Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 02:23 PM EDT

PDB ID	:	6D8W
Title	:	Crystal structure of InvbI.18715.a.KN11: Influenza hemagglutinin from strain A/Jiangsu/ALSI/2011
Authors	:	Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2018-04-27
Resolution	:	2.35 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:

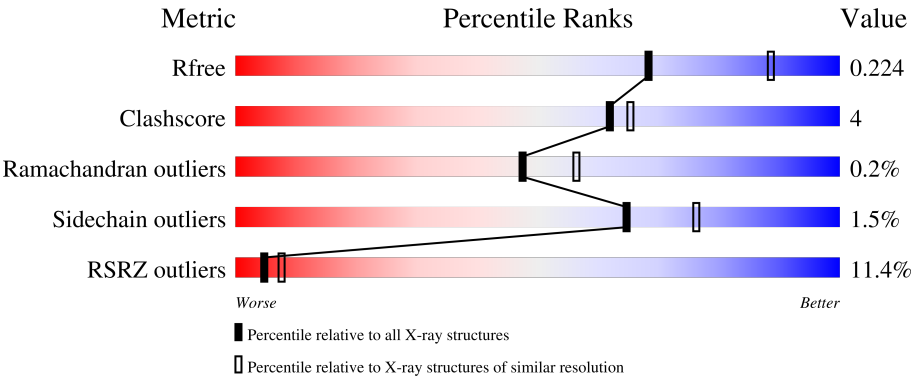
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.35 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}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 <=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	499	11% 81% 11% • 7%
1	B	499	11% 88% 10% •
1	C	499	12% 86% 9% 5%
1	D	499	13% 80% 9% 11%
1	E	499	8% 85% 10% •

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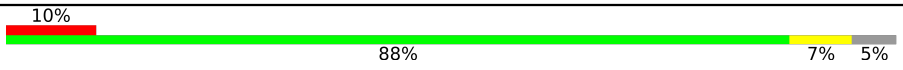
Mol	Chain	Length	Quality of chain
1	F	499	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OXM	B	502	-	X	-	-
3	OXM	E	502	-	X	-	-
3	OXM	F	503	-	X	-	-
3	OXM	F	504	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 22584 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	466	Total	C	N	O	S	0	4	0
			3577	2250	625	683	19			
1	B	491	Total	C	N	O	S	0	5	0
			3729	2352	650	708	19			
1	C	476	Total	C	N	O	S	0	7	0
			3630	2292	632	687	19			
1	D	443	Total	C	N	O	S	0	3	0
			3344	2108	582	639	15			
1	E	477	Total	C	N	O	S	0	4	0
			3631	2292	625	695	19			
1	F	476	Total	C	N	O	S	0	3	0
			3636	2286	637	694	19			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP G0Z9B7
A	2	SER	-	expression tag	UNP G0Z9B7
A	493	PHE	-	expression tag	UNP G0Z9B7
A	494	LEU	-	expression tag	UNP G0Z9B7
A	495	VAL	-	expression tag	UNP G0Z9B7
A	496	PRO	-	expression tag	UNP G0Z9B7
A	497	ARG	-	expression tag	UNP G0Z9B7
B	1	GLY	-	expression tag	UNP G0Z9B7
B	2	SER	-	expression tag	UNP G0Z9B7
B	495	PHE	-	expression tag	UNP G0Z9B7
B	496	LEU	-	expression tag	UNP G0Z9B7
B	497	VAL	-	expression tag	UNP G0Z9B7
B	498	PRO	-	expression tag	UNP G0Z9B7
B	499	ARG	-	expression tag	UNP G0Z9B7
C	1	GLY	-	expression tag	UNP G0Z9B7
C	2	SER	-	expression tag	UNP G0Z9B7
C	495	PHE	-	expression tag	UNP G0Z9B7

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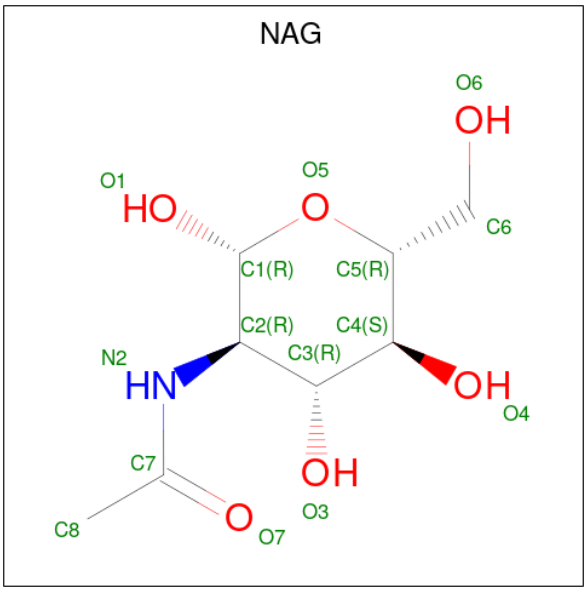
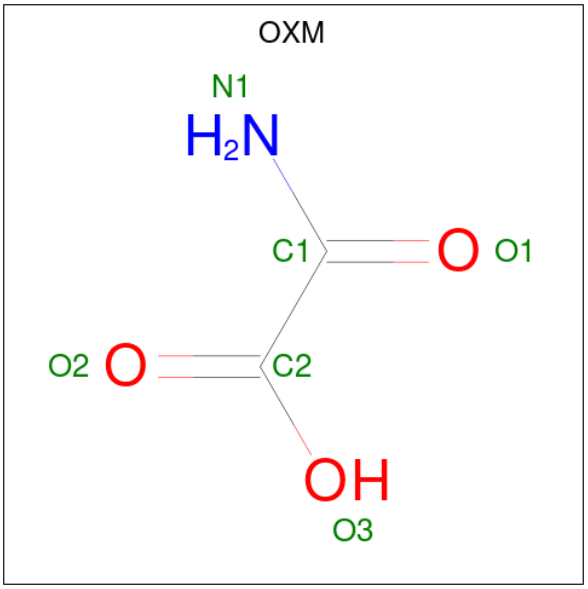
Chain	Residue	Modelled	Actual	Comment	Reference
C	496	LEU	-	expression tag	UNP G0Z9B7
C	497	VAL	-	expression tag	UNP G0Z9B7
C	498	PRO	-	expression tag	UNP G0Z9B7
C	499	ARG	-	expression tag	UNP G0Z9B7
D	1	GLY	-	expression tag	UNP G0Z9B7
D	2	SER	-	expression tag	UNP G0Z9B7
D	495	PHE	-	expression tag	UNP G0Z9B7
D	496	LEU	-	expression tag	UNP G0Z9B7
D	497	VAL	-	expression tag	UNP G0Z9B7
D	498	PRO	-	expression tag	UNP G0Z9B7
D	499	ARG	-	expression tag	UNP G0Z9B7
E	1	GLY	-	expression tag	UNP G0Z9B7
E	2	SER	-	expression tag	UNP G0Z9B7
E	495	PHE	-	expression tag	UNP G0Z9B7
E	496	LEU	-	expression tag	UNP G0Z9B7
E	497	VAL	-	expression tag	UNP G0Z9B7
E	498	PRO	-	expression tag	UNP G0Z9B7
E	499	ARG	-	expression tag	UNP G0Z9B7
F	1	GLY	-	expression tag	UNP G0Z9B7
F	2	SER	-	expression tag	UNP G0Z9B7
F	495	PHE	-	expression tag	UNP G0Z9B7
F	496	LEU	-	expression tag	UNP G0Z9B7
F	497	VAL	-	expression tag	UNP G0Z9B7
F	498	PRO	-	expression tag	UNP G0Z9B7
F	499	ARG	-	expression tag	UNP G0Z9B7

