94:GLN:HA	2:F:117:LEU:HA	2.03	0.41
2:F:280:GLY:HA3	2:F:301:GLN:NE2	2.36	0.41
1:A:527:ILE:HG23	1:A:695:SER:HB2	2.01	0.40
2:D:477:MET:HB2	2:D:523:ARG:NH1	2.35	0.40
1:C:449:ASN:ND2	5:C:906:HOH:O	2.51	0.40
2:F:484:ILE:HG22	2:F:527:HIS:CE1	2.55	0.40
2:E:263:LEU:HD13	2:E:272:PHE:HB3	2.03	0.40
1:A:601:GLY:O	1:A:651:VAL:HG23	2.22	0.40
2:D:73:SER:HB3	2:D:97:LEU:HG	2.02	0.40
2:D:260:CYS:HB3	2:D:278:ILE:HB	2.03	0.40
2:D:85:GLY:HA2	2:D:109:ASP:O	2.20	0.40
2:D:132:ARG:O	2:D:158:ILE:HD12	2.20	0.40
1:B:659:PRO:O	1:B:661:MET:HG2	2.21	0.40
2:F:124:ASN:HD22	2:F:124:ASN:N	2.20	0.40
2:D:286:CYS:SG	2:D:299:VAL:HG12	2.62	0.40
1:C:617:LEU:HD12	1:C:639:HIS:O	2.22	0.40
2:E:346:PHE:HD2	2:E:360:TYR:HB2	1.85	0.40
1:A:377:ASN:HD22	1:A:377:ASN:HA	1.73	0.40
1:B:345:ILE:HD13	1:B:642:LEU:HD21	2.04	0.40
1:B:469:GLU:OE2	1:B:487:ASP:HB2	2.22	0.40
2:F:71:SER:HB2	2:F:95:LEU:HD23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	484/486 (100%)	469 (97%)	15 (3%)	0	100	100
1	B	484/486 (100%)	469 (97%)	15 (3%)	0	100	100
1	C	484/486 (100%)	475 (98%)	9 (2%)	0	100	100
2	D	515/526 (98%)	488 (95%)	26 (5%)	1 (0%)	43	74
2	E	515/526 (98%)	491 (95%)	24 (5%)	0	100	100
2	F	515/526 (98%)	497 (96%)	18 (4%)	0	100	100
All	All	2997/3036 (99%)	2889 (96%)	107 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	522	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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	420/420 (100%)	416 (99%)	4 (1%)	68	75
1	B	420/420 (100%)	404 (96%)	16 (4%)	29	55
1	C	420/420 (100%)	407 (97%)	13 (3%)	35	59
2	D	474/483 (98%)	455 (96%)	19 (4%)	28	54
2	E	474/483 (98%)	452 (95%)	22 (5%)	24	50
2	F	474/483 (98%)	447 (94%)	27 (6%)	18	45
All	All	2682/2709 (99%)	2581 (96%)	101 (4%)	29	55

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	376	HIS
1	A	460	CYS
1	A	473	CYS
1	A	627	VAL

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Mol	Chain	Res	Type
2	D	45	VAL
2	D	88	LEU
2	D	138	LEU
2	D	162	LEU
2	D	168	VAL
2	D	175	PHE
2	D	192	ASN
2	D	267	HIS
2	D	274	ASN
2	D	282	SER
2	D	283	THR
2	D	291	ILE
2	D	306	SER
2	D	348	VAL
2	D	374	HIS
2	D	421	THR
2	D	444	VAL
2	D	517	LEU
2	D	556	SER
1	B	284	ARG
1	B	366	MET
1	B	397	THR
1	B	452	ILE
1	B	453	GLU
1	B	457	GLU
1	B	460	CYS
1	B	466	CYS
1	B	467	VAL
1	B	473	CYS
1	B	480	THR
1	B	563	THR
1	B	627	VAL
1	B	642	LEU
1	B	643	GLU
1	B	684	GLU
1	C	298	LYS
1	C	357	VAL
1	C	420	GLU
1	C	460	CYS
1	C	473	CYS
1	C	478	THR
1	C	521	SER

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Mol	Chain	Res	Type
1	C	589	THR
1	C	596	ARG
1	C	614	LEU
1	C	627	VAL
1	C	684	GLU
1	C	707	ILE
2	F	48	CYS
2	F	49	THR
2	F	56	GLU
2	F	162	LEU
2	F	168	VAL
2	F	176	ASN
2	F	181	LEU
2	F	219	PHE
2	F	241	THR
2	F	245	LEU
2	F	268	VAL
2	F	269	GLU
2	F	274	ASN
2	F	289	ILE
2	F	311	ARG
2	F	321	ILE
2	F	347	VAL
2	F	348	VAL
2	F	352	SER
2	F	374	HIS
2	F	421	THR
2	F	425	ASP
2	F	473	SER
2	F	474	ARG
2	F	505	ASP
2	F	547	ILE
2	F	554	ASP
2	E	42	CYS
2	E	131	SER
2	E	138	LEU
2	E	149	ASN
2	E	162	LEU
2	E	215	SER
2	E	241	THR
2	E	264	GLU
2	E	267	HIS

