Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:51 PM GMT

PDB ID	:	3V8X
Title	:	The crystal structure of transferrin binding protein A (TbpA) from Neisserial meningitidis serogroup B in complex with full length human transferrin
Authors	:	Noinaj, N.; Easley, N.; Buchanan, S.K.
Deposited on	:	2011-12-23
Resolution	:	2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

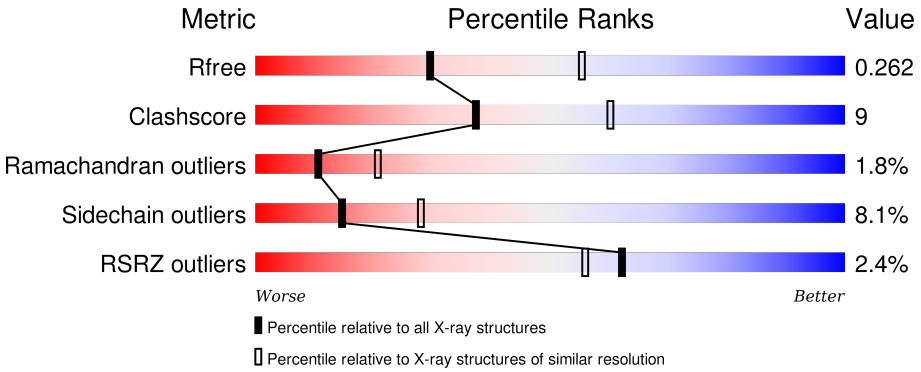
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

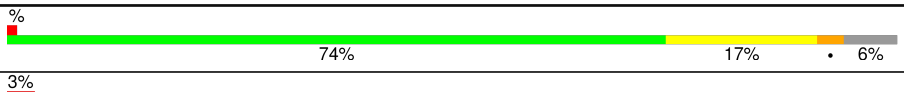
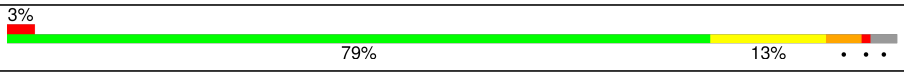
The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	904	
2	B	698	

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	C8E	A	1001	-	-	-	X
3	C8E	A	1002	-	-	-	X
5	SIA	B	717	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12233 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 Transferrin-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	853	6686	4176	1218	1282	10	0	2	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	EXPRESSION TAG	UNP Q9K0U9
A	13	ASP	-	EXPRESSION TAG	UNP Q9K0U9
A	14	ILE	-	EXPRESSION TAG	UNP Q9K0U9
A	15	HIS	-	EXPRESSION TAG	UNP Q9K0U9
A	16	HIS	-	EXPRESSION TAG	UNP Q9K0U9
A	17	HIS	-	EXPRESSION TAG	UNP Q9K0U9
A	18	HIS	-	EXPRESSION TAG	UNP Q9K0U9
A	19	HIS	-	EXPRESSION TAG	UNP Q9K0U9
A	20	HIS	-	EXPRESSION TAG	UNP Q9K0U9
A	21	HIS	-	EXPRESSION TAG	UNP Q9K0U9
A	22	HIS	-	EXPRESSION TAG	UNP Q9K0U9
A	23	HIS	-	EXPRESSION TAG	UNP Q9K0U9
A	24	HIS	-	EXPRESSION TAG	UNP Q9K0U9
A	435	VAL	ILE	VARIANT	UNP Q9K0U9
A	913	TYR	MET	ENGINEERED MUTATION	UNP Q9K0U9

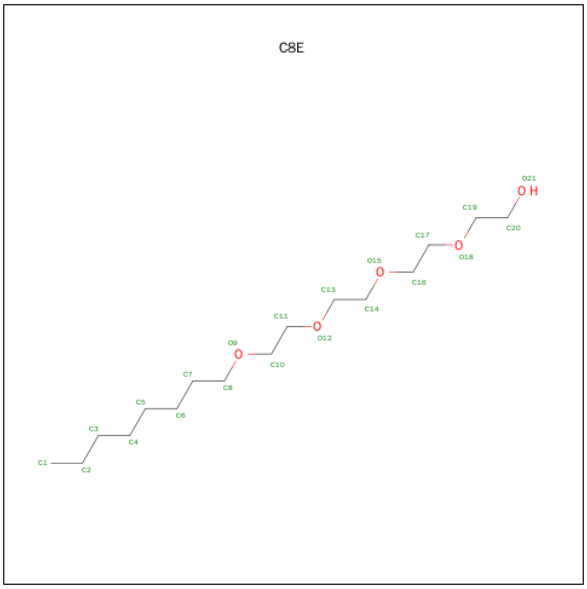
- Molecule 2 is a protein called Serotransferrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	676	5050	3160	868	977	45	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	429	VAL	ILE	VARIANT	UNP P02787

- Molecule 3 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: $C_{16}H_{34}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 21 16 5	0	0
3	A	1	Total C O 21 16 5	0	0

- Molecule 4 is a polymer of unknown type called SUGAR (10-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	10	Total C N O 131 73 5 53	0	0

- Molecule 5 is a polymer of unknown type called SUGAR (9-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	9	Total C N O 120 67 5 48	0	0

- Molecule 6 is water.