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



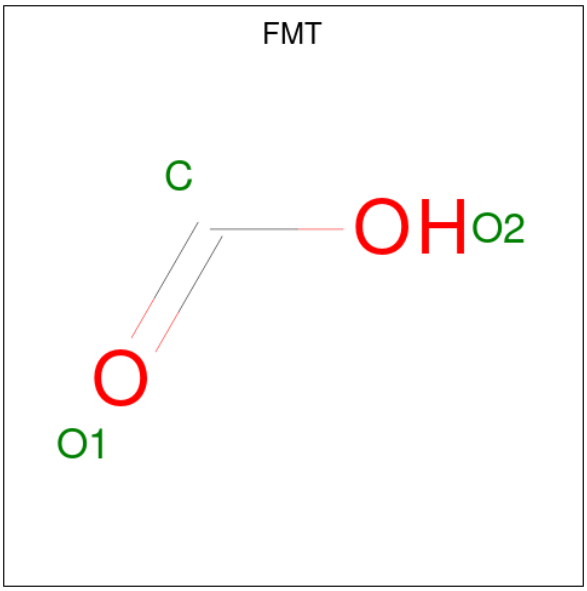
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	E	1	Total C N O 14 8 1 5	0	0
2	F	1	Total C N O 14 8 1 5	0	0
2	F	1	Total C N O 14 8 1 5	0	0

- Molecule 3 is OXAMIC ACID (three-letter code: OXM) (formula: $C_2H_3NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 6 2 1 3	0	0
3	A	1	Total C N O 6 2 1 3	0	0
3	B	1	Total C N O 6 2 1 3	0	0
3	C	1	Total C N O 6 2 1 3	0	0
3	D	1	Total C N O 6 2 1 3	0	0
3	E	1	Total C N O 6 2 1 3	0	0
3	F	1	Total C N O 6 2 1 3	0	0
3	F	1	Total C N O 6 2 1 3	0	0

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 3 1 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	215	Total O 216 216	0	2

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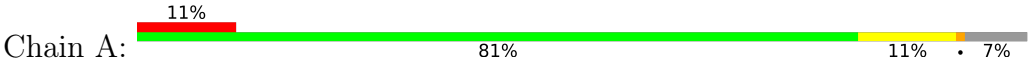
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	96	Total O 96 96	0	0
5	C	156	Total O 156 156	0	0
5	D	118	Total O 120 120	0	2
5	E	152	Total O 155 155	0	3
5	F	172	Total O 173 173	0	1

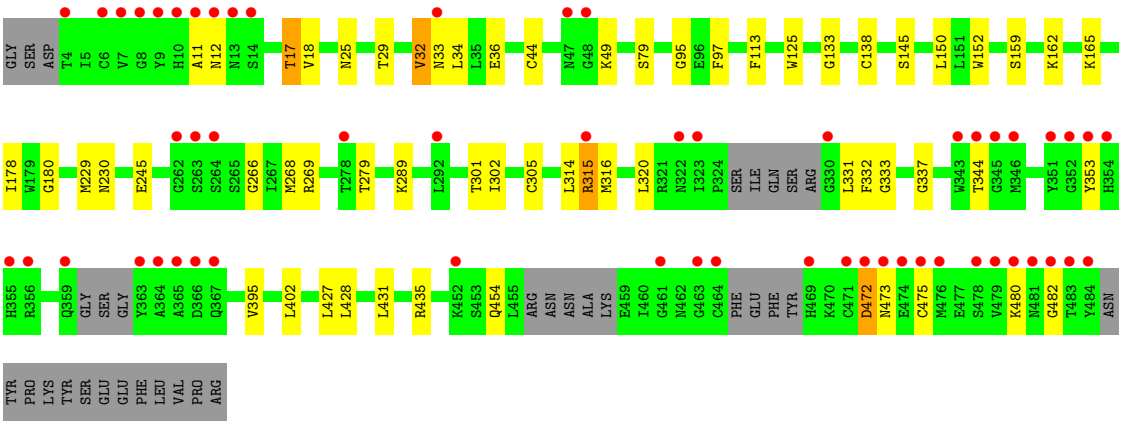
3 Residue-property plots (i)

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: Hemagglutinin

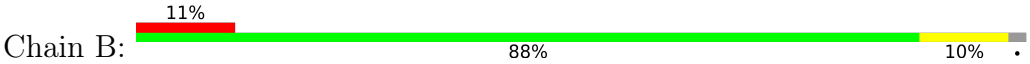
Chain A:

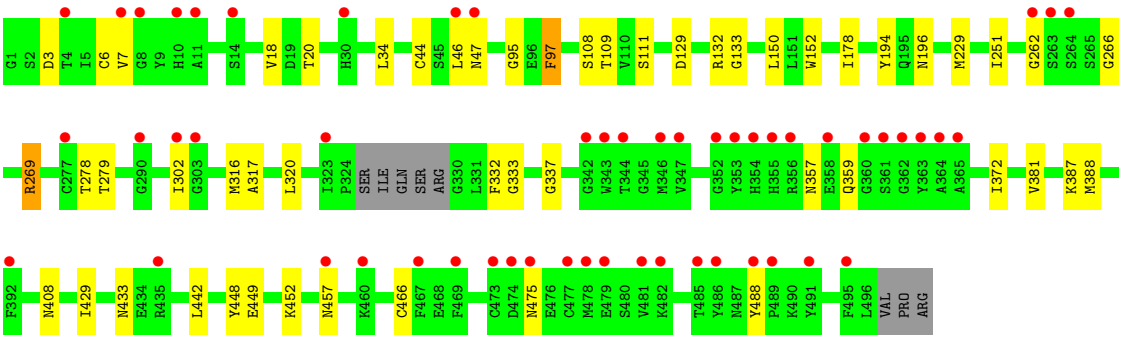




• Molecule 1: Hemagglutinin

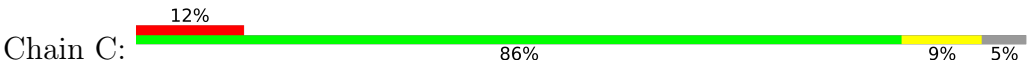
Chain B:

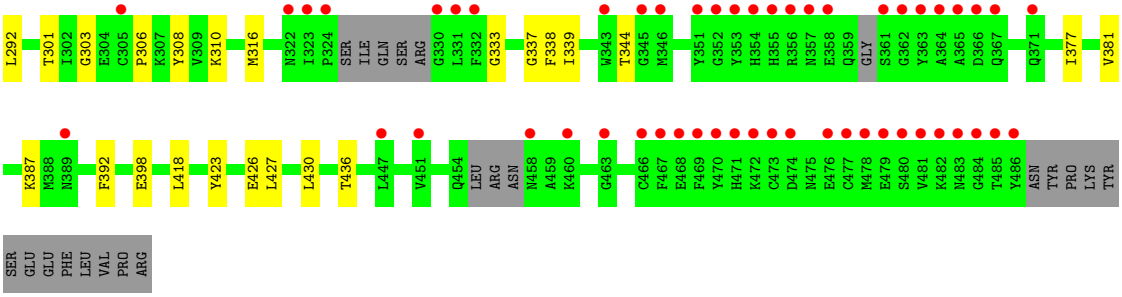




• Molecule 1: Hemagglutinin

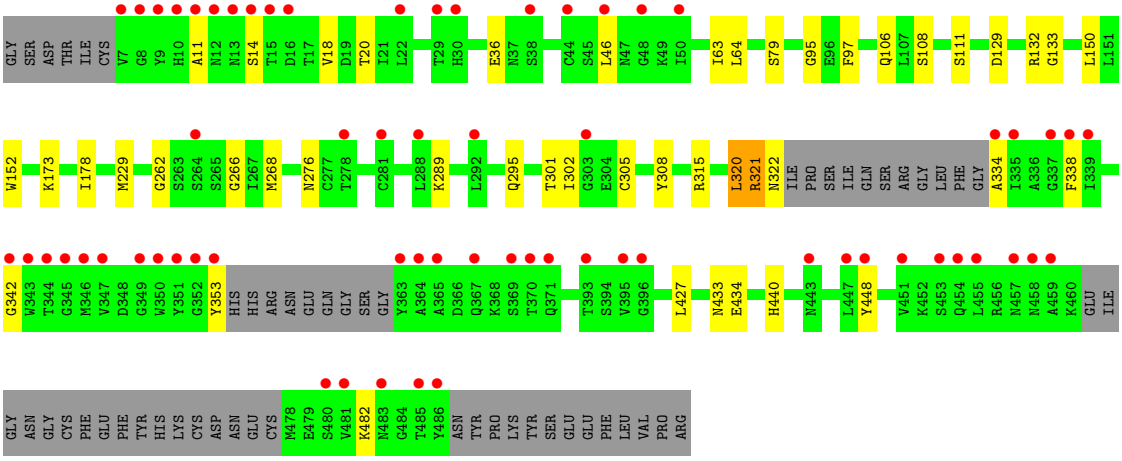
Chain C:





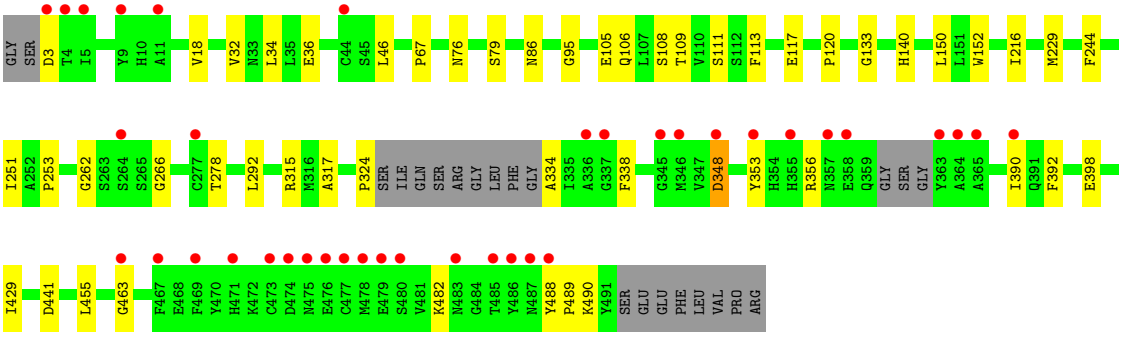
• Molecule 1: Hemagglutinin

Chain D:



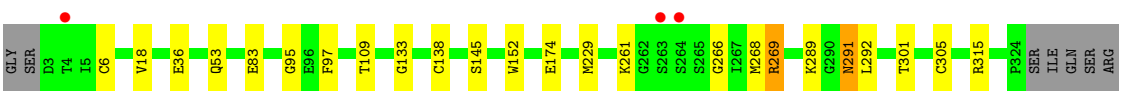
• Molecule 1: Hemagglutinin

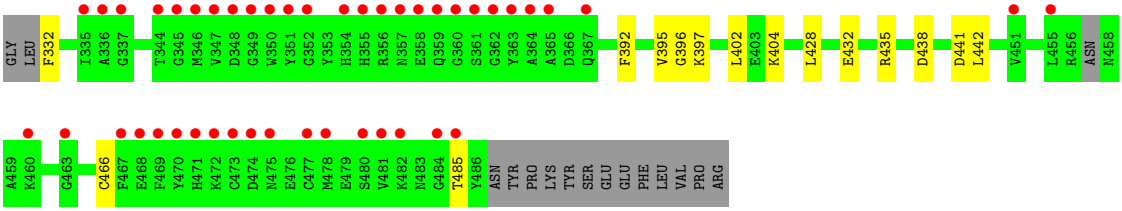
Chain E:



• Molecule 1: Hemagglutinin

Chain F:




GLY
LEU
F332
I335
A336
G337
T344
G345
M346
V347
D348
G349
W350
Y351
G352
Y353
H354
H355
R356
N357
E358
Q359
G360
S361
G362
Y363
A364
A365
D366
Q367
F392
V395
G396
K397
L402
E403
K404
L428
E432
R435
D438
D441
L442
V451
L455
R456
ASN
N458

A459
K460
G463
C466
F467
E468
F469
Y470
H471
K472
C473
D474
N475
E476
C477
M478
E479
S480
V481
K482
N483
G484
T485
Y486
ASN
TYR
PRO
LYS
TYR
SER
GLU
GLU
PHE
LEU
VAL
PRO
ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	67.30Å 113.33Å 130.12Å 110.16° 90.85° 90.28°	Depositor
Resolution (Å)	43.29 – 2.35 46.34 – 2.35	Depositor EDS
% Data completeness (in resolution range)	97.5 (43.29-2.35) 97.5 (46.34-2.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.179 , 0.225 0.180 , 0.224	Depositor DCC
R_{free} test set	2044 reflections (1.39%)	wwPDB-VP
Wilson B-factor (Å^2)	40.1	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 54.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	22584	wwPDB-VP
Average B, all atoms (Å^2)	60.0	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 22.75 % 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 5.3547e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: FMT, OXM, 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	0.43	0/3668	0.61	0/4985
1	B	0.39	0/3830	0.56	0/5216
1	C	0.41	0/3736	0.59	0/5086
1	D	0.40	0/3429	0.58	0/4672
1	E	0.41	0/3730	0.58	0/5086
1	F	0.43	0/3725	0.60	0/5066
All	All	0.41	0/22118	0.59	0/30111

There are no bond length outliers.

There are no bond angle outliers.

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	3577	0	3354	44	0
1	B	3729	0	3430	30	0
1	C	3630	0	3349	31	0
1	D	3344	0	3075	29	0
1	E	3631	0	3340	26	0
1	F	3636	0	3383	26	0
2	A	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	14	0	13	0	0
2	E	14	0	13	0	0
2	F	28	0	26	1	0
3	A	12	0	4	2	0
3	B	6	0	2	0	0
3	C	6	0	2	1	0
3	D	6	0	2	1	0
3	E	6	0	2	0	0
3	F	12	0	4	2	0
4	B	3	0	1	0	0
5	A	216	0	0	2	0
5	B	96	0	0	0	0
5	C	156	0	0	6	0
5	D	120	0	0	5	0
5	E	155	0	0	3	0
5	F	173	0	0	5	0
All	All	22584	0	20013	183	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 4.