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Mol	Chain	Res	Type
2	E	269	GLU
2	E	274	ASN
2	E	308	ILE
2	E	327	LEU
2	E	337	THR
2	E	346	PHE
2	E	348	VAL
2	E	374	HIS
2	E	390	THR
2	E	444	VAL
2	E	471	MET
2	E	486	ASN
2	E	547	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	255	HIS
1	A	427	ASN
1	A	574	ASN
1	A	594	ASN
1	A	660	GLN
1	A	705	HIS
1	A	718	ASN
2	D	52	ASN
2	D	57	ASN
2	D	143	HIS
2	D	148	ASN
2	D	307	HIS
2	D	333	ASN
2	D	485	ASN
1	B	691	ASN
1	B	718	ASN
1	C	247	ASN
1	C	280	GLN
2	F	124	ASN
2	F	126	ASN
2	F	148	ASN
2	F	150	ASN
2	F	254	GLN
2	F	301	GLN
2	F	333	ASN

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Mol	Chain	Res	Type
2	F	480	GLN
2	F	534	ASN
2	E	52	ASN
2	E	143	HIS
2	E	235	GLN
2	E	267	HIS
2	E	480	GLN
2	E	527	HIS

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 30 ligands modelled in this entry, 12 are monoatomic - leaving 18 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	$\# Z > 2$
3	NAG	B	803	1	14,14,15	0.45	0	17,19,21	0.47	0
3	NAG	B	802	1	14,14,15	0.25	0	17,19,21	0.52	0
3	NAG	B	801	1	14,14,15	0.51	0	17,19,21	1.37	2 (11%)
3	NAG	D	601	2	14,14,15	0.23	0	17,19,21	0.44	0
3	NAG	A	801	1	14,14,15	0.21	0	17,19,21	0.43	0
3	NAG	C	803	1	14,14,15	0.22	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	E	603	2	14,14,15	0.38	0	17,19,21	0.52	0
3	NAG	F	603	2	14,14,15	0.26	0	17,19,21	0.48	0
3	NAG	C	801	1	14,14,15	0.47	0	17,19,21	0.68	1 (5%)
3	NAG	D	602	2	14,14,15	0.19	0	17,19,21	0.41	0
3	NAG	D	603	2	14,14,15	0.22	0	17,19,21	0.45	0
3	NAG	A	802	1	14,14,15	0.84	1 (7%)	17,19,21	1.35	2 (11%)
3	NAG	F	601	2	14,14,15	0.72	1 (7%)	17,19,21	0.80	1 (5%)
3	NAG	E	601	2	14,14,15	0.46	0	17,19,21	1.34	2 (11%)
3	NAG	E	602	2	14,14,15	0.55	0	17,19,21	1.37	2 (11%)
3	NAG	F	602	2	14,14,15	0.41	0	17,19,21	0.47	0
3	NAG	A	803	1	14,14,15	0.88	1 (7%)	17,19,21	1.37	2 (11%)
3	NAG	C	802	1	14,14,15	0.21	0	17,19,21	0.40	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
3	NAG	B	803	1	-	4/6/23/26	0/1/1/1
3	NAG	B	802	1	-	4/6/23/26	0/1/1/1
3	NAG	B	801	1	-	6/6/23/26	0/1/1/1
3	NAG	D	601	2	-	4/6/23/26	0/1/1/1
3	NAG	A	801	1	-	4/6/23/26	0/1/1/1
3	NAG	C	803	1	-	2/6/23/26	0/1/1/1
3	NAG	E	603	2	-	4/6/23/26	0/1/1/1
3	NAG	F	603	2	-	4/6/23/26	0/1/1/1
3	NAG	C	801	1	-	4/6/23/26	0/1/1/1
3	NAG	D	602	2	-	3/6/23/26	0/1/1/1
3	NAG	D	603	2	-	3/6/23/26	0/1/1/1
3	NAG	A	802	1	-	5/6/23/26	0/1/1/1
3	NAG	F	601	2	-	4/6/23/26	0/1/1/1
3	NAG	E	601	2	-	6/6/23/26	0/1/1/1
3	NAG	E	602	2	-	4/6/23/26	0/1/1/1
3	NAG	F	602	2	-	2/6/23/26	0/1/1/1
3	NAG	A	803	1	-	6/6/23/26	0/1/1/1
3	NAG	C	802	1	-	3/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	803	NAG	C1-C2	3.02	1.56	1.52
3	A	802	NAG	C1-C2	2.84	1.56	1.52
3	F	601	NAG	C1-C2	2.39	1.55	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	NAG	C2-N2-C7	4.64	129.11	122.90
3	E	601	NAG	C2-N2-C7	4.64	129.11	122.90
3	B	801	NAG	C2-N2-C7	4.55	129.00	122.90
3	A	803	NAG	C2-N2-C7	4.55	129.00	122.90
3	E	602	NAG	C2-N2-C7	4.47	128.89	122.90
3	F	601	NAG	C1-O5-C5	2.77	115.90	112.19
3	A	802	NAG	C1-C2-N2	2.38	114.19	110.43
3	C	801	NAG	C1-O5-C5	2.26	115.21	112.19
3	E	601	NAG	C1-C2-N2	2.23	113.95	110.43
3	A	803	NAG	C1-C2-N2	2.22	113.94	110.43
3	B	801	NAG	C1-C2-N2	2.20	113.89	110.43
3	E	602	NAG	C1-O5-C5	2.13	115.04	112.19