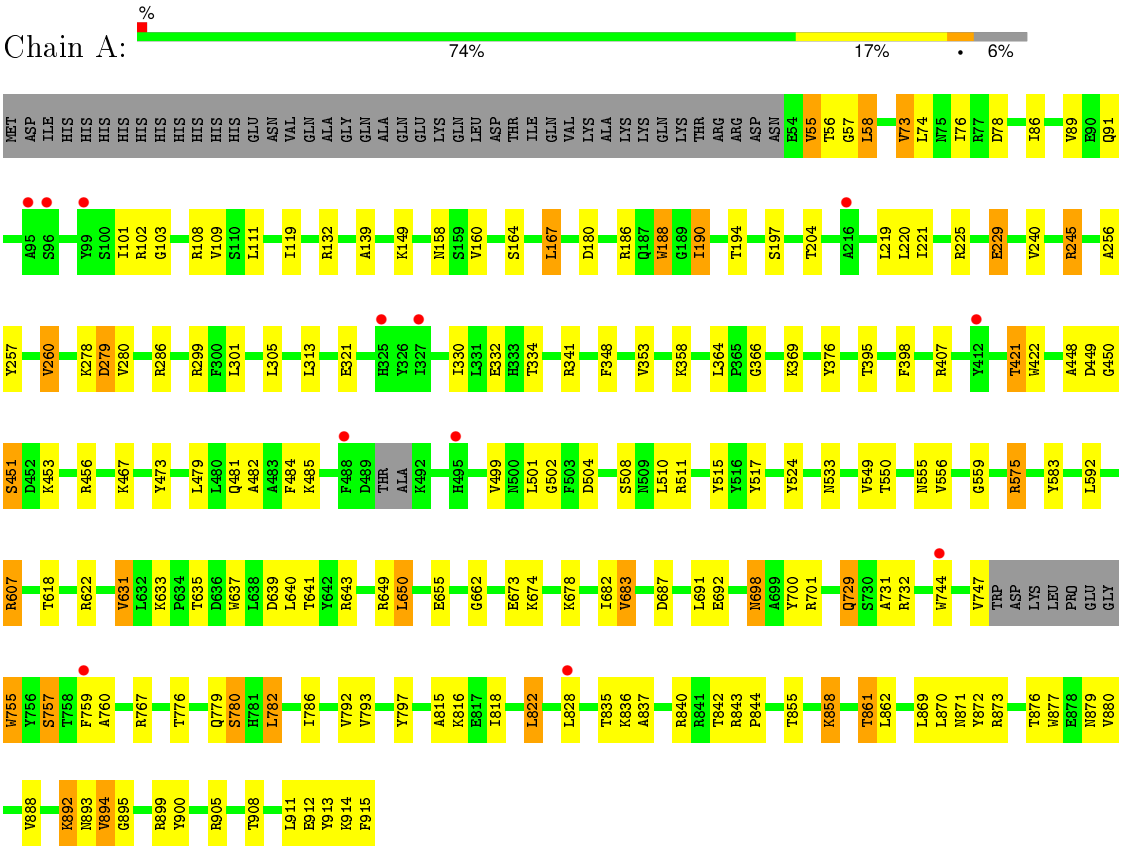
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	142	Total O 142 142	0	0
6	B	62	Total O 62 62	0	0

3 Residue-property plots (i)

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

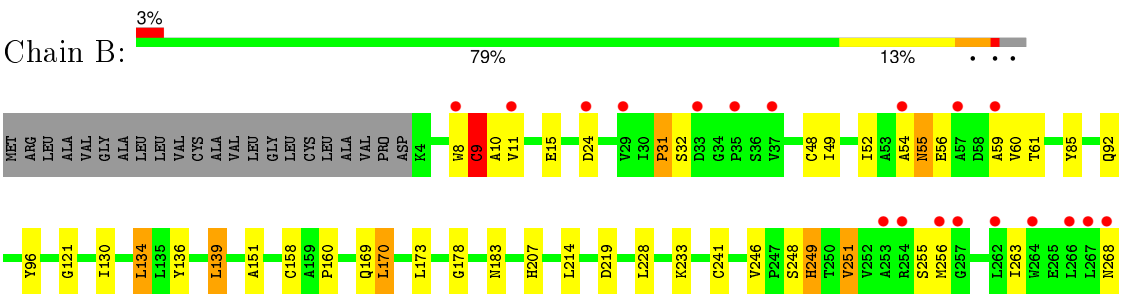
- Molecule 1: Transferrin-binding protein 1

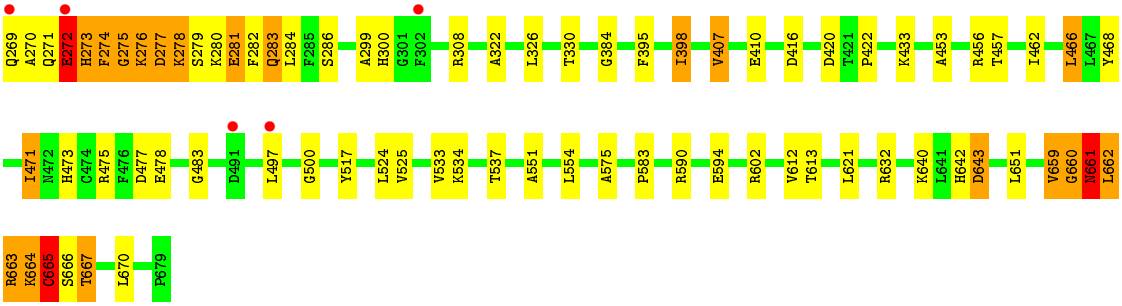
Chain A:



- Molecule 2: Serotransferrin

Chain B:




Q269
A270
Q271
E272
H273
F274
G275
K276
D277
K278
S279
K280
E281
F282
Q283
L284
F285
S286
A299
H300
G301
F302
R308
A322
L326
T330
G384
F395
I398
V407
E410
D416
D420
T421
P422
K433
A453
R456
T457
I462
L466
L467
Y468

I471
N472
H473
C474
R475
F476
D477
E478
G483
D491
L497
G500
Y517
L524
V525
V533
K534
T537
A551
L554
A575
P583
R590
E594
R602
V612
T613
L621
R632
K640
L641
H642
D643
L651
V659
G660
M661
L662

