



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:38 am GMT

PDB ID : 4YY0
Title : The structure of hemagglutinin from a H6N1 influenza virus (A/chicken/Taiwan/A2837/2013)
Authors : Wang, F.; Qi, J.; Bi, Y.; Zhang, W.; Wang, M.; Wang, M.; Liu, J.; Yan, J.; Shi, Y.; Gao, G.F.
Deposited on : 2015-03-23
Resolution : 2.59 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

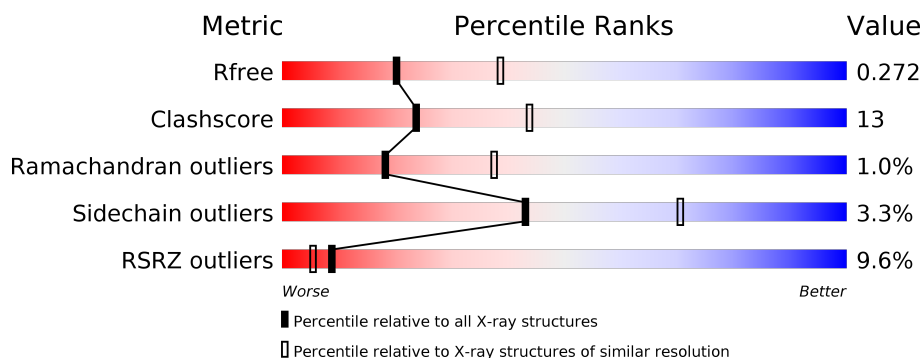
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (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 $\leq 5\%$. 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	325	<div> <div>2%</div> <div>85%</div> <div>13%</div> <div>..</div> </div>
1	C	325	<div> <div>5%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>
1	E	325	<div> <div>6%</div> <div>80%</div> <div>18%</div> <div>..</div> </div>
2	B	159	<div> <div>15%</div> <div>74%</div> <div>24%</div> <div>..</div> </div>
2	D	159	<div> <div>24%</div> <div>67%</div> <div>27%</div> <div>5%</div> <div>.</div> </div>
2	F	159	<div> <div>23%</div> <div>69%</div> <div>22%</div> <div>8%</div> <div>.</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11681 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.

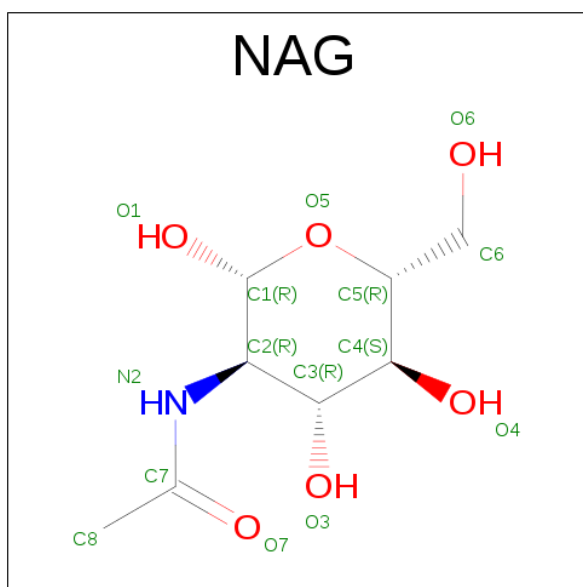
- Molecule 1 is a protein called HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	0	0
			2563	1625	436	489	13			
1	C	325	Total	C	N	O	S	0	0	0
			2563	1625	436	489	13			
1	E	325	Total	C	N	O	S	0	0	0
			2563	1625	436	489	13			

- Molecule 2 is a protein called HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	159	Total	C	N	O	S	0	0	0
			1275	794	221	253	7			
2	D	159	Total	C	N	O	S	0	0	0
			1275	794	221	253	7			
2	F	159	Total	C	N	O	S	0	0	0
			1275	794	221	253	7			

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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	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	D	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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	30	Total	O	0	0
			30	30		
4	B	1	Total	O	0	0
			1	1		
4	C	15	Total	O	0	0
			15	15		
4	D	5	Total	O	0	0
			5	5		
4	E	13	Total	O	0	0
			13	13		

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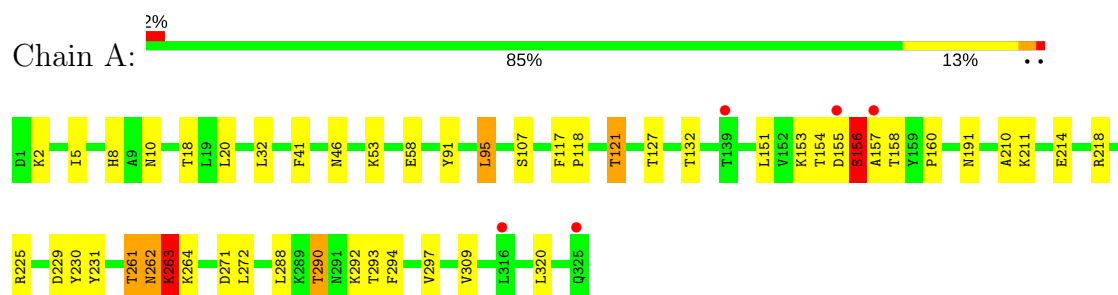
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	5	Total	O	0	0
			5	5		

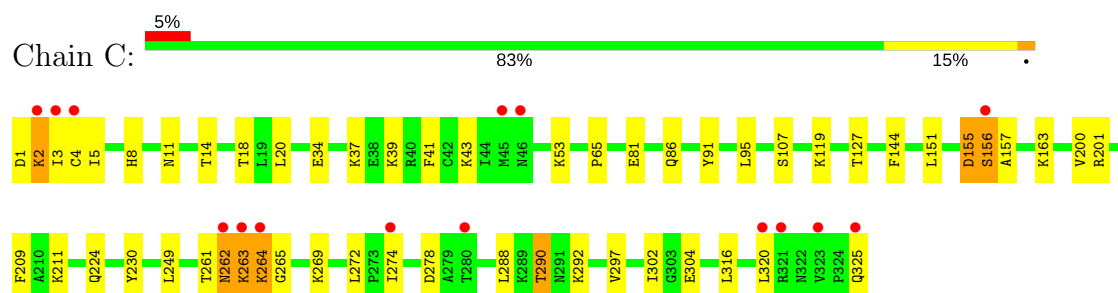
3 Residue-property plots [i](#)

