Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:00 PM GMT

PDB ID	:	4NDZ
Title	:	Structure of Maltose Binding Protein fusion to 2-O-Sulfotransferase with bound heptasaccharide and PAP
Authors	:	Liu, C.; Sheng, J.; Krahn, J.M.; Perera, L.; Xu, Y.; Hsieh, P.; Liu, J.; Pedersen, L.C.
Deposited on	:	2013-10-28
Resolution	:	3.45 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:

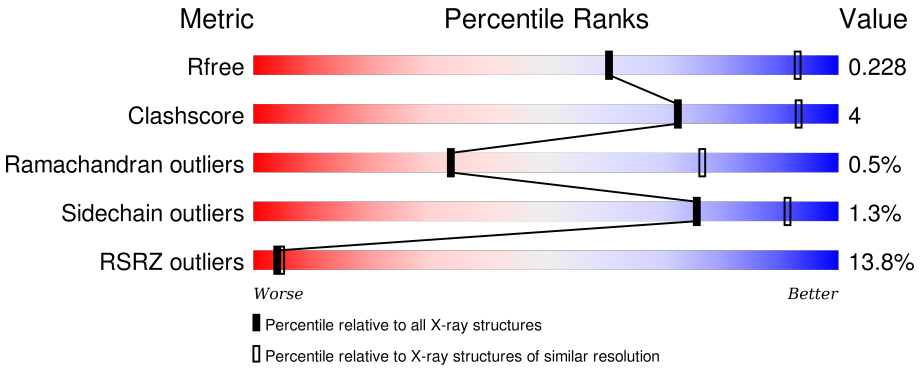
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.45 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	1000 (3.56-3.36)
Clashscore	102246	1090 (3.56-3.36)
Ramachandran outliers	100387	1057 (3.56-3.36)
Sidechain outliers	100360	1058 (3.56-3.36)
RSRZ outliers	91569	1005 (3.56-3.36)

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 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	658	38% 6% 56%
1	B	658	28% 86% 14%
1	C	658	10% 87% 12%
1	D	658	7% 86% 12%
1	E	658	5% 87% 13%

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Mol	Chain	Length	Quality of chain
1	F	658	

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	GNS	F	2009	-	-	-	X
4	NPO	A	2011	-	-	-	X
4	NPO	E	2011	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28764 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 Maltose-binding periplasmic protein, Heparan sulfate 2-O-sulfotransferase 1 fusion.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	1
			2352	1522	399	422	9			
1	B	654	Total	C	N	O	S	0	0	1
			5136	3314	852	955	15			
1	C	655	Total	C	N	O	S	0	0	1
			5128	3311	848	955	14			
1	D	654	Total	C	N	O	S	0	0	1
			5136	3313	853	955	15			
1	E	654	Total	C	N	O	S	0	0	1
			5110	3298	842	955	15			
1	F	654	Total	C	N	O	S	0	1	0
			5124	3307	846	956	15			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	359	ALA	GLU	ENGINEERED MUTATION	UNP P0AEX9
A	362	ALA	LYS	ENGINEERED MUTATION	UNP P0AEX9
A	363	ALA	ASP	ENGINEERED MUTATION	UNP P0AEX9
A	367	ASN	ARG	ENGINEERED MUTATION	UNP P0AEX9
A	368	ALA	-	LINKER	UNP P0AEX9
A	369	ALA	-	LINKER	UNP P0AEX9
A	370	ALA	-	LINKER	UNP P0AEX9
B	359	ALA	GLU	ENGINEERED MUTATION	UNP P0AEX9
B	362	ALA	LYS	ENGINEERED MUTATION	UNP P0AEX9
B	363	ALA	ASP	ENGINEERED MUTATION	UNP P0AEX9
B	367	ASN	ARG	ENGINEERED MUTATION	UNP P0AEX9
B	368	ALA	-	LINKER	UNP P0AEX9
B	369	ALA	-	LINKER	UNP P0AEX9
B	370	ALA	-	LINKER	UNP P0AEX9
C	359	ALA	GLU	ENGINEERED MUTATION	UNP P0AEX9
C	362	ALA	LYS	ENGINEERED MUTATION	UNP P0AEX9