All (183) 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:315:ARG:HA	1:A:315:ARG:CZ	1.90	1.00
1:A:33:ASN:HA	1:A:315:ARG:NH2	1.82	0.94
1:D:64:LEU:HD23	1:D:178[B]:ILE:HD11	1.51	0.91
1:A:32:VAL:O	1:A:315:ARG:NH1	2.12	0.82
1:F:266:GLY:HA3	1:F:395:VAL:HG11	1.61	0.79
1:A:33:ASN:HA	1:A:315:ARG:CZ	2.15	0.77
3:A:502:OXM:N1	5:A:601:HOH:O	2.16	0.75
1:E:34:LEU:HD12	1:E:429:ILE:HD11	1.70	0.73
3:C:700:OXM:N1	5:C:801:HOH:O	2.14	0.72
1:C:219[A]:ARG:NH2	5:C:804:HOH:O	2.23	0.70
1:D:133:GLY:HA3	1:D:152:TRP:HB3	1.73	0.70
1:F:133:GLY:HA3	1:F:152:TRP:HB3	1.74	0.70
1:A:315:ARG:NH1	1:A:316:MET:H	1.92	0.68
1:A:162:LYS:NZ	1:A:245:GLU:OE2	2.28	0.66
1:A:315:ARG:HA	1:A:315:ARG:NH2	2.11	0.66
1:D:111:SER:HB3	1:D:262:GLY:HA3	1.77	0.65
1:B:457:ASN:OD1	1:B:488:TYR:OH	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:ARG:NH2	1:C:155:LYS:O	2.31	0.64
1:D:268:MET:HE3	1:D:302:ILE:HD12	1.81	0.62
1:B:46:LEU:HD21	1:B:302:ILE:HG22	1.81	0.61
1:E:86:ASN:ND2	5:E:602:HOH:O	2.33	0.61
1:A:314:LEU:O	1:A:315:ARG:NH2	2.34	0.61
1:A:95:GLY:HA3	1:A:229:MET:O	2.01	0.60
1:F:332:PHE:HE2	1:F:438:ASP:HB3	1.65	0.60
1:F:95:GLY:HA3	1:F:229:MET:O	2.01	0.59
1:F:83:GLU:OE1	3:F:504:OXM:N1	2.35	0.59
1:C:283:THR:HG22	1:C:301:THR:HG22	1.83	0.59
1:C:316:MET:HE3	1:C:381:VAL:HG22	1.84	0.59
1:F:269:ARG:NH1	5:F:601:HOH:O	2.29	0.59
1:D:129:ASP:OD2	1:D:132:ARG:NH1	2.36	0.58
2:F:502:NAG:H3	2:F:502:NAG:H83	1.86	0.58
1:B:95:GLY:HA3	1:B:229:MET:O	2.05	0.57
1:C:133:GLY:HA3	1:C:152:TRP:HB3	1.86	0.57
1:E:67:PRO:HB2	1:E:140:HIS:HB2	1.87	0.56
1:C:95:GLY:HA3	1:C:229:MET:O	2.06	0.56
1:D:95:GLY:HA3	1:D:229:MET:O	2.06	0.55
1:D:322:ASN:OD1	5:D:801:HOH:O	2.18	0.55
1:B:129:ASP:OD2	1:B:132:ARG:NH1	2.40	0.55
1:A:315:ARG:HA	1:A:315:ARG:NE	2.22	0.55
1:A:34:LEU:H	1:A:315:ARG:NH2	2.05	0.55
1:E:133:GLY:HA3	1:E:152:TRP:HB3	1.88	0.55
1:D:64:LEU:CD2	1:D:178[B]:ILE:HD11	2.30	0.55
1:E:348:ASP:OD1	1:E:348:ASP:N	2.32	0.55
1:B:34:LEU:HD12	1:B:429:ILE:HD11	1.89	0.54
1:A:427:LEU:HD21	1:F:428:LEU:HD13	1.90	0.54
1:B:316:MET:HE3	1:B:381:VAL:HG22	1.90	0.54
1:D:276:ASN:ND2	5:D:804:HOH:O	2.35	0.53
1:C:56:ASN:HB2	5:C:911:HOH:O	2.08	0.53
1:F:397[A]:LYS:HB3	5:F:746:HOH:O	2.09	0.53
1:B:108:SER:HB3	1:B:266:GLY:HA2	1.91	0.53
1:D:320:LEU:HD12	1:D:321:ARG:O	2.09	0.52
1:B:133:GLY:HA3	1:B:152:TRP:HB3	1.91	0.52
1:E:18:VAL:HG21	1:E:317:ALA:HB2	1.90	0.52
1:E:398:GLU:OE1	5:E:601:HOH:O	2.19	0.52
1:A:353:TYR:CD1	1:A:480:LYS:HG2	2.45	0.52
1:F:432:GLU:OE2	1:F:435:ARG:NH1	2.43	0.52
1:A:454:GLN:HE22	1:A:482:GLY:HA2	1.76	0.51
1:A:12:ASN:HD21	1:A:29:THR:HB	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:95:GLY:HA3	1:E:229:MET:O	2.10	0.51
1:A:431:LEU:O	1:A:435:ARG:HG3	2.11	0.51
1:D:353:TYR:CD1	1:D:482:LYS:HG2	2.45	0.51
1:D:108:SER:HB2	1:D:266:GLY:HA2	1.92	0.50
1:F:397[B]:LYS:HB3	5:F:746:HOH:O	2.10	0.50
1:C:303:GLY:HA2	1:C:392:PHE:CE2	2.45	0.50
1:B:387:LYS:HD2	1:C:426:GLU:HB3	1.92	0.50
1:F:18:VAL:HG12	1:F:315:ARG:HG2	1.94	0.50
1:D:150:LEU:HD21	1:D:178[A]:ILE:HG13	1.93	0.50
1:F:53[B]:GLN:NE2	5:F:604:HOH:O	2.44	0.50
1:F:269:ARG:HG2	3:F:504:OXM:N1	2.27	0.50
1:E:488:TYR:O	1:E:490:LYS:N	2.38	0.49
3:D:700:OXM:N1	5:D:802:HOH:O	2.24	0.49
1:E:3:ASP:HA	1:E:356:ARG:O	2.11	0.49
1:A:268:MET:HE3	1:A:302:ILE:HD12	1.95	0.49
1:C:215[B]:GLU:OE1	5:C:802:HOH:O	2.19	0.49
1:D:18:VAL:HG12	1:D:315:ARG:HG2	1.94	0.49
1:D:301:THR:HB	1:D:305:CYS:SG	2.53	0.49
1:D:334:ALA:HA	1:D:338:PHE:CE1	2.47	0.48
1:F:6:CYS:HA	1:F:466:CYS:HA	1.95	0.48
1:A:133:GLY:HA3	1:A:152:TRP:HB3	1.95	0.48
1:D:63:ILE:HG22	1:D:178[B]:ILE:HD12	1.95	0.48
1:F:395:VAL:HG23	1:F:396:GLY:O	2.13	0.48
1:E:111:SER:HB3	1:E:262:GLY:HA3	1.96	0.48
1:E:46:LEU:HB2	1:E:79:SER:HB2	1.95	0.48
1:A:12:ASN:ND2	1:A:29:THR:HB	2.28	0.48
1:B:150:LEU:HD21	1:B:178[A]:ILE:HG23	1.95	0.48
1:A:17:THR:OG1	1:A:25:ASN:HA	2.13	0.48
1:C:308:TYR:CD2	1:C:418:LEU:HD13	2.49	0.48
1:B:20:THR:HG22	1:B:433:ASN:HB3	1.96	0.47
1:A:49:LYS:HB3	1:A:79:SER:HB3	1.97	0.47
1:C:11:ALA:O	1:C:344:THR:HA	2.15	0.47
1:C:338:PHE:CD1	1:C:339:ILE:HG13	2.50	0.47
1:E:106:GLN:O	1:E:109:THR:HG22	2.14	0.47
1:A:125:TRP:CZ3	1:A:165[B]:LYS:HG3	2.50	0.47
1:C:129:ASP:OD2	1:C:132:ARG:NH1	2.48	0.47
1:F:289:LYS:HB3	1:F:291:ASN:ND2	2.30	0.47