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	601	NAG	C1-C2-N2-C7
3	C	801	NAG	O5-C5-C6-O6
3	A	803	NAG	C4-C5-C6-O6
3	C	801	NAG	C4-C5-C6-O6
3	E	601	NAG	C4-C5-C6-O6
3	B	802	NAG	O5-C5-C6-O6
3	F	601	NAG	O5-C5-C6-O6
3	B	802	NAG	C4-C5-C6-O6
3	A	801	NAG	C8-C7-N2-C2
3	A	801	NAG	O7-C7-N2-C2
3	A	802	NAG	C8-C7-N2-C2
3	A	802	NAG	O7-C7-N2-C2
3	A	803	NAG	C8-C7-N2-C2
3	A	803	NAG	O7-C7-N2-C2
3	D	601	NAG	C8-C7-N2-C2
3	D	601	NAG	O7-C7-N2-C2
3	D	602	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	D	602	NAG	O7-C7-N2-C2
3	D	603	NAG	C8-C7-N2-C2
3	D	603	NAG	O7-C7-N2-C2
3	B	801	NAG	C8-C7-N2-C2
3	B	801	NAG	O7-C7-N2-C2
3	B	802	NAG	C8-C7-N2-C2
3	B	802	NAG	O7-C7-N2-C2
3	B	803	NAG	C8-C7-N2-C2
3	B	803	NAG	O7-C7-N2-C2
3	C	801	NAG	C8-C7-N2-C2
3	C	801	NAG	O7-C7-N2-C2
3	C	802	NAG	C8-C7-N2-C2
3	C	802	NAG	O7-C7-N2-C2
3	C	803	NAG	C8-C7-N2-C2
3	C	803	NAG	O7-C7-N2-C2
3	F	601	NAG	C8-C7-N2-C2
3	F	601	NAG	O7-C7-N2-C2
3	F	603	NAG	C8-C7-N2-C2
3	F	603	NAG	O7-C7-N2-C2
3	E	601	NAG	C8-C7-N2-C2
3	E	601	NAG	O7-C7-N2-C2
3	E	602	NAG	C8-C7-N2-C2
3	E	602	NAG	O7-C7-N2-C2
3	E	603	NAG	C8-C7-N2-C2
3	E	603	NAG	O7-C7-N2-C2
3	E	601	NAG	O5-C5-C6-O6
3	C	802	NAG	O5-C5-C6-O6
3	F	601	NAG	C4-C5-C6-O6
3	A	803	NAG	O5-C5-C6-O6
3	F	603	NAG	C4-C5-C6-O6
3	B	801	NAG	O5-C5-C6-O6
3	F	602	NAG	O5-C5-C6-O6
3	A	801	NAG	O5-C5-C6-O6
3	F	602	NAG	C4-C5-C6-O6
3	A	802	NAG	O5-C5-C6-O6
3	F	603	NAG	O5-C5-C6-O6
3	D	602	NAG	O5-C5-C6-O6
3	E	603	NAG	C4-C5-C6-O6
3	B	803	NAG	C1-C2-N2-C7
3	D	601	NAG	C4-C5-C6-O6
3	E	602	NAG	C3-C2-N2-C7
3	E	603	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	B	801	NAG	C4-C5-C6-O6
3	A	802	NAG	C1-C2-N2-C7
3	A	803	NAG	C1-C2-N2-C7
3	B	801	NAG	C1-C2-N2-C7
3	E	601	NAG	C1-C2-N2-C7
3	E	602	NAG	C1-C2-N2-C7
3	A	802	NAG	C3-C2-N2-C7
3	A	803	NAG	C3-C2-N2-C7
3	B	801	NAG	C3-C2-N2-C7
3	B	803	NAG	C3-C2-N2-C7
3	E	601	NAG	C3-C2-N2-C7
3	D	603	NAG	C4-C5-C6-O6
3	A	801	NAG	C4-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	803	NAG	6	0
3	B	801	NAG	1	0
3	D	601	NAG	4	0
3	E	603	NAG	4	0
3	A	802	NAG	2	0
3	F	601	NAG	2	0
3	E	601	NAG	1	0
3	E	602	NAG	2	0
3	A	803	NAG	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, 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	486/486 (100%)	0.26	11 (2%) 61 37	102, 169, 251, 286	0
1	B	486/486 (100%)	-0.17	1 (0%) 91 82	35, 61, 118, 156	0
1	C	486/486 (100%)	-0.06	4 (0%) 82 60	48, 95, 174, 215	0
2	D	517/526 (98%)	0.27	9 (1%) 69 43	80, 130, 178, 202	0