R663
K664
C665
S666
T667
L670
P679

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	91.01Å 129.36Å 198.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.92 – 2.60 49.47 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (29.92-2.60) 98.0 (49.47-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.208 , 0.267 0.202 , 0.262	Depositor DCC
R_{free} test set	3604 reflections (5.03%)	DCC
Wilson B-factor (Å^2)	57.3	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 47.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 71726 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12233	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, SIA, GAL, C8E, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.29	0/6834	0.47	1/9244 (0.0%)
2	B	0.29	0/5166	0.44	1/7025 (0.0%)
All	All	0.29	0/12000	0.45	2/16269 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	275	GLY	N-CA-C	-5.57	99.18	113.10
1	A	448	ALA	N-CA-C	-5.07	97.30	111.00

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	6686	0	6396	91	0
2	B	5050	0	4646	120	0
3	A	42	0	68	6	0
4	B	131	0	110	7	0
5	B	120	0	101	2	0
6	A	142	0	0	2	0
6	B	62	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12233	0	11321	217	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 9.

All (217) 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)
2:B:282:PHE:O	2:B:283:GLN:HG2	1.46	1.15
2:B:275:GLY:HA2	2:B:281:GLU:O	1.48	1.12
2:B:659:VAL:HG23	2:B:660:GLY:H	0.91	1.05
2:B:269:GLN:HA	2:B:272:GLU:HG3	1.39	1.02
2:B:659:VAL:CG2	2:B:660:GLY:H	1.69	1.00
2:B:659:VAL:HG23	2:B:660:GLY:N	1.54	1.00
2:B:274:PHE:HB2	2:B:279:SER:HB3	1.40	0.98
2:B:661:ASN:H	2:B:661:ASN:ND2	1.65	0.94
2:B:274:PHE:CB	2:B:279:SER:HB3	2.01	0.89
2:B:277:ASP:CB	2:B:283:GLN:HA	2.02	0.89
2:B:283:GLN:HE21	2:B:286:SER:HB3	1.38	0.87
2:B:661:ASN:HD22	2:B:661:ASN:N	1.77	0.82
2:B:277:ASP:HA	2:B:283:GLN:HA	1.62	0.81
1:A:229:GLU:HG2	1:A:305:LEU:H	1.45	0.81
2:B:660:GLY:O	2:B:663:ARG:CB	2.30	0.80
2:B:270:ALA:O	2:B:276:LYS:CB	2.30	0.79
2:B:275:GLY:CA	2:B:281:GLU:O	2.30	0.79
2:B:274:PHE:C	2:B:276:LYS:N	2.29	0.78
2:B:277:ASP:CA	2:B:283:GLN:HA	2.13	0.78
2:B:282:PHE:O	2:B:283:GLN:CG	2.30	0.77
2:B:269:GLN:CA	2:B:272:GLU:HG3	2.15	0.77
1:A:510:LEU:HB3	1:A:575:ARG:HG3	1.67	0.76
2:B:52:ILE:HD11	2:B:60:VAL:HG23	1.67	0.76
2:B:659:VAL:CG2	2:B:660:GLY:N	2.30	0.75
2:B:10:ALA:HB1	2:B:15:GLU:HG3	1.66	0.75
2:B:277:ASP:CB	2:B:284:LEU:H	2.00	0.74
2:B:661:ASN:H	2:B:661:ASN:HD22	1.31	0.73
2:B:274:PHE:HB2	2:B:279:SER:CB	2.18	0.72
2:B:661:ASN:ND2	2:B:661:ASN:N	2.30	0.72
2:B:271:GLN:O	2:B:272:GLU:C	2.30	0.70
1:A:631:VAL:HG12	1:A:641:THR:HG22	1.74	0.70
2:B:48:CYS:HB3	2:B:60:VAL:HG21	1.73	0.69
1:A:256:ALA:HB1	1:A:279:ASP:HB2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:663:ARG:O	2:B:664:LYS:C	2.29	0.68
1:A:58:LEU:HD13	1:A:643:ARG:HD2	1.76	0.68
2:B:273:HIS:C	2:B:275:GLY:H	1.98	0.68
1:A:779:GLN:NE2	1:A:835:THR:OG1	2.26	0.67
2:B:660:GLY:O	2:B:661:ASN:C	2.33	0.67
2:B:283:GLN:O	2:B:283:GLN:HG2	1.93	0.67
2:B:274:PHE:C	2:B:276:LYS:H	1.99	0.66
2:B:273:HIS:C	2:B:275:GLY:N	2.47	0.66
2:B:273:HIS:O	2:B:275:GLY:N	2.29	0.66
2:B:276:LYS:O	2:B:284:LEU:N	2.29	0.65
2:B:661:ASN:O	2:B:663:ARG:N	2.29	0.65
2:B:268:ASN:O	2:B:272:GLU:HG2	1.96	0.65
2:B:61:THR:HG1	2:B:249:HIS:HD1	1.43	0.65
2:B:272:GLU:O	2:B:274:PHE:N	2.30	0.65
2:B:660:GLY:O	2:B:663:ARG:N	2.31	0.64
1:A:760:ALA:HB3	1:A:792:VAL:HG13	1.81	0.62
1:A:755:TRP:HB3	1:A:797:TYR:HD2	1.65	0.62
2:B:272:GLU:O	2:B:274:PHE:HD2	1.82	0.61
1:A:358:LYS:NZ	6:A:1195:HOH:O	2.32	0.61
2:B:433:LYS:NZ	2:B:524:LEU:O	2.34	0.60
2:B:272:GLU:O	2:B:274:PHE:CD2	2.54	0.60