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

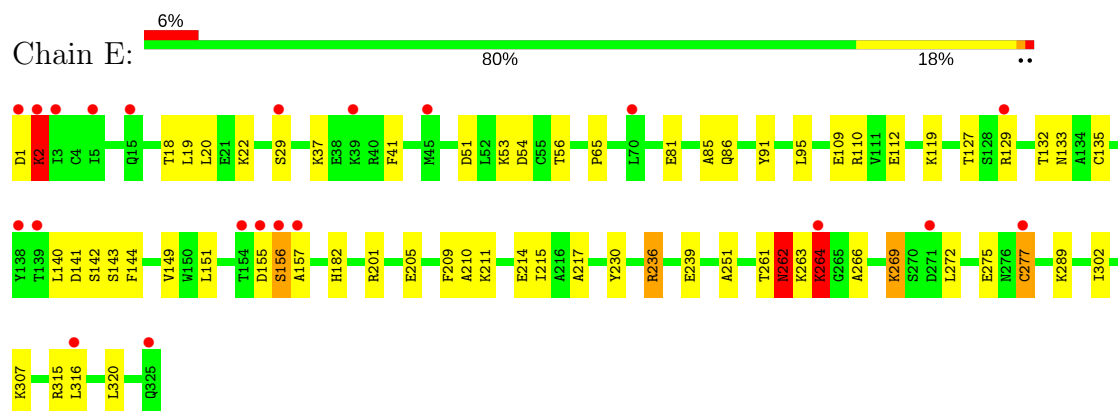
• Molecule 1: HA1



• Molecule 1: HA1

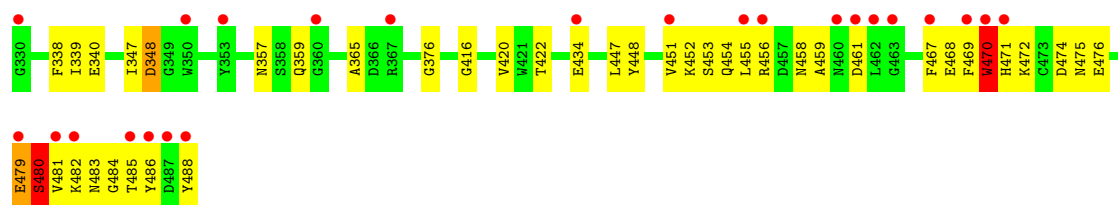


• Molecule 1: HA1

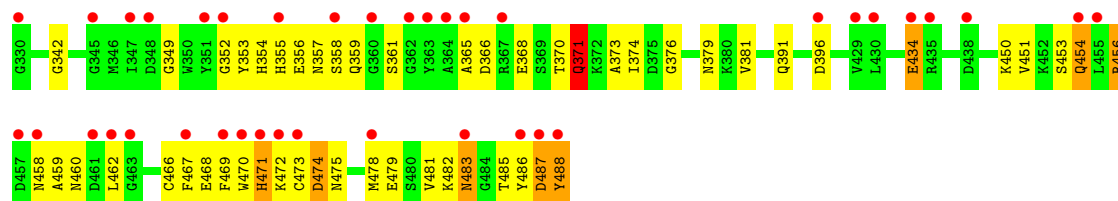


• Molecule 2: HA2

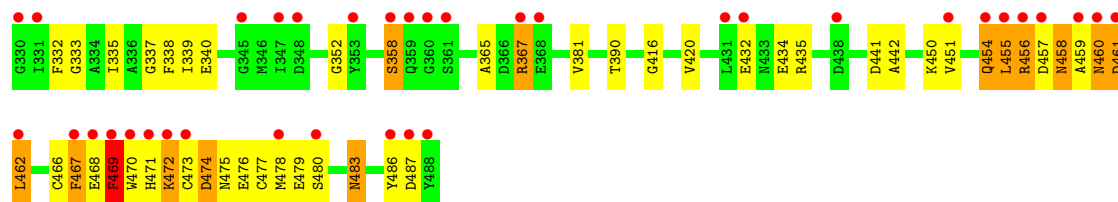




• Molecule 2: HA2



• Molecule 2: HA2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.61Å 106.26Å 125.28Å 90.00° 102.75° 90.00°	Depositor
Resolution (Å)	41.37 – 2.59 41.37 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.2 (41.37-2.59) 99.2 (41.37-2.59)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.63 (at 2.58Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.4_1496)	Depositor
R, R_{free}	0.220 , 0.271 0.222 , 0.272	Depositor DCC
R_{free} test set	2711 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	51.1	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11681	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.31	0/2625	0.61	4/3571 (0.1%)
1	C	0.31	0/2625	0.56	1/3571 (0.0%)
1	E	0.34	0/2625	0.63	1/3571 (0.0%)
2	B	0.48	0/1301	0.85	2/1754 (0.1%)
2	D	0.52	1/1301 (0.1%)	0.76	3/1754 (0.2%)
2	F	0.56	3/1301 (0.2%)	0.87	6/1754 (0.3%)
All	All	0.40	4/11778 (0.0%)	0.68	17/15975 (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
2	B	0	2
2	F	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	469	PHE	CG-CD1	-7.08	1.28	1.38
2	D	434	GLU	CB-CG	-5.66	1.41	1.52
2	F	467	PHE	CD1-CE1	-5.56	1.28	1.39
2	F	469	PHE	CD1-CE1	-5.09	1.29	1.39