2	E	517/526 (98%)	0.25	12 (2%) 61 37	60, 98, 165, 212	0
2	F	517/526 (98%)	-0.03	2 (0%) 88 72	42, 106, 177, 217	0
All	All	3009/3036 (99%)	0.09	39 (1%) 75 50	35, 112, 196, 286	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	181	LEU	6.1
2	E	159	PHE	3.2
2	E	333	ASN	3.2
1	A	637	GLY	3.1
2	E	62	PRO	3.0
2	D	72	LEU	2.9
1	C	486	SER	2.8
1	C	355	GLY	2.8
2	D	260	CYS	2.8
1	A	422	TYR	2.7
1	A	649	GLY	2.7
2	E	177	CYS	2.7
1	B	382	SER	2.6
2	F	221	CYS	2.6
1	A	525	PRO	2.5
2	E	154	LEU	2.5
2	E	498	PHE	2.4
1	A	312	PHE	2.4
2	E	121	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	164	SER	2.3
1	C	601	GLY	2.3
2	D	62	PRO	2.3
1	A	638	GLY	2.2
2	D	135	PHE	2.2
1	A	452	ILE	2.2
2	D	302	LEU	2.2
2	E	123	GLU	2.2
2	F	242	PHE	2.2
1	A	489	LEU	2.1
2	E	128	LYS	2.1
2	D	84	GLU	2.1
2	D	48	CYS	2.1
1	C	357	VAL	2.1
1	A	358	ASN	2.1
2	E	260	CYS	2.1
1	A	245	ILE	2.0
1	A	256	ARG	2.0
2	E	365	ASN	2.0
2	E	484	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	A	801	14/15	-0.03	0.14	224,252,264,266	0
3	NAG	F	601	14/15	0.21	0.10	167,193,208,210	0
3	NAG	D	602	14/15	0.30	0.15	187,209,214,217	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	E	601	14/15	0.37	0.14	200,211,220,221	0
3	NAG	C	802	14/15	0.52	0.11	168,184,191,192	0
3	NAG	A	803	14/15	0.54	0.09	222,240,246,247	0
3	NAG	B	801	14/15	0.58	0.11	112,133,141,150	0
3	NAG	D	603	14/15	0.59	0.15	139,151,164,167	0
3	NAG	D	601	14/15	0.62	0.09	118,164,181,183	0
3	NAG	F	603	14/15	0.63	0.13	122,130,135,140	0
3	NAG	C	803	14/15	0.63	0.09	121,157,163,167	0
3	NAG	A	802	14/15	0.66	0.11	178,183,189,189	0
3	NAG	B	802	14/15	0.75	0.17	60,84,112,134	0
3	NAG	E	602	14/15	0.75	0.13	104,135,157,161	0
3	NAG	C	801	14/15	0.79	0.10	101,118,137,142	0
3	NAG	B	803	14/15	0.82	0.14	78,101,123,124	0
3	NAG	F	602	14/15	0.85	0.09	96,107,123,132	0
3	NAG	E	603	14/15	0.89	0.08	131,145,158,162	0
4	CA	A	806	1/1	0.89	0.07	281,281,281,281	0
4	CA	F	604	1/1	0.92	0.14	54,54,54,54	0
4	CA	C	806	1/1	0.94	0.05	129,129,129,129	0
4	CA	B	804	1/1	0.95	0.08	82,82,82,82	0
4	CA	A	805	1/1	0.95	0.04	181,181,181,181	0
4	CA	A	804	1/1	0.95	0.04	169,169,169,169	0
4	CA	D	604	1/1	0.96	0.06	82,82,82,82	0
4	CA	E	604	1/1	0.96	0.13	71,71,71,71	0
4	CA	C	805	1/1	0.98	0.05	44,44,44,44	0
4	CA	B	806	1/1	0.98	0.04	34,34,34,34	0
4	CA	C	804	1/1	0.99	0.02	72,72,72,72	0
4	CA	B	805	1/1	1.00	0.02	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.