2:B:269:GLN:HA	2:B:272:GLU:CG	2.22	0.60
2:B:277:ASP:CB	2:B:284:LEU:N	2.64	0.60
1:A:755:TRP:HE3	1:A:797:TYR:HB2	1.67	0.59
2:B:659:VAL:O	2:B:661:ASN:N	2.35	0.59
2:B:663:ARG:O	2:B:665:CYS:HB3	2.03	0.59
1:A:911:LEU:HD22	1:A:913:TYR:HE2	1.68	0.59
2:B:277:ASP:CB	2:B:283:GLN:CA	2.79	0.58
2:B:274:PHE:CB	2:B:279:SER:CB	2.79	0.58
2:B:271:GLN:O	2:B:276:LYS:CB	2.52	0.58
1:A:73:VAL:HG23	1:A:78:ASP:HB2	1.85	0.58
1:A:524:TYR:H	4:B:704:MAN:H61	1.67	0.58
2:B:61:THR:HA	2:B:251:VAL:HA	1.86	0.57
2:B:273:HIS:O	2:B:276:LYS:N	2.29	0.57
2:B:662:LEU:C	2:B:663:ARG:O	2.40	0.57
1:A:662:GLY:O	2:B:602:ARG:NH2	2.34	0.57
1:A:313:LEU:HD11	1:A:330:ILE:HD11	1.86	0.57
1:A:674:LYS:HD2	1:A:701:ARG:HH12	1.70	0.57
1:A:197:SER:HA	1:A:908:THR:HG22	1.88	0.56
2:B:274:PHE:HD1	2:B:278:LYS:C	2.08	0.56
2:B:517:TYR:CZ	2:B:534:LYS:HD3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:661:ASN:C	2:B:663:ARG:N	2.57	0.56
1:A:861:THR:HG23	1:A:912:GLU:HB2	1.87	0.55
1:A:221:ILE:HD12	1:A:313:LEU:HD23	1.89	0.55
1:A:732:ARG:HG3	1:A:767:ARG:HB2	1.89	0.55
1:A:453:LYS:O	1:A:456:ARG:NH2	2.41	0.54
2:B:283:GLN:O	2:B:283:GLN:CG	2.55	0.54
2:B:664:LYS:O	2:B:665:CYS:CB	2.55	0.54
1:A:449:ASP:CG	1:A:451:SER:OG	2.46	0.54
2:B:8:TRP:HD1	2:B:9:CYS:O	1.91	0.54
2:B:279:SER:OG	2:B:280:LYS:N	2.40	0.53
1:A:842:THR:HG21	1:A:877:TRP:HB2	1.90	0.53
1:A:55:VAL:HG13	1:A:631:VAL:HG22	1.91	0.53
4:B:704:MAN:H3	4:B:705:NAG:C7	2.39	0.52
2:B:158:CYS:HB2	2:B:173:LEU:HB2	1.91	0.52
1:A:482:ALA:HB3	1:A:501:LEU:HB2	1.91	0.52
1:A:869:LEU:O	1:A:905:ARG:NH1	2.41	0.52
2:B:283:GLN:HE21	2:B:286:SER:CB	2.18	0.51
1:A:484:PHE:HB2	1:A:499:VAL:HG22	1.93	0.51
2:B:8:TRP:HD1	2:B:9:CYS:H	1.58	0.51
1:A:816:LYS:HB2	1:A:842:THR:HG22	1.93	0.51
1:A:449:ASP:OD1	1:A:451:SER:OG	2.29	0.50
2:B:662:LEU:O	2:B:663:ARG:O	2.29	0.50
2:B:282:PHE:O	2:B:283:GLN:O	2.30	0.50
1:A:870:LEU:O	1:A:872:TYR:N	2.42	0.50
2:B:666:SER:OG	2:B:667:THR:N	2.44	0.50
1:A:103:GLY:HA2	1:A:786:ILE:HG12	1.93	0.50
2:B:661:ASN:O	2:B:662:LEU:C	2.50	0.49
2:B:271:GLN:O	2:B:272:GLU:O	2.30	0.49
2:B:661:ASN:O	2:B:663:ARG:O	2.30	0.49
2:B:433:LYS:HE3	2:B:525:VAL:HA	1.93	0.49
1:A:729:GLN:NE2	1:A:780:SER:O	2.37	0.49
2:B:660:GLY:O	2:B:661:ASN:O	2.30	0.49
1:A:257:TYR:CZ	1:A:278:LYS:HE2	2.48	0.49
1:A:640:LEU:HD12	1:A:682:ILE:HD13	1.94	0.49
1:A:473:TYR:HH	1:A:508:SER:HG	1.58	0.49
1:A:502:GLY:HA3	1:A:583:TYR:CE2	2.47	0.49
1:A:843:ARG:HE	3:A:1002:C8E:H172	1.77	0.49
2:B:280:LYS:O	2:B:281:GLU:O	2.30	0.49
1:A:332:GLU:HB3	1:A:407:ARG:HB3	1.96	0.48
1:A:398:PHE:CG	1:A:453:LYS:HG3	2.49	0.48
1:A:449:ASP:OD2	1:A:451:SER:OG	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:274:PHE:CD1	2:B:278:LYS:CB	2.97	0.48
2:B:272:GLU:O	2:B:273:HIS:C	2.50	0.47
1:A:108:ARG:HG2	1:A:167:LEU:HD12	1.95	0.47
1:A:744:TRP:NE1	1:A:757:SER:HB2	2.30	0.47
1:A:479:LEU:HD13	1:A:504:ASP:HB2	1.97	0.47
1:A:892:LYS:HA	1:A:893:ASN:HA	1.68	0.47
1:A:101:ILE:HG22	1:A:102:ARG:HG2	1.97	0.47
2:B:471:ILE:HB	2:B:473:HIS:NE2	2.30	0.47
1:A:782:LEU:HG	1:A:837:ALA:HB2	1.97	0.47
1:A:450:GLY:HA3	1:A:451:SER:HA	1.57	0.47
2:B:178:GLY:HA3	2:B:183:ASN:HB2	1.97	0.47
1:A:876:THR:O	1:A:880:VAL:HG23	2.15	0.47
2:B:643:ASP:OD1	2:B:643:ASP:N	2.48	0.46
1:A:91:GLN:HG3	1:A:139:ALA:HB2	1.96	0.46
2:B:422:PRO:HG3	2:B:640:LYS:O	2.15	0.46
2:B:9:CYS:HB3	2:B:60:VAL:HG22	1.98	0.46
1:A:56:THR:HA	1:A:57:GLY:HA2	1.48	0.46
2:B:8:TRP:CD1	2:B:9:CYS:N	2.83	0.46
3:A:1002:C8E:H171	3:A:1002:C8E:H142	1.51	0.46
2:B:134:LEU:HD13	2:B:322:ALA:HB2	1.97	0.46
1:A:524:TYR:H	4:B:704:MAN:C6	2.28	0.45
2:B:130:ILE:HD11	2:B:246:VAL:HG21	1.97	0.45
1:A:759:PHE:CD1	1:A:793:VAL:HG12	2.51	0.45
1:A:639:ASP:HB2	1:A:683:VAL:HG13	1.98	0.45