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	262	ASN	N-CA-CB	-12.28	88.49	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	261	THR	N-CA-C	-11.74	79.31	111.00
1	A	262	ASN	N-CA-CB	-9.79	92.98	110.60
2	F	462	LEU	CA-CB-CG	8.92	135.81	115.30
1	C	265	GLY	N-CA-C	-7.33	94.77	113.10
2	F	469	PHE	CB-CG-CD2	7.16	125.81	120.80
2	B	455	LEU	CA-CB-CG	6.70	130.72	115.30
1	A	261	THR	CB-CA-C	-6.59	93.81	111.60
2	F	455	LEU	CA-CB-CG	6.44	130.12	115.30
2	F	469	PHE	CB-CG-CD1	-6.40	116.32	120.80
2	F	467	PHE	CB-CG-CD1	-6.28	116.41	120.80
2	D	371	GLN	CA-CB-CG	6.24	127.12	113.40
2	D	471	HIS	N-CA-C	-5.63	95.79	111.00
2	B	470	TRP	N-CA-CB	-5.45	100.80	110.60
2	F	469	PHE	N-CA-CB	-5.26	101.13	110.60
1	A	263	LYS	CA-CB-CG	5.16	124.74	113.40
2	D	488	TYR	CD1-CE1-CZ	5.06	124.35	119.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	470	TRP	Peptide
2	B	479	GLU	Peptide
2	F	358	SER	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	2563	0	2508	41	0
1	C	2563	0	2508	52	0
1	E	2563	0	2507	72	0
2	B	1275	0	1180	50	0
2	D	1275	0	1178	57	0
2	F	1275	0	1180	54	0
3	A	28	0	26	0	0
3	C	28	0	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	14	0	13	3	0
3	E	28	0	26	0	0
4	A	30	0	0	4	0
4	B	1	0	0	0	0
4	C	15	0	0	2	0
4	D	5	0	0	0	0
4	E	13	0	0	3	0
4	F	5	0	0	0	0
All	All	11681	0	11152	286	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 13.