1:E:108:SER:HB3	1:E:266:GLY:HA2	1.96	0.46
1:B:269:ARG:HH21	1:B:269:ARG:HG3	1.81	0.46
1:F:174:GLU:HG2	5:F:681:HOH:O	2.15	0.46
1:B:3:ASP:OD1	1:B:357:ASN:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:LEU:HG	1:F:442:LEU:HD23	1.97	0.46
1:A:301:THR:HB	1:A:305:CYS:SG	2.54	0.46
1:B:359:GLN:NE2	1:B:475:ASN:H	2.14	0.46
1:E:338:PHE:HB2	1:E:463:GLY:O	2.16	0.46
1:E:36:GLU:HG3	1:E:292:LEU:HB2	1.98	0.46
1:F:332:PHE:N	1:F:441:ASP:OD2	2.49	0.46
1:A:428:LEU:HD13	1:D:427:LEU:HD21	1.98	0.46
1:F:301:THR:HB	1:F:305:CYS:SG	2.55	0.46
1:A:333:GLY:O	1:A:337:GLY:HA3	2.16	0.46
1:A:266:GLY:HA3	1:A:395:VAL:HG11	1.99	0.45
1:C:398:GLU:OE1	5:C:803:HOH:O	2.21	0.45
1:C:377:ILE:HD12	1:C:436:THR:HG23	1.98	0.45
1:F:109:THR:OG1	1:F:261:LYS:HD2	2.16	0.45
1:C:183:HIS:CE1	1:C:214:PRO:HA	2.52	0.45
1:E:76:ASN:HA	1:E:113:PHE:HB3	1.97	0.45
1:C:377:ILE:O	1:C:381:VAL:HG23	2.17	0.45
1:A:315:ARG:CZ	1:A:315:ARG:CA	2.81	0.45
1:C:269:ARG:NH1	5:C:817:HOH:O	2.49	0.44
1:A:36:GLU:OE2	1:A:289:LYS:N	2.49	0.44
1:D:295:GLN:O	1:D:308:TYR:HA	2.17	0.44
1:A:18:VAL:HG12	1:A:315:ARG:HG3	1.98	0.44
1:D:20:THR:HB	1:D:434:GLU:HB2	1.98	0.44
1:D:36:GLU:OE2	1:D:289:LYS:N	2.51	0.44
1:B:333:GLY:O	1:B:337:GLY:HA3	2.18	0.43
1:C:423:TYR:CE2	1:C:427:LEU:HD22	2.52	0.43
1:C:117:GLU:HG2	1:C:120:PRO:HA	1.99	0.43
1:E:18:VAL:HG12	1:E:315:ARG:HG2	2.01	0.43
1:B:150:LEU:HB3	1:B:251:ILE:HG22	2.01	0.43
1:D:20:THR:HG22	1:D:433:ASN:HB3	2.00	0.43
1:D:106:GLN:NE2	1:F:404:LYS:HG3	2.33	0.43
1:B:388:MET:HG2	1:C:423:TYR:CE1	2.53	0.43
1:A:138:CYS:O	1:A:145:SER:HB3	2.18	0.43
1:D:353:TYR:CE1	1:D:482:LYS:HG2	2.54	0.43
1:B:97:PHE:CZ	1:B:178[A]:ILE:HD11	2.54	0.43
1:B:332:PHE:CD1	1:B:442:LEU:HD13	2.54	0.43
1:C:292:LEU:O	1:C:306:PRO:HB3	2.19	0.43
1:A:11:ALA:O	1:A:344:THR:HA	2.19	0.42
1:C:316:MET:HE1	1:C:381:VAL:HA	2.00	0.42
1:A:331:LEU:HD23	1:A:332:PHE:CE1	2.54	0.42
1:E:46:LEU:HD23	1:E:46:LEU:HA	1.93	0.42
1:E:334:ALA:HB3	1:E:441:ASP:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:THR:HG22	1:C:264:SER:HA	2.00	0.42
1:C:338:PHE:CE1	1:C:339:ILE:HG13	2.55	0.42
1:B:18:VAL:HG21	1:B:317:ALA:HB2	2.01	0.42
1:D:14:SER:N	5:D:801:HOH:O	2.52	0.42
1:B:449:GLU:HA	1:B:452:LYS:HB3	2.01	0.42
1:C:333:GLY:O	1:C:337:GLY:HA3	2.19	0.42
1:A:315:ARG:NH1	1:A:316:MET:N	2.65	0.42
1:C:387:LYS:HD3	1:C:387:LYS:HA	1.88	0.42
1:E:150:LEU:HB3	1:E:251:ILE:HG22	2.02	0.42
1:C:310:LYS:HG3	1:C:418:LEU:HD11	2.00	0.42
1:A:472:ASP:CG	1:A:473:ASN:H	2.23	0.42
1:B:44:CYS:HB2	1:B:279:THR:HG22	2.00	0.42
1:B:408:ASN:ND2	1:E:105:GLU:OE2	2.32	0.42
1:B:111:SER:HB3	1:B:262:GLY:HA3	2.01	0.41
1:D:46:LEU:HB3	1:D:79:SER:HB2	2.01	0.41
1:C:92:CYS:O	1:C:223:ARG:NE	2.34	0.41
1:F:36:GLU:HG3	1:F:292:LEU:HB2	2.02	0.41
1:E:390:ILE:HA	5:E:727:HOH:O	2.21	0.41
1:A:32:VAL:C	1:A:315:ARG:NH1	2.73	0.41
1:B:6:CYS:HA	1:B:466:CYS:HA	2.03	0.41
1:A:18:VAL:HG12	1:A:315:ARG:CG	2.50	0.41
1:A:269:ARG:NH2	3:A:503:OXM:O1	2.54	0.41
1:A:402:LEU:HD23	1:A:402:LEU:HA	1.94	0.41
1:E:117:GLU:HG2	1:E:120:PRO:HA	2.02	0.41
1:A:150:LEU:HD21	1:A:178[A]:ILE:HG13	2.03	0.41
1:A:180:GLY:HA2	1:A:230:ASN:O	2.21	0.41
1:B:316:MET:CE	1:B:381:VAL:HG22	2.51	0.41
1:B:320:LEU:H	1:B:320:LEU:HG	1.72	0.41
1:D:97:PHE:HB2	5:D:873:HOH:O	2.21	0.41
1:D:320:LEU:HB3	1:D:440:HIS:CG	2.55	0.41
1:E:353:TYR:CD1	1:E:482:LYS:HG2	2.56	0.41
1:F:138:CYS:O	1:F:145:SER:HB3	2.21	0.41
1:A:44:CYS:HB2	1:A:279:THR:HG22	2.03	0.41
1:D:11:ALA:HB2	1:D:342:GLY:HA3	2.03	0.41
1:F:402:LEU:HD23	1:F:402:LEU:HA	1.91	0.41
1:A:395:VAL:HG22	5:A:690:HOH:O	2.20	0.40
1:B:194:TYR:O	1:B:196:ASN:N	2.51	0.40
1:C:132:ARG:HH21	1:C:154:VAL:HG23	1.86	0.40
1:F:485:THR:O	1:F:485:THR:OG1	2.36	0.40
1:A:32:VAL:O	1:A:315:ARG:CZ	2.67	0.40
1:B:7:VAL:HG21	1:B:448:TYR:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:244:PHE:CZ	1:E:253:PRO:HG2	2.56	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	460/499 (92%)	443 (96%)	16 (4%)	1 (0%)	47	56
1	B	492/499 (99%)	474 (96%)	17 (4%)	1 (0%)	47	56
1	C	475/499 (95%)	463 (98%)	12 (2%)	0	100	100
1	D	438/499 (88%)	425 (97%)	13 (3%)	0	100	100
1	E	475/499 (95%)	457 (96%)	16 (3%)	2 (0%)	34	38
1	F	473/499 (95%)	458 (97%)	14 (3%)	1 (0%)	47	56
All	All	2813/2994 (94%)	2720 (97%)	88 (3%)	5 (0%)	47	56