1:A:555:ASN:OD1	4:B:707:SIA:O4	2.28	0.45
2:B:398:ILE:HD11	2:B:670:LEU:HG	1.99	0.45
2:B:283:GLN:NE2	2:B:286:SER:HB3	2.19	0.45
1:A:755:TRP:HB3	1:A:797:TYR:CD2	2.47	0.45
3:A:1002:C8E:H192	3:A:1002:C8E:H162	1.59	0.45
1:A:190:ILE:HG23	1:A:915:PHE:HB2	1.99	0.45
2:B:281:GLU:HA	2:B:282:PHE:HA	1.55	0.45
2:B:395:PHE:HA	2:B:398:ILE:HG23	1.98	0.45
1:A:649:ARG:HD3	1:A:673:GLU:OE1	2.17	0.44
1:A:149:LYS:HD3	1:A:180:ASP:OD1	2.17	0.44
1:A:759:PHE:HD1	1:A:793:VAL:HG12	1.82	0.44
1:A:607[B]:ARG:O	1:A:607[B]:ARG:NH1	2.50	0.44
2:B:214:LEU:HG	2:B:219:ASP:HB3	2.00	0.44
2:B:407:VAL:HG13	2:B:594:GLU:HG3	1.99	0.44
1:A:341:ARG:CZ	1:A:451:SER:HB2	2.48	0.44
2:B:276:LYS:O	2:B:277:ASP:CB	2.64	0.44
2:B:274:PHE:HB3	2:B:279:SER:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:ALA:HB1	2:B:169:GLN:HB2	1.99	0.44
2:B:583:PRO:HG3	2:B:651:LEU:HD23	1.99	0.44
1:A:894:VAL:HA	1:A:895:GLY:HA3	1.61	0.44
2:B:410:GLU:OE1	2:B:632:ARG:HG2	2.17	0.44
1:A:575:ARG:H	1:A:575:ARG:HG2	1.58	0.44
1:A:836:LYS:HD3	3:A:1002:C8E:H31	1.98	0.44
2:B:136:TYR:HA	2:B:139:LEU:HD22	2.00	0.44
1:A:366:GLY:HA2	1:A:524:TYR:CZ	2.53	0.43
2:B:121:GLY:HA2	2:B:160:PRO:HG2	2.00	0.43
1:A:132:ARG:O	1:A:467:LYS:NZ	2.52	0.43
1:A:74:LEU:O	1:A:225:ARG:NH2	2.51	0.43
2:B:468:TYR:CD2	2:B:661:ASN:HB3	2.54	0.43
2:B:575:ALA:HB1	4:B:703:BMA:O6	2.19	0.43
1:A:683:VAL:HB	1:A:692:GLU:HG3	2.01	0.43
2:B:533:VAL:HG21	2:B:537:THR:HG21	2.00	0.43
2:B:31:PRO:HB2	2:B:32:SER:H	1.56	0.42
2:B:274:PHE:HB3	2:B:279:SER:HB3	1.94	0.42
2:B:255:SER:OG	2:B:256:MET:N	2.51	0.42
1:A:635:THR:C	1:A:637:TRP:H	2.22	0.42
2:B:85:TYR:CD2	2:B:299:ALA:HA	2.55	0.42
2:B:384:GLY:HA2	2:B:590:ARG:NH1	2.34	0.42
2:B:134:LEU:HA	2:B:134:LEU:HD12	1.86	0.42
4:B:707:SIA:H8	4:B:707:SIA:N5	2.34	0.42
1:A:479:LEU:HG	1:A:481:GLN:HG3	2.02	0.42
1:A:700:TYR:N	1:A:731:ALA:O	2.51	0.42
5:B:713:BMA:H61	5:B:714:MAN:H2	1.22	0.42
1:A:815:ALA:HB2	1:A:844:PRO:HD3	2.01	0.42
1:A:229:GLU:H	1:A:229:GLU:HG3	1.42	0.41
1:A:840:ARG:HH21	3:A:1002:C8E:H141	1.85	0.41
2:B:59:ALA:HB2	2:B:263:ILE:HD13	2.02	0.41
2:B:274:PHE:HD1	2:B:278:LYS:CB	2.32	0.41
1:A:524:TYR:O	4:B:704:MAN:H62	2.20	0.41
1:A:167:LEU:HD13	1:A:700:TYR:HD1	1.85	0.41
2:B:326:LEU:HD12	2:B:326:LEU:HA	1.90	0.41
2:B:233:LYS:HD2	2:B:241:CYS:HB2	2.03	0.41
1:A:879:ASN:HB3	1:A:900:TYR:HB3	2.02	0.41
1:A:260:VAL:HA	1:A:549:VAL:O	2.20	0.41
2:B:462:ILE:O	2:B:466:LEU:HD22	2.20	0.41
2:B:151:ALA:HB2	2:B:170:LEU:HD13	2.03	0.41
1:A:633:LYS:HG2	1:A:639:ASP:OD1	2.19	0.41
5:B:714:MAN:H3	5:B:715:NAG:C7	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:LYS:HD3	1:A:549:VAL:HG21	2.01	0.41
1:A:186:ARG:NH1	1:A:188:TRP:O	2.53	0.41
1:A:421:THR:HG22	1:A:422:TRP:H	1.85	0.41
2:B:96:TYR:HB2	2:B:207:HIS:HB3	2.03	0.41
3:A:1001:C8E:H51	3:A:1001:C8E:H82	1.91	0.41
2:B:453:ALA:HB3	2:B:456:ARG:HD3	2.03	0.41
1:A:485:LYS:HB2	1:A:485:LYS:HE3	1.91	0.41
1:A:245:ARG:HG2	1:A:348:PHE:HB3	2.02	0.41
1:A:164:SER:HB2	1:A:650:LEU:HD22	2.02	0.41
1:A:818:ILE:HG12	1:A:822:LEU:HD22	2.03	0.41
1:A:858:LYS:O	1:A:914:LYS:HB2	2.21	0.41
2:B:475:ARG:O	2:B:478:GLU:HG2	2.21	0.41
2:B:269:GLN:C	2:B:272:GLU:HG3	2.42	0.40
1:A:698:ASN:HB2	6:A:1158:HOH:O	2.21	0.40
2:B:551:ALA:HA	2:B:554:LEU:HG	2.03	0.40
2:B:483:GLY:HA2	2:B:497:LEU:HD11	2.04	0.40
2:B:660:GLY:O	2:B:663:ARG:CA	2.69	0.40
1:A:517:TYR:CZ	1:A:559:GLY:HA3	2.57	0.40
1:A:892:LYS:HB2	1:A:893:ASN:OD1	2.22	0.40
1:A:649:ARG:HH22	1:A:655:GLU:CD	2.25	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	849/904 (94%)	807 (95%)	39 (5%)	3 (0%)	39 65
2	B	674/698 (97%)	593 (88%)	57 (8%)	24 (4%)	4 6
All	All	1523/1602 (95%)	1400 (92%)	96 (6%)	27 (2%)	11 21