All (286) 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:E:109:GLU:HB2	1:E:261:THR:CG2	1.86	1.04
1:A:261:THR:O	1:A:261:THR:CG2	2.03	1.02
1:A:261:THR:HG22	1:A:261:THR:O	1.63	0.96
2:B:471:HIS:HD2	2:B:472:LYS:H	1.11	0.94
1:C:2:LYS:NZ	1:C:4:CYS:SG	2.41	0.92
2:B:452:LYS:HG2	2:B:456:ARG:HE	1.33	0.91
2:D:379:ASN:ND2	1:E:19:LEU:O	2.07	0.87
1:C:11:ASN:ND2	4:C:501:HOH:O	2.08	0.86
2:F:474:ASP:OD1	2:F:477:CYS:N	2.08	0.86
2:B:471:HIS:CD2	2:B:472:LYS:H	1.94	0.85
1:C:20:LEU:N	2:D:434:GLU:OE2	2.12	0.83
1:C:325:GLN:NE2	2:D:342:GLY:O	2.11	0.83
2:D:458:ASN:ND2	2:D:486:TYR:OH	2.13	0.82
1:E:109:GLU:HB2	1:E:261:THR:HG22	1.58	0.82
1:E:205:GLU:OE1	4:E:501:HOH:O	1.97	0.82
1:C:263:LYS:O	1:C:264:LYS:CG	2.28	0.81
1:A:107:SER:OG	4:A:501:HOH:O	1.99	0.81
1:E:264:LYS:HB2	1:E:302:ILE:HD11	1.63	0.80
2:B:357:ASN:ND2	2:B:359:GLN:OE1	2.14	0.80
1:E:109:GLU:HB2	1:E:261:THR:HG21	1.63	0.79
2:D:460:ASN:HB2	2:D:470:TRP:CZ2	2.18	0.79
2:D:359:GLN:OE1	2:D:475:ASN:ND2	2.16	0.79
1:A:154:THR:C	1:A:156:SER:H	1.86	0.78
2:B:482:LYS:HD2	2:B:482:LYS:O	1.84	0.77
2:D:456:ARG:NH2	2:F:461:ASP:O	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:THR:HG23	1:C:292:LYS:H	1.50	0.75
2:B:357:ASN:ND2	2:B:475:ASN:OD1	2.20	0.75
1:C:261:THR:HG23	1:C:263:LYS:H	1.52	0.73
2:F:462:LEU:HD13	2:F:466:CYS:HB2	1.70	0.73
2:F:468:GLU:OE1	2:F:468:GLU:N	2.22	0.73
2:D:458:ASN:HB3	2:D:471:HIS:CE1	2.23	0.73
1:E:261:THR:HB	1:E:263:LYS:HD3	1.70	0.72
2:B:454:GLN:NE2	2:B:484:GLY:O	2.22	0.72
1:A:261:THR:HG23	1:A:261:THR:O	1.90	0.72
1:C:263:LYS:O	1:C:264:LYS:HG3	1.89	0.71
2:B:348:ASP:OD1	2:B:348:ASP:N	2.24	0.71
1:E:264:LYS:HD2	1:E:264:LYS:H	1.54	0.70
2:B:454:GLN:HE22	2:B:484:GLY:C	1.93	0.70
2:F:469:PHE:CE1	2:F:473:CYS:HB2	2.26	0.70
1:A:156:SER:OG	1:A:157:ALA:N	2.25	0.70
1:C:18:THR:HB	2:D:434:GLU:CG	2.22	0.69
1:E:217:ALA:O	4:E:502:HOH:O	2.09	0.69
1:C:18:THR:HB	2:D:434:GLU:HG2	1.74	0.69
1:E:109:GLU:CB	1:E:261:THR:CG2	2.69	0.69
1:A:18:THR:HB	2:B:434:GLU:HG3	1.74	0.68
1:E:1:ASP:N	4:E:504:HOH:O	2.26	0.68
2:F:477:CYS:O	2:F:480:SER:HB2	1.93	0.68
1:A:117:PHE:O	4:A:502:HOH:O	2.10	0.67
1:C:263:LYS:O	1:C:264:LYS:HG2	1.94	0.67
2:D:453:SER:O	2:D:456:ARG:NH1	2.27	0.67
2:B:452:LYS:O	2:B:456:ARG:HG2	1.94	0.67
1:E:2:LYS:HD3	2:F:469:PHE:HD2	1.60	0.67
2:B:471:HIS:CD2	2:B:472:LYS:N	2.62	0.67
2:D:356:GLU:HG3	2:D:361:SER:HB2	1.77	0.66
2:B:470:TRP:CG	2:B:471:HIS:HB2	2.31	0.65
1:E:109:GLU:CB	1:E:261:THR:HG22	2.25	0.65
1:E:29:SER:OG	1:E:315:ARG:NE	2.30	0.65
1:C:316:LEU:HD23	2:D:381:VAL:HG22	1.79	0.65
1:E:129:ARG:HG2	1:E:129:ARG:O	1.97	0.65
2:F:460:ASN:ND2	2:F:461:ASP:H	1.94	0.64
2:F:475:ASN:O	2:F:479:GLU:HG2	1.98	0.64
1:A:262:ASN:OD1	1:A:263:LYS:N	2.30	0.64
1:A:154:THR:C	1:A:156:SER:N	2.51	0.64
1:A:210:ALA:O	1:A:211:LYS:HG2	1.98	0.64
1:E:209:PHE:CZ	1:E:211:LYS:HG3	2.34	0.63
1:A:127:THR:HG22	1:A:151:LEU:HD22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:471:HIS:HD2	2:B:472:LYS:N	1.91	0.63
2:D:475:ASN:HA	2:D:478:MET:HB2	1.81	0.63
1:E:275:GLU:HB2	1:E:277:CYS:SG	2.39	0.63
1:C:290:THR:CG2	1:C:292:LYS:H	2.12	0.62
1:E:20:LEU:HG	2:F:434:GLU:OE2	1.99	0.62
1:C:3:ILE:CD1	2:D:481:VAL:HG21	2.28	0.62
2:F:462:LEU:N	2:F:468:GLU:OE2	2.32	0.62
2:B:470:TRP:CD1	2:B:471:HIS:HB2	2.35	0.62
1:E:263:LYS:HB3	1:E:264:LYS:HG2	1.81	0.62
1:E:127:THR:HG22	1:E:151:LEU:HD22	1.83	0.61
2:D:352:GLY:HA3	2:D:365:ALA:HA	1.81	0.61
1:E:262:ASN:N	1:E:263:LYS:HD2	2.15	0.61
1:E:140:LEU:CD1	1:E:143:SER:HB2	2.31	0.60
1:E:263:LYS:HD2	1:E:263:LYS:H	1.65	0.60
1:E:54:ASP:OD1	1:E:86:GLN:N	2.32	0.60
1:C:262:ASN:O	1:C:263:LYS:HG2	2.01	0.60
1:A:153:LYS:NZ	1:A:191:ASN:O	2.35	0.59
1:E:266:ALA:HB2	1:E:302:ILE:HD13	1.84	0.59
2:D:359:GLN:HE22	2:D:474:ASP:HA	1.67	0.59
1:A:20:LEU:HG	2:B:434:GLU:OE2	2.02	0.59
2:B:480:SER:OG	2:B:481:VAL:N	2.35	0.59
1:C:261:THR:HG23	1:C:263:LYS:N	2.18	0.59
1:C:264:LYS:O	1:C:302:ILE:HD11	2.02	0.58
2:F:474:ASP:OD1	2:F:476:GLU:N	2.36	0.58
2:B:452:LYS:HB3	2:B:456:ARG:HH21	1.67	0.58
1:C:156:SER:OG	1:C:157:ALA:N	2.37	0.58
1:E:316:LEU:HD23	2:F:381:VAL:HG22	1.86	0.58
1:E:110:ARG:NH2	1:E:112:GLU:OE2	2.37	0.57
2:F:460:ASN:HB3	2:F:468:GLU:HB2	1.85	0.57
1:A:154:THR:O	1:A:156:SER:N	2.33	0.57
1:E:51:ASP:HB3	1:E:53:LYS:HE3	1.86	0.57
2:B:482:LYS:HD2	2:B:482:LYS:C	2.24	0.57