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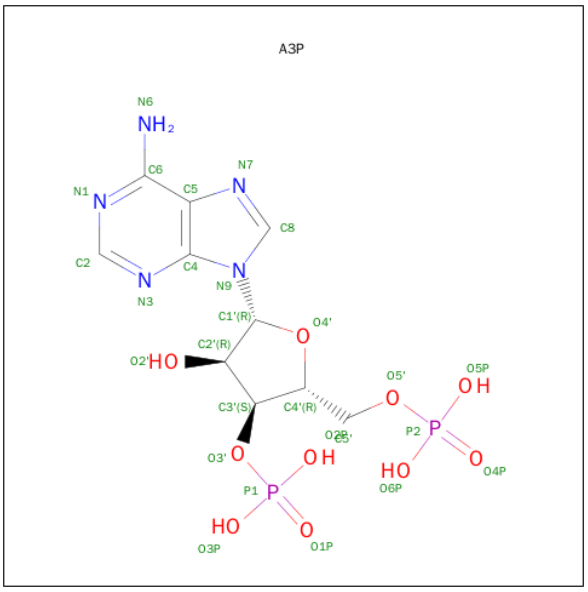
Chain	Residue	Modelled	Actual	Comment	Reference
C	363	ALA	ASP	ENGINEERED MUTATION	UNP P0AEX9
C	367	ASN	ARG	ENGINEERED MUTATION	UNP P0AEX9
C	368	ALA	-	LINKER	UNP P0AEX9
C	369	ALA	-	LINKER	UNP P0AEX9
C	370	ALA	-	LINKER	UNP P0AEX9
D	359	ALA	GLU	ENGINEERED MUTATION	UNP P0AEX9
D	362	ALA	LYS	ENGINEERED MUTATION	UNP P0AEX9
D	363	ALA	ASP	ENGINEERED MUTATION	UNP P0AEX9
D	367	ASN	ARG	ENGINEERED MUTATION	UNP P0AEX9
D	368	ALA	-	LINKER	UNP P0AEX9
D	369	ALA	-	LINKER	UNP P0AEX9
D	370	ALA	-	LINKER	UNP P0AEX9
E	359	ALA	GLU	ENGINEERED MUTATION	UNP P0AEX9
E	362	ALA	LYS	ENGINEERED MUTATION	UNP P0AEX9
E	363	ALA	ASP	ENGINEERED MUTATION	UNP P0AEX9
E	367	ASN	ARG	ENGINEERED MUTATION	UNP P0AEX9
E	368	ALA	-	LINKER	UNP P0AEX9
E	369	ALA	-	LINKER	UNP P0AEX9
E	370	ALA	-	LINKER	UNP P0AEX9
F	359	ALA	GLU	ENGINEERED MUTATION	UNP P0AEX9
F	362	ALA	LYS	ENGINEERED MUTATION	UNP P0AEX9
F	363	ALA	ASP	ENGINEERED MUTATION	UNP P0AEX9
F	367	ASN	ARG	ENGINEERED MUTATION	UNP P0AEX9
F	368	ALA	-	LINKER	UNP P0AEX9
F	369	ALA	-	LINKER	UNP P0AEX9
F	370	ALA	-	LINKER	UNP P0AEX9

- Molecule 2 is ADENOSINE-3'-5'-DIPHOSPHATE (three-letter code: A3P) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