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	780	SER
2	B	31	PRO
2	B	272	GLU
2	B	281	GLU
2	B	283	GLN
2	B	659	VAL
2	B	663	ARG
2	B	665	CYS
1	A	871	ASN
2	B	273	HIS
2	B	274	PHE
2	B	276	LYS
2	B	277	ASP
2	B	660	GLY
2	B	661	ASN
2	B	24	ASP
2	B	9	CYS
2	B	278	LYS
2	B	457	THR
2	B	500	GLY
2	B	662	LEU
2	B	664	LYS
1	A	158	ASN
2	B	55	ASN
2	B	248	SER
2	B	54	ALA
2	B	612	VAL

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	685/741 (92%)	616 (90%)	69 (10%)	9 17
2	B	520/585 (89%)	490 (94%)	30 (6%)	25 49
All	All	1205/1326 (91%)	1106 (92%)	99 (8%)	15 27

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	VAL
1	A	58	LEU
1	A	73	VAL
1	A	76	ILE
1	A	86	ILE
1	A	89	VAL
1	A	109	VAL
1	A	111	LEU
1	A	119	ILE
1	A	160	VAL
1	A	167	LEU
1	A	188	TRP
1	A	190	ILE
1	A	194	THR
1	A	204	THR
1	A	219	LEU
1	A	220	LEU
1	A	229	GLU
1	A	240	VAL
1	A	245	ARG
1	A	260	VAL
1	A	279	ASP
1	A	280	VAL
1	A	286	ARG
1	A	299	ARG
1	A	301	LEU
1	A	321	GLU
1	A	334	THR
1	A	353	VAL
1	A	364	LEU
1	A	376	TYR
1	A	395	THR
1	A	421	THR
1	A	451	SER
1	A	511	ARG
1	A	515	TYR
1	A	533	ASN
1	A	550	THR
1	A	556	VAL
1	A	575	ARG
1	A	592	LEU
1	A	607[A]	ARG
1	A	607[B]	ARG

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Mol	Chain	Res	Type
1	A	618	THR
1	A	622	ARG
1	A	631	VAL
1	A	650	LEU
1	A	678	LYS
1	A	683	VAL
1	A	687	ASP
1	A	691	LEU
1	A	698	ASN
1	A	729	GLN
1	A	747	VAL
1	A	755	TRP
1	A	757	SER
1	A	776	THR
1	A	782	LEU
1	A	822	LEU
1	A	828	LEU
1	A	855	THR
1	A	858	LYS
1	A	861	THR
1	A	862	LEU
1	A	873	ARG
1	A	888	VAL
1	A	892	LYS
1	A	894	VAL
1	A	899	ARG
2	B	9	CYS
2	B	11	VAL
2	B	49	ILE
2	B	55	ASN
2	B	56	GLU
2	B	92	GLN
2	B	134	LEU
2	B	139	LEU
2	B	170	LEU
2	B	228	LEU
2	B	249	HIS
2	B	251	VAL
2	B	272	GLU
2	B	300	HIS
2	B	308	ARG
2	B	330	THR