2:D:483:ASN:OD1	3:D:501:NAG:C7	2.52	0.57
2:D:357:ASN:ND2	2:D:473:CYS:O	2.32	0.57
1:E:262:ASN:HD22	1:E:263:LYS:HE3	1.70	0.57
1:E:129:ARG:NH2	1:E:155:ASP:OD2	2.35	0.57
2:F:479:GLU:O	2:F:483:ASN:HB3	2.05	0.57
2:F:460:ASN:HB2	2:F:470:TRP:CZ2	2.40	0.56
1:C:201:ARG:HD3	1:E:215:ILE:O	2.04	0.56
1:C:37:LYS:HE3	1:C:39:LYS:HE2	1.86	0.56
2:F:462:LEU:HD13	2:F:466:CYS:CB	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:LYS:NZ	2:D:466:CYS:SG	2.71	0.56
2:F:469:PHE:HB2	2:F:471:HIS:CE1	2.40	0.56
2:B:357:ASN:HD21	2:B:359:GLN:HB2	1.70	0.56
1:C:5:ILE:HD11	2:D:451:VAL:HG21	1.88	0.56
1:E:140:LEU:HD11	1:E:143:SER:HB2	1.88	0.55
2:B:476:GLU:O	2:B:480:SER:HB3	2.05	0.55
1:A:262:ASN:N	1:A:262:ASN:OD1	2.40	0.55
2:B:470:TRP:CD2	2:B:471:HIS:HB2	2.42	0.55
1:C:3:ILE:HD12	2:D:481:VAL:HG21	1.88	0.55
1:E:2:LYS:CD	2:F:469:PHE:HD2	2.20	0.55
2:D:371:GLN:HA	2:D:374:ILE:HB	1.88	0.54
2:F:456:ARG:O	2:F:456:ARG:HG3	2.05	0.54
2:B:459:ALA:HB2	2:B:469:PHE:HA	1.90	0.54
2:F:458:ASN:O	2:F:469:PHE:HA	2.08	0.54
1:A:229:ASP:HB3	1:A:231:TYR:CE2	2.43	0.54
2:D:485:THR:CG2	3:D:501:NAG:H82	2.37	0.54
2:B:447:LEU:O	2:B:451:VAL:HG12	2.07	0.54
1:A:211:LYS:NZ	1:A:231:TYR:OH	2.33	0.54
1:C:2:LYS:HZ3	2:D:466:CYS:CB	2.20	0.54
2:B:471:HIS:CD2	2:B:472:LYS:O	2.61	0.53
2:F:337:GLY:O	2:F:340:GLU:HG2	2.08	0.53
1:A:2:LYS:HB3	2:B:468:GLU:OE1	2.09	0.53
1:A:263:LYS:HG2	1:A:264:LYS:O	2.09	0.52
2:D:370:THR:O	2:D:373:ALA:HB3	2.10	0.52
1:C:95:LEU:HA	1:C:230:TYR:HB2	1.91	0.52
2:B:448:TYR:O	2:B:452:LYS:HB2	2.10	0.52
1:A:118:PRO:O	1:A:121:THR:OG1	2.21	0.52
1:A:158:THR:O	1:A:160:PRO:HD3	2.09	0.51
1:C:43:LYS:HE3	1:C:278:ASP:OD1	2.10	0.51
1:E:140:LEU:HD13	1:E:142:SER:O	2.11	0.51
2:F:352:GLY:HA3	2:F:365:ALA:HA	1.92	0.51
2:B:459:ALA:CB	2:B:469:PHE:HA	2.40	0.51
2:D:454:GLN:O	2:D:488:TYR:HE2	1.93	0.51
1:E:129:ARG:HH12	1:E:155:ASP:CG	2.13	0.51
2:B:452:LYS:HG2	2:B:456:ARG:NE	2.15	0.51
2:F:459:ALA:HA	2:F:468:GLU:O	2.09	0.51
3:C:402:NAG:O6	4:C:502:HOH:O	2.18	0.51
1:E:95:LEU:HA	1:E:230:TYR:HB2	1.93	0.50
2:B:452:LYS:CG	2:B:456:ARG:HE	2.14	0.50
2:D:458:ASN:HB3	2:D:471:HIS:HE1	1.71	0.50
1:E:18:THR:HB	2:F:434:GLU:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:THR:HB	1:A:292:LYS:H	1.77	0.50
1:C:304:GLU:OE1	2:D:391:GLN:NE2	2.45	0.50
1:E:129:ARG:NH1	1:E:155:ASP:OD2	2.42	0.50
2:D:379:ASN:OD1	1:E:22:LYS:HD2	2.12	0.50
2:F:333:GLY:O	2:F:337:GLY:HA3	2.12	0.50
2:D:371:GLN:HB2	2:D:374:ILE:HB	1.92	0.50
1:E:2:LYS:HG2	2:F:468:GLU:HA	1.93	0.50
2:D:357:ASN:HD21	2:D:475:ASN:ND2	2.10	0.50
2:F:450:LYS:O	2:F:454:GLN:HG2	2.12	0.50
2:F:483:ASN:C	2:F:483:ASN:OD1	2.50	0.49
1:E:289:LYS:O	1:E:289:LYS:HG3	2.12	0.49
2:B:434:GLU:OE1	2:F:435:ARG:NH1	2.44	0.49
2:B:461:ASP:HB2	2:B:467:PHE:CE2	2.48	0.49
2:D:355:HIS:O	2:D:361:SER:OG	2.12	0.49
2:F:455:LEU:HD23	2:F:486:TYR:CD2	2.47	0.49
2:B:470:TRP:CE2	2:B:471:HIS:HB2	2.47	0.49
1:C:5:ILE:HD13	2:D:467:PHE:HE1	1.78	0.49
2:D:462:LEU:HD11	2:D:468:GLU:HB2	1.94	0.49
1:C:81:GLU:O	1:C:269:LYS:HA	2.13	0.48
1:C:127:THR:HG22	1:C:151:LEU:HD22	1.93	0.48
1:C:18:THR:HB	2:D:434:GLU:HG3	1.93	0.48
1:E:262:ASN:H	1:E:263:LYS:HD2	1.77	0.48
2:F:460:ASN:ND2	2:F:461:ASP:N	2.61	0.48
2:D:371:GLN:HA	2:D:374:ILE:H	1.77	0.48
2:B:479:GLU:O	2:B:483:ASN:HB2	2.14	0.48
1:E:119:LYS:HD3	1:E:127:THR:HB	1.96	0.48
2:B:480:SER:HB2	2:B:486:TYR:HB2	1.96	0.48
1:A:95:LEU:HA	1:A:230:TYR:HB2	1.95	0.47
1:E:91:TYR:HD2	1:E:132:THR:HG21	1.79	0.47
2:D:359:GLN:CD	2:D:359:GLN:H	2.16	0.47
1:E:1:ASP:O	1:E:2:LYS:HD3	2.14	0.47
1:A:271:ASP:N	1:A:271:ASP:OD2	2.41	0.47
1:A:293:THR:HG23	1:A:294:PHE:CD2	2.49	0.47
2:B:340:GLU:HG2	2:B:340:GLU:H	1.52	0.47
2:F:457:ASP:C	2:F:459:ALA:N	2.68	0.47
1:E:2:LYS:HD2	2:F:469:PHE:N	2.30	0.47
2:F:332:PHE:CE1	2:F:442:ALA:HB2	2.51	0.46
2:D:472:LYS:HE3	2:D:472:LYS:HB3	1.70	0.46
2:F:461:ASP:HA	2:F:468:GLU:OE1	2.15	0.46
2:B:458:ASN:OD1	2:B:488:TYR:CE1	2.69	0.46
2:D:357:ASN:ND2	2:D:359:GLN:OE1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:TYR:HD2	1:A:132:THR:HG21	1.81	0.46
1:A:53:LYS:HD3	1:A:53:LYS:HA	1.80	0.46
2:B:348:ASP:OD2	2:B:365:ALA:N	2.48	0.46
1:C:200:VAL:HG13	1:C:249:LEU:HD13	1.98	0.46
2:F:338:PHE:CE1	2:F:339:ILE:HG13	2.50	0.46
1:E:2:LYS:HD3	2:F:469:PHE:CD2	2.45	0.46
2:F:432:GLU:OE1	2:F:435:ARG:NH2	2.38	0.46