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	392	PHE
1	B	47	ASN
1	A	472	ASP
1	E	489	PRO
1	E	392	PHE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	376/435 (86%)	368 (98%)	8 (2%)	53	65
1	B	378/435 (87%)	373 (99%)	5 (1%)	69	80
1	C	370/435 (85%)	364 (98%)	6 (2%)	62	75
1	D	337/435 (78%)	333 (99%)	4 (1%)	71	82
1	E	375/435 (86%)	369 (98%)	6 (2%)	62	75
1	F	377/435 (87%)	373 (99%)	4 (1%)	73	84
All	All	2213/2610 (85%)	2180 (98%)	33 (2%)	65	76

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	THR
1	A	32	VAL
1	A	97	PHE
1	A	113	PHE
1	A	159	SER
1	A	315	ARG
1	A	320	LEU
1	A	475	CYS
1	B	97	PHE
1	B	109	THR
1	B	269	ARG
1	B	278	THR
1	B	372	ILE
1	C	97	PHE
1	C	215[A]	GLU
1	C	215[B]	GLU
1	C	216	ILE
1	C	269	ARG
1	C	430	LEU
1	D	173	LYS
1	D	320	LEU
1	D	321	ARG
1	D	448	TYR
1	E	32	VAL
1	E	216	ILE
1	E	278	THR
1	E	324	PRO

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Mol	Chain	Res	Type
1	E	348	ASP
1	E	455	LEU
1	F	97	PHE
1	F	268	MET
1	F	269	ARG
1	F	291	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	GLN
1	A	454	GLN
1	B	389	ASN
1	B	487	ASN
1	E	471	HIS
1	E	483	ASN
1	F	291	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

14 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	OXM	F	503	-	5,5,5	3.18	2 (40%)	4,6,6	1.51	1 (25%)
3	OXM	F	504	-	5,5,5	2.35	1 (20%)	4,6,6	1.68	1 (25%)
3	OXM	C	700	-	5,5,5	3.81	1 (20%)	4,6,6	1.48	0
2	NAG	A	501	1	14,14,15	0.24	0	17,19,21	0.38	0
3	OXM	A	503	-	5,5,5	2.37	1 (20%)	4,6,6	1.93	1 (25%)
2	NAG	E	501	1	14,14,15	0.33	0	17,19,21	0.36	0
2	NAG	B	501	1	14,14,15	0.68	1 (7%)	17,19,21	0.44	0
3	OXM	A	502	-	5,5,5	3.95	2 (40%)	4,6,6	0.96	0
3	OXM	B	502	-	5,5,5	3.54	2 (40%)	4,6,6	1.96	2 (50%)
4	FMT	B	503	-	2,2,2	0.65	0	1,1,1	0.25	0
3	OXM	D	700	-	5,5,5	3.28	2 (40%)	4,6,6	1.34	0
3	OXM	E	502	-	5,5,5	3.11	2 (40%)	4,6,6	1.50	1 (25%)
2	NAG	F	501	1	14,14,15	0.59	0	17,19,21	0.68	1 (5%)
2	NAG	F	502	1	14,14,15	0.53	0	17,19,21	1.49	2 (11%)

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	OXM	F	503	-	-	3/3/4/4	-
3	OXM	F	504	-	-	3/3/4/4	-
3	OXM	C	700	-	-	3/3/4/4	-
2	NAG	A	501	1	-	2/6/23/26	0/1/1/1
3	OXM	A	503	-	-	3/3/4/4	-
2	NAG	E	501	1	-	2/6/23/26	0/1/1/1
2	NAG	B	501	1	-	2/6/23/26	0/1/1/1
3	OXM	A	502	-	-	3/3/4/4	-
3	OXM	B	502	-	-	3/3/4/4	-
3	OXM	D	700	-	-	3/3/4/4	-
3	OXM	E	502	-	-	3/3/4/4	-
2	NAG	F	501	1	-	2/6/23/26	0/1/1/1
2	NAG	F	502	1	-	5/6/23/26	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	OXM	C1-C2	-8.35	1.44	1.55
3	C	700	OXM	C1-C2	-8.22	1.45	1.55
3	B	502	OXM	C1-C2	-7.57	1.45	1.55
3	D	700	OXM	C1-C2	-6.93	1.46	1.55
3	F	503	OXM	C1-C2	-6.73	1.46	1.55
3	E	502	OXM	C1-C2	-6.37	1.47	1.55
3	A	503	OXM	C1-C2	-4.83	1.49	1.55
3	F	504	OXM	C1-C2	-4.71	1.49	1.55
3	A	502	OXM	O3-C2	-2.76	1.22	1.30
3	E	502	OXM	O3-C2	-2.68	1.22	1.30
3	B	502	OXM	O3-C2	-2.31	1.23	1.30
2	B	501	NAG	O5-C1	-2.29	1.40	1.43
3	D	700	OXM	O3-C2	-2.29	1.23	1.30
3	F	503	OXM	O3-C2	-2.18	1.24	1.30

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	502	NAG	C2-N2-C7	4.43	129.21	122.90
3	A	503	OXM	O3-C2-C1	3.10	121.00	113.84
3	B	502	OXM	O3-C2-C1	3.08	120.96	113.84
2	F	502	NAG	C1-C2-N2	2.90	115.45	110.49
3	F	504	OXM	O3-C2-C1	2.72	120.13	113.84
3	E	502	OXM	O3-C2-C1	2.47	119.55	113.84
3	F	503	OXM	O3-C2-C1	2.43	119.46	113.84
3	B	502	OXM	O2-C2-C1	-2.16	117.26	122.06
2	F	501	NAG	C1-O5-C5	2.08	115.00	112.19

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	OXM	N1-C1-C2-O2
3	A	502	OXM	N1-C1-C2-O3
3	A	503	OXM	N1-C1-C2-O2
3	A	503	OXM	N1-C1-C2-O3
3	B	502	OXM	N1-C1-C2-O3
3	C	700	OXM	N1-C1-C2-O2
3	C	700	OXM	N1-C1-C2-O3
3	D	700	OXM	N1-C1-C2-O2
3	D	700	OXM	N1-C1-C2-O3