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Mol	Chain	Res	Type
2	B	398	ILE
2	B	407	VAL
2	B	416	ASP
2	B	420	ASP
2	B	466	LEU
2	B	471	ILE
2	B	477	ASP
2	B	613	THR
2	B	621	LEU
2	B	642	HIS
2	B	643	ASP
2	B	661	ASN
2	B	665	CYS
2	B	667	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	GLN
1	A	779	GLN
2	B	283	GLN
2	B	469	ASN
2	B	661	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)

19 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	B	701	2,4	14,14,15	0.65	0	15,19,21	1.05	2 (13%)
4	NAG	B	702	4	14,14,15	0.50	0	15,19,21	1.15	2 (13%)
4	BMA	B	703	4	11,11,12	1.09	1 (9%)	14,15,17	1.76	5 (35%)
4	MAN	B	704	4	11,11,12	0.78	0	14,15,17	1.81	4 (28%)
4	NAG	B	705	4	14,14,15	0.55	0	15,19,21	1.44	1 (6%)
4	GAL	B	706	4	11,11,12	0.64	0	14,15,17	0.60	0
4	SIA	B	707	4	16,20,21	0.52	0	18,28,31	1.74	4 (22%)
4	MAN	B	708	4	11,11,12	0.62	0	14,15,17	1.49	2 (14%)
4	NAG	B	709	4	14,14,15	0.59	0	15,19,21	1.00	0
4	GAL	B	710	4	11,11,12	0.66	0	14,15,17	1.72	1 (7%)
5	NAG	B	711	2,5	14,14,15	0.67	0	15,19,21	1.15	1 (6%)
5	NAG	B	712	5	14,14,15	0.48	0	15,19,21	1.70	2 (13%)
5	BMA	B	713	5	11,11,12	1.94	3 (27%)	14,15,17	2.17	7 (50%)
5	MAN	B	714	5	11,11,12	0.56	0	14,15,17	0.80	0
5	NAG	B	715	5	14,14,15	0.48	0	15,19,21	1.05	1 (6%)
5	GAL	B	716	5	11,11,12	0.56	0	14,15,17	2.27	4 (28%)
5	SIA	B	717	5	16,20,21	0.46	0	18,28,31	1.85	3 (16%)
5	MAN	B	718	5	11,11,12	0.64	0	14,15,17	1.43	2 (14%)
5	NAG	B	719	5	14,14,15	0.51	0	15,19,21	0.57	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	701	2,4	-	0/6/23/26	0/1/1/1
4	NAG	B	702	4	-	0/6/23/26	0/1/1/1
4	BMA	B	703	4	-	0/2/19/22	0/1/1/1
4	MAN	B	704	4	-	0/2/19/22	0/1/1/1
4	NAG	B	705	4	-	0/6/23/26	0/1/1/1
4	GAL	B	706	4	-	0/2/19/22	0/1/1/1
4	SIA	B	707	4	-	0/14/34/38	0/1/1/1
4	MAN	B	708	4	-	0/2/19/22	1/1/1/1
4	NAG	B	709	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GAL	B	710	4	-	0/2/19/22	0/1/1/1
5	NAG	B	711	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	712	5	-	0/6/23/26	0/1/1/1
5	BMA	B	713	5	-	0/2/19/22	0/1/1/1
5	MAN	B	714	5	-	0/2/19/22	0/1/1/1
5	NAG	B	715	5	-	0/6/23/26	0/1/1/1
5	GAL	B	716	5	-	0/2/19/22	0/1/1/1
5	SIA	B	717	5	-	0/14/34/38	0/1/1/1
5	MAN	B	718	5	-	0/2/19/22	0/1/1/1
5	NAG	B	719	5	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	713	BMA	O5-C1	2.06	1.47	1.43
4	B	703	BMA	C2-C3	2.29	1.55	1.52
5	B	713	BMA	C2-C3	2.50	1.56	1.52
5	B	713	BMA	C1-C2	4.84	1.63	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	717	SIA	C7-C6-C5	-4.53	107.47	114.32
5	B	713	BMA	C3-C4-C5	-3.27	104.50	110.20
4	B	704	MAN	C6-C5-C4	-3.19	105.14	113.02
5	B	716	GAL	O6-C6-C5	-2.93	101.66	111.33
5	B	718	MAN	O5-C1-C2	-2.91	106.13	110.86
5	B	717	SIA	C3-C4-C5	-2.89	108.25	111.47
4	B	703	BMA	C1-C2-C3	-2.87	106.14	109.54
4	B	703	BMA	C2-C3-C4	-2.77	106.33	111.04
4	B	702	NAG	C2-N2-C7	-2.67	119.60	123.04
5	B	713	BMA	O2-C2-C3	-2.48	105.14	110.12
4	B	708	MAN	O5-C1-C2	-2.45	106.88	110.86
4	B	703	BMA	C3-C4-C5	-2.40	106.01	110.20
5	B	713	BMA	O3-C3-C4	-2.23	105.31	110.34
4	B	703	BMA	C6-C5-C4	-2.15	107.71	113.02
4	B	707	SIA	C3-C4-C5	-2.13	109.10	111.47
4	B	704	MAN	O3-C3-C2	-2.09	106.22	110.00
5	B	713	BMA	O2-C2-C1	2.05	113.32	109.21
4	B	703	BMA	O3-C3-C2	2.10	113.80	110.00
4	B	707	SIA	C8-C7-C6	2.10	117.24	113.01
4	B	701	NAG	C3-C4-C5	2.12	113.89	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	708	MAN	O4-C4-C5	2.13	114.87	109.24
5	B	716	GAL	O5-C5-C6	2.17	112.05	107.35
4	B	702	NAG	C1-O5-C5	2.20	115.04	112.25
4	B	701	NAG	C4-C3-C2	2.28	114.77	111.23
4	B	704	MAN	C2-C3-C4	2.32	114.99	111.04
5	B	715	NAG	C1-O5-C5	2.65	115.61	112.25
5	B	712	NAG	O4-C4-C3	2.88	116.83	110.34
5	B	713	BMA	O5-C1-C2	3.06	115.83	110.86
5	B	713	BMA	C1-C2-C3	3.11	113.22	109.54
5	B	713	BMA	C1-O5-C5	3.22	116.33	112.25
5	B	718	MAN	C3-C4-C5	3.52	116.33	110.20
5	B	711	NAG	C4-C3-C2	3.58	116.79	111.23
4	B	707	SIA	O6-C2-C3	3.94	117.43	109.86
4	B	707	SIA	C6-C5-N5	4.06	118.14	111.07
4	B	704	MAN	O4-C4-C3	4.48	120.43	110.34
4	B	705	NAG	C1-O5-C5	4.53	118.00	112.25
5	B	712	NAG	C1-O5-C5	5.00	118.59	112.25
5	B	717	SIA	O6-C6-C5	5.04	116.73	108.48
5	B	716	GAL	O2-C2-C1	5.08	119.39	109.21
5	B	716	GAL	O2-C2-C3	5.10	120.37	110.12
4	B	710	GAL	C1-C2-C3	5.38	115.91	109.54