2:F:457:ASP:O	2:F:470:TRP:CD1	2.69	0.46
2:F:469:PHE:HD1	2:F:471:HIS:NE2	2.14	0.46
1:E:156:SER:OG	1:E:157:ALA:N	2.48	0.45
2:D:479:GLU:O	2:D:483:ASN:HB2	2.17	0.45
1:A:218:ARG:O	1:A:225:ARG:HG2	2.16	0.45
1:C:155:ASP:O	1:C:156:SER:HB3	2.16	0.45
1:E:129:ARG:O	1:E:129:ARG:CG	2.63	0.45
1:C:34:GLU:OE1	1:C:290:THR:OG1	2.34	0.45
2:D:478:MET:O	2:D:481:VAL:HG22	2.17	0.45
2:B:458:ASN:O	2:B:470:TRP:HB2	2.16	0.45
2:F:462:LEU:HD12	2:F:468:GLU:CD	2.37	0.45
2:B:453:SER:OG	2:B:453:SER:O	2.35	0.45
2:B:376:GLY:HA2	1:C:20:LEU:O	2.17	0.45
2:D:376:GLY:O	2:D:379:ASN:HB3	2.16	0.44
1:E:1:ASP:HB3	2:F:469:PHE:CE2	2.51	0.44
1:C:209:PHE:CZ	1:C:211:LYS:HG3	2.53	0.44
2:D:487:ASP:OD1	2:D:487:ASP:N	2.51	0.44
1:E:210:ALA:C	1:E:211:LYS:HG2	2.38	0.44
1:E:41:PHE:CE2	1:E:272:LEU:HB2	2.52	0.44
2:F:416:GLY:O	2:F:420:VAL:HG13	2.17	0.44
2:B:416:GLY:O	2:B:420:VAL:HG13	2.17	0.44
2:B:461:ASP:HB2	2:B:467:PHE:HE2	1.81	0.44
2:D:485:THR:HG21	3:D:501:NAG:H82	1.98	0.44
1:E:263:LYS:N	1:E:263:LYS:HD2	2.30	0.44
1:C:91:TYR:OH	1:C:224:GLN:NE2	2.51	0.44
2:F:475:ASN:HA	2:F:478:MET:HB2	2.00	0.44
1:A:10:ASN:ND2	4:A:503:HOH:O	2.10	0.44
2:B:458:ASN:C	2:B:470:TRP:HB2	2.38	0.44
1:C:41:PHE:CE2	1:C:272:LEU:HB2	2.53	0.44
2:F:457:ASP:C	2:F:459:ALA:H	2.19	0.44
1:A:263:LYS:HE3	1:A:263:LYS:HB3	1.68	0.43
1:E:56:THR:HG22	1:E:85:ALA:HB3	2.00	0.43
1:A:309:VAL:CG2	2:B:422:THR:HA	2.49	0.43
2:F:458:ASN:HD22	2:F:458:ASN:HA	1.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:GLN:NE2	2:D:342:GLY:N	2.67	0.43
2:D:371:GLN:CA	2:D:374:ILE:HB	2.49	0.43
1:C:107:SER:O	1:C:261:THR:HG22	2.19	0.43
1:C:288:LEU:HD21	1:C:297:VAL:HG21	2.00	0.43
1:C:2:LYS:HD2	1:C:3:ILE:N	2.34	0.43
1:C:53:LYS:HB3	1:C:53:LYS:HE3	1.63	0.43
1:C:119:LYS:HD3	1:C:127:THR:HB	2.01	0.43
2:D:459:ALA:HA	2:D:468:GLU:O	2.19	0.42
1:E:1:ASP:O	1:E:2:LYS:CB	2.66	0.42
1:C:8:HIS:ND1	2:D:349:GLY:O	2.52	0.42
1:E:81:GLU:O	1:E:269:LYS:HA	2.19	0.42
1:A:5:ILE:CD1	2:B:451:VAL:HG11	2.49	0.42
2:B:483:ASN:OD1	2:B:485:THR:OG1	2.36	0.42
1:C:263:LYS:C	1:C:264:LYS:HG2	2.39	0.42
1:E:236:ARG:HG3	1:E:239:GLU:CD	2.40	0.42
1:E:263:LYS:HB3	1:E:264:LYS:CG	2.47	0.42
1:A:41:PHE:CE2	1:A:272:LEU:HB2	2.55	0.42
2:D:352:GLY:HA2	2:D:366:ASP:H	1.84	0.42
2:D:353:TYR:CD1	2:D:482:LYS:HE2	2.54	0.42
2:D:376:GLY:HA2	1:E:20:LEU:O	2.20	0.42
1:C:1:ASP:OD2	2:D:472:LYS:HB3	2.20	0.42
1:E:262:ASN:HB3	1:E:263:LYS:HD2	2.02	0.42
1:E:307:LYS:HE3	2:F:390:THR:O	2.19	0.42
1:A:8:HIS:O	1:A:320:LEU:HD11	2.20	0.42
2:B:347:ILE:N	2:B:348:ASP:OD1	2.53	0.42
1:E:302:ILE:HD12	1:E:302:ILE:HA	1.96	0.42
2:D:359:GLN:NE2	2:D:474:ASP:HA	2.35	0.42
1:E:2:LYS:CG	2:F:469:PHE:H	2.33	0.42
1:A:32:LEU:HB3	1:A:293:THR:CG2	2.50	0.41
1:C:65:PRO:HG3	1:C:144:PHE:O	2.19	0.41
1:C:37:LYS:HD3	1:C:297:VAL:HG13	2.02	0.41
1:E:182:HIS:CE1	1:E:214:GLU:HG3	2.55	0.41
2:B:338:PHE:CE1	2:B:339:ILE:HG13	2.55	0.41
1:E:135:CYS:O	1:E:143:SER:HB3	2.20	0.41
1:A:58:GLU:OE2	4:A:504:HOH:O	2.22	0.41
1:A:5:ILE:HD11	2:B:451:VAL:HG11	2.02	0.41
2:F:469:PHE:HE1	2:F:472:LYS:C	2.23	0.41
1:E:133:ASN:HA	1:E:141:ASP:O	2.20	0.41
1:C:263:LYS:C	1:C:264:LYS:CG	2.85	0.41
1:E:1:ASP:O	1:E:2:LYS:HB2	2.20	0.41
1:A:210:ALA:C	1:A:211:LYS:HG2	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:149:VAL:HG13	1:E:251:ALA:HB3	2.02	0.41
1:E:65:PRO:HG3	1:E:144:PHE:O	2.20	0.41
2:F:486:TYR:CD1	2:F:487:ASP:N	2.89	0.41
1:C:8:HIS:O	1:C:320:LEU:HD11	2.21	0.41
1:E:261:THR:C	1:E:263:LYS:H	2.24	0.41
2:D:355:HIS:CE1	2:D:361:SER:HA	2.56	0.41
2:D:458:ASN:O	2:D:469:PHE:HA	2.21	0.41
1:E:201:ARG:HG2	1:E:210:ALA:CB	2.51	0.41
2:F:451:VAL:HG22	2:F:467:PHE:CZ	2.56	0.41
1:A:214:GLU:CD	1:E:210:ALA:HB3	2.41	0.40
1:C:41:PHE:HB2	1:C:274:ILE:HG12	2.03	0.40
1:A:288:LEU:HD21	1:A:297:VAL:HG21	2.02	0.40
2:D:354:HIS:CE1	2:D:361:SER:OG	2.75	0.40
2:F:367:ARG:HD2	2:F:367:ARG:HA	1.76	0.40
2:F:335:ILE:N	2:F:441:ASP:OD1	2.50	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	323/325 (99%)	306 (95%)	15 (5%)	2 (1%)	28	53
1	C	323/325 (99%)	306 (95%)	13 (4%)	4 (1%)	15	32
1	E	323/325 (99%)	308 (95%)	12 (4%)	3 (1%)	20	40
2	B	157/159 (99%)	148 (94%)	6 (4%)	3 (2%)	9	18
2	D	157/159 (99%)	147 (94%)	8 (5%)	2 (1%)	14	29
2	F	157/159 (99%)	150 (96%)	6 (4%)	1 (1%)	28	53
All	All	1440/1452 (99%)	1365 (95%)	60 (4%)	15 (1%)	18	37