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Mol	Chain	Res	Type	Atoms
3	D	700	OXM	O1-C1-C2-O2
3	E	502	OXM	N1-C1-C2-O2
3	E	502	OXM	N1-C1-C2-O3
3	F	503	OXM	N1-C1-C2-O2
3	F	503	OXM	N1-C1-C2-O3
3	F	504	OXM	N1-C1-C2-O2
3	F	504	OXM	N1-C1-C2-O3
2	E	501	NAG	C4-C5-C6-O6
2	F	502	NAG	O5-C5-C6-O6
2	E	501	NAG	O5-C5-C6-O6
2	F	502	NAG	C4-C5-C6-O6
2	F	502	NAG	C8-C7-N2-C2
2	F	502	NAG	O7-C7-N2-C2
2	B	501	NAG	O5-C5-C6-O6
2	B	501	NAG	C4-C5-C6-O6
3	A	503	OXM	O1-C1-C2-O2
2	A	501	NAG	C4-C5-C6-O6
3	A	502	OXM	O1-C1-C2-O2
3	C	700	OXM	O1-C1-C2-O2
3	E	502	OXM	O1-C1-C2-O2
3	F	503	OXM	O1-C1-C2-O2
3	F	504	OXM	O1-C1-C2-O2
2	A	501	NAG	O5-C5-C6-O6
2	F	502	NAG	C3-C2-N2-C7
3	B	502	OXM	N1-C1-C2-O2
3	B	502	OXM	O1-C1-C2-O2
2	F	501	NAG	C3-C2-N2-C7
2	F	501	NAG	C1-C2-N2-C7

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	504	OXM	2	0
3	C	700	OXM	1	0
3	A	503	OXM	1	0
3	A	502	OXM	1	0
3	D	700	OXM	1	0
2	F	502	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	466/499 (93%)	0.67	56 (12%) 4 7	21, 50, 123, 145	0
1	B	491/499 (98%)	0.53	54 (10%) 5 8	28, 65, 108, 125	0
1	C	476/499 (95%)	0.60	61 (12%) 3 6	22, 58, 116, 150	0
1	D	443/499 (88%)	0.67	65 (14%) 2 3	26, 61, 129, 151	0
1	E	477/499 (95%)	0.38	38 (7%) 12 18	25, 55, 104, 132	0
1	F	476/499 (95%)	0.45	48 (10%) 7 11	23, 51, 108, 133	0
All	All	2829/2994 (94%)	0.55	322 (11%) 5 7	21, 57, 115, 151	0