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	708	MAN	C1-C2-C3-C4-C5-O5

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	703	BMA	1	0
4	B	704	MAN	4	0
4	B	705	NAG	1	0
4	B	707	SIA	2	0
5	B	713	BMA	1	0
5	B	714	MAN	2	0
5	B	715	NAG	1	0

5.6 Ligand geometry (i)

2 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	C8E	A	1001	-	20,20,20	0.40	0	19,19,19	0.34	0
3	C8E	A	1002	-	20,20,20	0.43	0	19,19,19	0.67	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	C8E	A	1001	-	-	0/18/18/18	0/0/0/0
3	C8E	A	1002	-	-	0/18/18/18	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	C8E	1	0
3	A	1002	C8E	5	0

5.7 Other polymers (i)

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	853/904 (94%)	-0.10	12 (1%)	78	74	37, 69, 111, 155	0
2	B	676/698 (96%)	-0.04	24 (3%)	46	38	43, 82, 152, 212	0
All	All	1529/1602 (95%)	-0.07	36 (2%)	62	56	37, 74, 136, 212	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	267	LEU	5.0
2	B	256	MET	4.5
2	B	37	VAL	4.3
2	B	24	ASP	4.2
2	B	302	PHE	4.1
2	B	59	ALA	3.8
2	B	8	TRP	3.7
2	B	253	ALA	3.7
2	B	262	LEU	3.5
2	B	29	VAL	3.3
2	B	35	PRO	3.2
2	B	254	ARG	3.1
1	A	488	PHE	3.1
2	B	33	ASP	3.1
2	B	11	VAL	3.0
1	A	216	ALA	3.0
1	A	95	ALA	2.9
2	B	497	LEU	2.7
2	B	257	GLY	2.6
2	B	491	ASP	2.5
2	B	266	LEU	2.5
2	B	264	TRP	2.5
1	A	495	HIS	2.4
1	A	325	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	759	PHE	2.4
1	A	412	TYR	2.3
2	B	57	ALA	2.3
2	B	272	GLU	2.3
1	A	99	TYR	2.2
1	A	96	SER	2.2
1	A	327	ILE	2.2
2	B	269	GLN	2.2
2	B	54	ALA	2.2
1	A	744	TRP	2.1
1	A	828	LEU	2.0
2	B	268	ASN	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)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	SIA	B	717	20/21	0.88	0.32	3.80	73,91,144,146	0
4	NAG	B	701	14/15	0.95	0.14	-0.32	54,67,82,86	0
5	NAG	B	711	14/15	0.90	0.18	-0.64	67,113,122,131	0
4	NAG	B	702	14/15	0.97	0.10	-2.56	55,66,71,80	0
5	NAG	B	719	14/15	0.62	0.36	-	157,178,187,187	0
5	NAG	B	715	14/15	0.86	0.23	-	113,135,143,144	0
5	MAN	B	718	11/12	0.60	0.22	-	167,175,185,187	0
5	BMA	B	713	11/12	0.63	0.19	-	150,169,201,202	0
4	MAN	B	708	11/12	0.79	0.25	-	85,118,141,153	0
4	NAG	B	709	14/15	0.90	0.15	-	118,125,145,150	0
4	SIA	B	707	20/21	0.62	0.43	-	149,166,174,174	0
4	NAG	B	705	14/15	0.91	0.25	-	81,103,113,123	0
4	MAN	B	704	11/12	0.83	0.28	-	79,95,116,128	0
4	GAL	B	706	11/12	0.60	0.28	-	30,142,156,165	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	BMA	B	703	11/12	0.95	0.14	-	54,64,85,108	0
4	GAL	B	710	11/12	0.77	0.16	-	139,154,157,160	0
5	GAL	B	716	11/12	0.51	0.40	-	30,133,150,153	0
5	NAG	B	712	14/15	0.85	0.21	-	111,144,158,162	0
5	MAN	B	714	11/12	0.83	0.18	-	137,153,155,157	0

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	C8E	A	1001	21/21	0.79	0.24	4.07	70,101,117,118	0
3	C8E	A	1002	21/21	0.83	0.25	3.97	48,77,98,106	0

6.5 Other polymers

There are no such residues in this entry.