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	ASP
2	B	480	SER
1	C	156	SER
1	C	263	LYS
2	D	483	ASN
1	E	264	LYS
2	B	474	ASP
1	C	155	ASP
1	E	2	LYS
1	E	156	SER
2	F	474	ASP
1	A	156	SER
2	B	470	TRP
2	D	474	ASP
1	C	262	ASN

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	285/285 (100%)	279 (98%)	6 (2%)	59	83
1	C	285/285 (100%)	279 (98%)	6 (2%)	59	83
1	E	285/285 (100%)	277 (97%)	8 (3%)	49	76
2	B	134/134 (100%)	131 (98%)	3 (2%)	57	81
2	D	134/134 (100%)	126 (94%)	8 (6%)	22	44
2	F	134/134 (100%)	124 (92%)	10 (8%)	16	31
All	All	1257/1257 (100%)	1216 (97%)	41 (3%)	43	70

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	95	LEU
1	A	121	THR
1	A	156	SER

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Mol	Chain	Res	Type
1	A	263	LYS
1	A	290	THR
2	B	348	ASP
2	B	470	TRP
2	B	480	SER
1	C	2	LYS
1	C	14	THR
1	C	86	GLN
1	C	163	LYS
1	C	264	LYS
1	C	290	THR
2	D	358	SER
2	D	368	GLU
2	D	371	GLN
2	D	396	ASP
2	D	450	LYS
2	D	454	GLN
2	D	456	ARG
2	D	487	ASP
1	E	2	LYS
1	E	37	LYS
1	E	236	ARG
1	E	262	ASN
1	E	264	LYS
1	E	269	LYS
1	E	277	CYS
1	E	320	LEU
2	F	358	SER
2	F	367	ARG
2	F	454	GLN
2	F	456	ARG
2	F	458	ASN
2	F	460	ASN
2	F	461	ASP
2	F	469	PHE
2	F	472	LYS
2	F	483	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	357	ASN

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Mol	Chain	Res	Type
2	B	454	GLN
2	B	471	HIS
1	C	224	GLN
2	D	458	ASN
2	D	471	HIS
2	D	475	ASN
1	E	262	ASN
2	F	458	ASN
2	F	460	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

7 ligands 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	$\# Z > 2$
3	NAG	A	401	1	14,14,15	0.27	0	15,19,21	0.73	1 (6%)
3	NAG	A	402	1	14,14,15	0.23	0	15,19,21	0.65	1 (6%)
3	NAG	C	401	1	14,14,15	0.51	0	15,19,21	0.60	0
3	NAG	C	402	1	14,14,15	0.31	0	15,19,21	0.96	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	D	501	2	14,14,15	0.61	0	15,19,21	1.02	1 (6%)
3	NAG	E	401	1	14,14,15	1.33	2 (14%)	15,19,21	1.07	1 (6%)
3	NAG	E	402	1	14,14,15	0.22	0	15,19,21	0.86	1 (6%)

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	A	401	1	-	0/6/23/26	0/1/1/1
3	NAG	A	402	1	-	0/6/23/26	0/1/1/1
3	NAG	C	401	1	-	0/6/23/26	0/1/1/1
3	NAG	C	402	1	-	0/6/23/26	0/1/1/1
3	NAG	D	501	2	-	0/6/23/26	0/1/1/1
3	NAG	E	401	1	-	0/6/23/26	0/1/1/1
3	NAG	E	402	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	401	NAG	O5-C1	2.97	1.48	1.43
3	E	401	NAG	C1-C2	3.74	1.57	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	NAG	C1-O5-C5	-2.60	108.58	112.17
3	A	402	NAG	C1-O5-C5	2.04	114.98	112.17
3	A	401	NAG	C1-O5-C5	2.26	115.28	112.17
3	E	401	NAG	O3-C3-C4	2.44	115.66	110.36
3	E	402	NAG	C1-O5-C5	2.50	115.61	112.17
3	C	402	NAG	C1-O5-C5	2.86	116.11	112.17