All (322) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	484	TYR	10.9
1	D	345	GLY	9.5
1	A	352	GLY	9.0
1	C	467	PHE	7.6
1	D	8	GLY	7.4
1	D	364	ALA	7.1
1	D	346	MET	7.0
1	F	360	GLY	6.9
1	A	364	ALA	6.8
1	C	481	VAL	6.6
1	A	345	GLY	6.4
1	D	343	TRP	6.4
1	C	451	VAL	6.3
1	A	476	MET	6.3
1	F	460	LYS	6.1
1	F	364	ALA	6.1
1	A	8	GLY	6.0
1	E	469	PHE	6.0
1	A	463	GLY	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	363	TYR	5.8
1	D	334	ALA	5.6
1	C	469	PHE	5.6
1	A	6	CYS	5.6
1	B	354	HIS	5.5
1	F	478	MET	5.5
1	D	352	GLY	5.4
1	B	364	ALA	5.4
1	A	4	THR	5.4
1	C	473	CYS	5.4
1	F	337	GLY	5.3
1	F	475	ASN	5.2
1	A	472	ASP	5.1
1	A	471	CYS	5.1
1	B	362	GLY	5.1
1	A	343	TRP	5.1
1	E	473	CYS	5.0
1	F	451	VAL	5.0
1	C	482	LYS	5.0
1	C	478	MET	5.0
1	E	337	GLY	5.0
1	A	475	CYS	4.9
1	B	478	MET	4.9
1	A	461	GLY	4.9
1	A	14	SER	4.9
1	E	346	MET	4.9
1	D	454	GLN	4.9
1	D	447	LEU	4.8
1	A	353	TYR	4.8
1	C	463	GLY	4.8
1	A	351	TYR	4.7
1	D	7	VAL	4.7
1	C	477	CYS	4.7
1	E	355	HIS	4.7
1	C	483	ASN	4.7
1	C	355	HIS	4.7
1	B	360	GLY	4.7
1	A	264	SER	4.6
1	D	485	THR	4.6
1	C	264	SER	4.6
1	C	458	ASN	4.6
1	D	396	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	483	THR	4.6
1	C	351	TYR	4.6
1	C	486	TYR	4.5
1	B	46	LEU	4.5
1	A	7	VAL	4.5
1	C	364	ALA	4.4
1	D	483	ASN	4.4
1	E	358	GLU	4.4
1	C	356	ARG	4.4
1	D	486	TYR	4.4
1	B	290	GLY	4.3
1	B	264	SER	4.3
1	D	453	SER	4.3
1	F	470	TYR	4.3
1	D	365	ALA	4.3
1	D	13	ASN	4.3
1	E	478	MET	4.3
1	A	346	MET	4.2
1	F	473	CYS	4.2
1	D	363	TYR	4.2
1	F	471	HIS	4.2
1	B	365	ALA	4.1
1	F	362	GLY	4.1
1	A	330	GLY	4.1
1	E	486	TYR	4.0
1	C	474	ASP	4.0
1	E	365	ALA	4.0
1	F	356	ARG	4.0
1	B	457	ASN	4.0
1	C	353	TYR	3.9
1	D	10	HIS	3.9
1	C	476	GLU	3.9
1	B	352	GLY	3.9
1	D	347	VAL	3.9
1	B	353	TYR	3.8
1	C	470	TYR	3.8
1	E	348	ASP	3.8
1	A	474	GLU	3.8
1	C	330	GLY	3.8
1	A	355	HIS	3.8
1	F	355	HIS	3.8
1	C	354	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	480	SER	3.8
1	B	7	VAL	3.8
1	E	4	THR	3.8
1	C	466	CYS	3.8
1	F	352	GLY	3.7
1	B	481	VAL	3.7
1	F	469	PHE	3.7
1	C	361	SER	3.7
1	F	467	PHE	3.7
1	F	363	TYR	3.7
1	C	362	GLY	3.7
1	A	464	CYS	3.7
1	A	323	ILE	3.6
1	F	361	SER	3.6
1	F	345	GLY	3.6
1	C	332	PHE	3.6
1	A	354	HIS	3.6
1	C	47	ASN	3.6
1	F	4	THR	3.6
1	D	353	TYR	3.6
1	F	336	ALA	3.5
1	A	263	SER	3.5
1	D	337	GLY	3.5
1	D	349	GLY	3.5
1	B	469	PHE	3.5
1	F	474	ASP	3.5
1	D	480	SER	3.4
1	E	477	CYS	3.4
1	F	455	LEU	3.4
1	F	335	ILE	3.4
1	F	348	ASP	3.4
1	D	351	TYR	3.4
1	D	292	LEU	3.4
1	E	480	SER	3.3
1	D	9	TYR	3.3
1	C	46	LEU	3.3
1	C	363	TYR	3.3
1	B	392	PHE	3.3
1	D	14	SER	3.3
1	B	4	THR	3.3
1	F	357	ASN	3.3
1	D	44	CYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	480	LYS	3.3
1	F	463	GLY	3.3
1	F	359	GLN	3.3
1	D	12	ASN	3.3
1	A	262	GLY	3.3
1	F	349	GLY	3.3
1	F	468	GLU	3.3
1	D	30	HIS	3.2
1	B	482	LYS	3.2
1	F	477	CYS	3.2
1	B	8	GLY	3.2
1	C	365	ALA	3.2
1	A	322	ASN	3.2
1	D	15	THR	3.2
1	B	479	GLU	3.2
1	D	459	ALA	3.2
1	A	356	ARG	3.2
1	E	363	TYR	3.1
1	D	29	THR	3.1
1	E	488	TYR	3.1
1	A	13	ASN	3.1
1	D	443	ASN	3.1
1	B	347	VAL	3.1
1	D	448	TYR	3.1
1	F	482	LYS	3.1
1	B	302	ILE	3.1
1	E	474	ASP	3.0
1	E	471	HIS	3.0
1	D	393	THR	3.0
1	E	364	ALA	3.0
1	A	315	ARG	3.0
1	F	472	LYS	3.0
1	D	344	THR	3.0
1	B	477	CYS	3.0
1	E	463	GLY	2.9
1	F	354	HIS	2.9
1	A	12	ASN	2.9
1	D	264	SER	2.9
1	C	479	GLU	2.9
1	D	369	SER	2.9
1	E	336	ALA	2.9
1	C	323	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	16	ASP	2.9
1	F	264	SER	2.9
1	B	488	TYR	2.9
1	C	305	CYS	2.9
1	C	13	ASN	2.9
1	B	358	GLU	2.9
1	B	474	ASP	2.9
1	E	9	TYR	2.9
1	B	342	GLY	2.8
1	D	451	VAL	2.8
1	D	367	GLN	2.8
1	C	352	GLY	2.8
1	E	5	ILE	2.8
1	A	365	ALA	2.8
1	E	357	ASN	2.8
1	E	487	ASN	2.8
1	D	342	GLY	2.8
1	D	288	LEU	2.8
1	D	335	ILE	2.8
1	B	361	SER	2.7
1	E	475	ASN	2.7
1	E	345	GLY	2.7
1	C	447	LEU	2.7
1	B	355	HIS	2.7
1	E	11	ALA	2.7
1	F	480	SER	2.7
1	C	343	TRP	2.7
1	A	367	GLN	2.7
1	A	482	GLY	2.7
1	C	6	CYS	2.7
1	D	395	VAL	2.7
1	E	3	ASP	2.7
1	C	484	GLY	2.7
1	A	366	ASP	2.6
1	A	33	ASN	2.6
1	D	50	ILE	2.6
1	B	467	PHE	2.6
1	D	278	THR	2.6
1	A	48	GLY	2.6
1	A	481	ASN	2.6
1	C	468	GLU	2.6
1	C	3	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	491	TYR	2.6
1	F	350	TRP	2.6
1	E	264	SER	2.6
1	A	479	VAL	2.6
1	C	472	LYS	2.6
1	B	346	MET	2.6
1	A	469	HIS	2.6
1	C	471	HIS	2.6
1	D	303	GLY	2.6
1	D	455	LEU	2.5
1	C	358	GLU	2.5
1	C	346	MET	2.5
1	C	322	ASN	2.5
1	F	344	THR	2.5
1	B	262	GLY	2.5
1	D	457	ASN	2.5
1	F	347	VAL	2.5
1	D	281	CYS	2.5
1	A	359	GLN	2.5
1	F	481	VAL	2.5
1	F	365	ALA	2.5
1	B	303	GLY	2.5
1	C	367	GLN	2.5
1	C	331	LEU	2.5
1	A	11	ALA	2.4
1	D	338	PHE	2.4
1	F	485	THR	2.4
1	D	370	THR	2.4
1	B	343	TRP	2.4
1	D	46	LEU	2.4
1	F	263	SER	2.4
1	B	10	HIS	2.4
1	B	435	ARG	2.4
1	E	277	CYS	2.4
1	D	371	GLN	2.4
1	B	47	ASN	2.4
1	F	358	GLU	2.4
1	B	363	TYR	2.4
1	D	350	TRP	2.4
1	F	346	MET	2.4
1	A	344	THR	2.4
1	B	263	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	475	ASN	2.4
1	C	44	CYS	2.4
1	E	390	ILE	2.3
1	A	478	SER	2.3
1	D	458	ASN	2.3
1	A	278	THR	2.3
1	E	476	GLU	2.3
1	C	345	GLY	2.3
1	A	9	TYR	2.3
1	B	486	TYR	2.3
1	E	483	ASN	2.3
1	D	38	SER	2.3
1	B	460	LYS	2.3
1	A	10	HIS	2.3
1	B	30	HIS	2.3
1	C	324	PRO	2.3
1	B	485	THR	2.3
1	C	460	LYS	2.3
1	B	344	THR	2.2
1	E	479	GLU	2.2
1	A	47	ASN	2.2
1	C	389	ASN	2.2
1	B	14	SER	2.2
1	D	339	ILE	2.2
1	C	366	ASP	2.2
1	E	44	CYS	2.2
1	D	22	LEU	2.2
1	E	467	PHE	2.2
1	A	452	LYS	2.2
1	F	484	GLY	2.2
1	B	277	CYS	2.2
1	B	473	CYS	2.2
1	F	367	GLN	2.1
1	C	357	ASN	2.1
1	B	495	PHE	2.1
1	E	485	THR	2.1
1	A	292	LEU	2.1
1	D	11	ALA	2.1
1	E	353	TYR	2.1
1	A	473	ASN	2.1
1	C	371	GLN	2.1
1	C	7	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	48	GLY	2.1
1	C	485	THR	2.1
1	D	481	VAL	2.1
1	F	351	TYR	2.1
1	C	50	ILE	2.0
1	B	11	ALA	2.0
1	B	489	PRO	2.0
1	B	323	ILE	2.0
1	B	356	ARG	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 monosaccharides 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	F	502	14/15	0.72	0.27	92,104,110,113	0
2	NAG	E	501	14/15	0.75	0.34	78,102,109,111	0
2	NAG	F	501	14/15	0.76	0.35	85,102,110,113	0
4	FMT	B	503	3/3	0.79	0.12	91,91,92,93	0
3	OXM	A	503	6/6	0.85	0.40	90,90,93,96	0
3	OXM	F	504	6/6	0.86	0.24	75,81,82,87	0
2	NAG	B	501	14/15	0.87	0.23	73,94,110,113	0
2	NAG	A	501	14/15	0.89	0.18	75,85,89,91	0
3	OXM	D	700	6/6	0.92	0.29	61,65,83,93	0
3	OXM	C	700	6/6	0.93	0.29	50,65,83,84	0
3	OXM	F	503	6/6	0.93	0.28	56,61,76,80	0
3	OXM	B	502	6/6	0.94	0.26	47,55,61,74	0
3	OXM	A	502	6/6	0.95	0.25	44,55,60,64	0
3	OXM	E	502	6/6	0.96	0.17	45,56,63,74	0

6.5 Other polymers (i)

There are no such residues in this entry.