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
3	C	402	NAG	1	0
3	D	501	NAG	3	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	325/325 (100%)	0.20	5 (1%) 74 69	32, 54, 92, 147	0
1	C	325/325 (100%)	0.29	15 (4%) 33 26	33, 57, 106, 154	0
1	E	325/325 (100%)	0.50	21 (6%) 20 14	39, 71, 110, 168	0
2	B	159/159 (100%)	0.99	24 (15%) 3 1	40, 85, 164, 215	0
2	D	159/159 (100%)	1.39	38 (23%) 1 0	37, 96, 166, 232	0
2	F	159/159 (100%)	1.34	36 (22%) 1 0	37, 95, 174, 220	0
All	All	1452/1452 (100%)	0.63	139 (9%) 9 5	32, 67, 146, 232	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	488	TYR	15.9
2	B	488	TYR	9.4
2	B	487	ASP	7.9
2	F	467	PHE	7.5
2	F	455	LEU	7.3
1	E	325	GLN	7.0
1	A	155	ASP	6.4
2	F	471	HIS	6.3
2	D	467	PHE	6.3
2	F	358	SER	6.0
2	F	469	PHE	5.7
1	E	138	TYR	5.5
2	D	455	LEU	5.4
2	F	472	LYS	5.3
2	B	455	LEU	5.1
2	F	367	ARG	5.0
2	F	488	TYR	5.0
2	D	347	ILE	5.0
2	F	460	ASN	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	157	ALA	4.9
2	D	478	MET	4.8
2	F	347	ILE	4.8
2	D	360	GLY	4.7
1	C	264	LYS	4.6
2	D	487	ASP	4.6
2	F	470	TRP	4.6
1	C	263	LYS	4.5
2	F	456	ARG	4.5
2	D	457	ASP	4.4
2	D	351	TYR	4.3
2	B	470	TRP	4.3
2	B	451	VAL	4.2
2	B	486	TYR	4.2
2	B	485	THR	4.2
2	F	459	ALA	4.2
2	F	480	SER	4.2
2	B	353	TYR	4.1
2	D	434	GLU	4.1
2	D	470	TRP	4.1
1	E	264	LYS	4.0
1	E	157	ALA	4.0
2	F	331	ILE	3.9
2	F	487	ASP	3.9
2	D	345	GLY	3.9
2	D	364	ALA	3.8
2	D	461	ASP	3.8
2	F	451	VAL	3.7
2	D	367	ARG	3.7
2	F	468	GLU	3.7
2	B	463	GLY	3.7
1	E	39	LYS	3.6
2	D	463	GLY	3.6
2	B	467	PHE	3.6
2	F	345	GLY	3.6
2	B	479	GLU	3.6
1	E	155	ASP	3.5
1	E	45	MET	3.5
2	F	454	GLN	3.5
1	C	3	ILE	3.4
2	D	352	GLY	3.4
1	E	277	CYS	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	469	PHE	3.4
2	F	360	GLY	3.3
2	D	348	ASP	3.3
1	E	1	ASP	3.3
2	D	486	TYR	3.3
2	B	471	HIS	3.2
2	D	355	HIS	3.2
2	B	482	LYS	3.2
2	D	473	CYS	3.2
2	D	462	LEU	3.1
2	F	348	ASP	3.1
2	D	438	ASP	3.1
2	F	432	GLU	3.1
2	D	458	ASN	3.1
2	F	478	MET	3.0
1	E	271	ASP	2.9
1	E	156	SER	2.9
2	D	429	VAL	2.9
2	B	469	PHE	2.8
2	D	362	GLY	2.7
2	D	358	SER	2.7
1	C	262	ASN	2.6
1	C	321	ARG	2.6
2	F	368	GLU	2.6
1	E	29	SER	2.6
2	F	486	TYR	2.6
2	B	456	ARG	2.6
2	B	461	ASP	2.6
2	F	473	CYS	2.5
2	D	483	ASN	2.5
1	C	325	GLN	2.5
1	A	316	LEU	2.5
2	B	330	GLY	2.5
2	D	435	ARG	2.5
2	F	353	TYR	2.5
2	F	431	LEU	2.5
1	C	4	CYS	2.5
2	F	461	ASP	2.5
2	D	472	LYS	2.4
1	C	45	MET	2.4
2	F	330	GLY	2.4
2	B	462	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	460	ASN	2.4
1	E	316	LEU	2.4
2	D	454	GLN	2.4
1	C	46	ASN	2.4
1	E	70	LEU	2.4
2	F	438	ASP	2.3
1	E	154	THR	2.3
2	F	359	GLN	2.3
2	B	481	VAL	2.3
2	D	430	LEU	2.3
2	D	471	HIS	2.3
2	D	396	ASP	2.3
1	A	139	THR	2.3
2	F	361	SER	2.2
1	C	280	THR	2.2
2	B	367	ARG	2.2
1	C	323	VAL	2.2
2	B	360	GLY	2.2
1	E	129	ARG	2.2
1	E	139	THR	2.2
2	D	330	GLY	2.2
1	C	274	ILE	2.2
1	A	325	GLN	2.1
2	D	365	ALA	2.1
2	B	434	GLU	2.1
2	D	363	TYR	2.1
1	C	320	LEU	2.0
1	C	2	LYS	2.0
2	F	457	ASP	2.0
1	C	156	SER	2.0
1	E	15	GLN	2.0
1	E	2	LYS	2.0
1	E	3	ILE	2.0
1	E	5	ILE	2.0
2	B	350	TRP	2.0
2	F	462	LEU	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 carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	C	402	14/15	0.86	0.18	0.43	78,93,104,107	0
3	NAG	E	402	14/15	0.90	0.20	0.25	64,80,88,88	0
3	NAG	A	401	14/15	0.73	0.36	-	119,124,128,129	0
3	NAG	C	401	14/15	0.42	0.37	-	140,159,164,164	0
3	NAG	D	501	14/15	0.71	0.35	-	166,171,173,174	0
3	NAG	A	402	14/15	0.86	0.15	-	66,80,93,95	0
3	NAG	E	401	14/15	0.79	0.20	-	140,148,152,154	0

6.5 Other polymers [i](#)

There are no such residues in this entry.