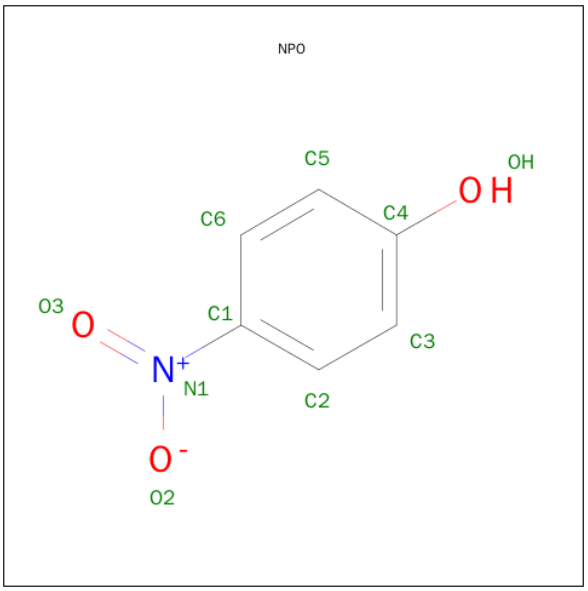


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	7	Total	C	N	O	S	0	0
			92	44	3	43	2		
3	B	7	Total	C	N	O	S	0	0
			92	44	3	43	2		
3	D	7	Total	C	N	O	S	0	0
			92	44	3	43	2		
3	E	7	Total	C	N	O	S	0	0
			92	44	3	43	2		
3	F	7	Total	C	N	O	S	0	0
			93	44	3	44	2		

- Molecule 4 is P-NITROPHENOL (three-letter code: NPO) (formula: $C_6H_5NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 10 6 1 3	0	0
4	B	1	Total C N O 10 6 1 3	0	0
4	D	1	Total C N O 10 6 1 3	0	0
4	E	1	Total C N O 10 6 1 3	0	0

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

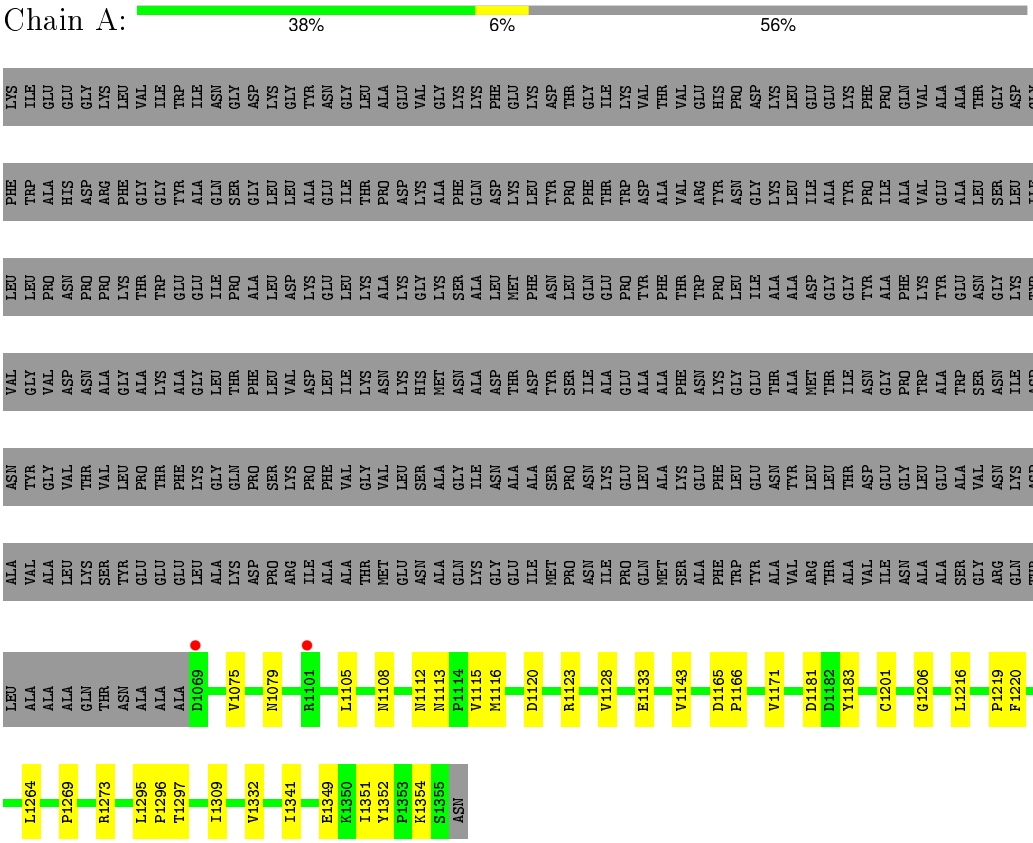
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	2	Total C O 23 12 11	0	0
5	C	2	Total C O 23 12 11	0	0
5	D	2	Total C O 23 12 11	0	0
5	E	2	Total C O 23 12 11	0	0
5	F	2	Total C O 23 12 11	0	0

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.

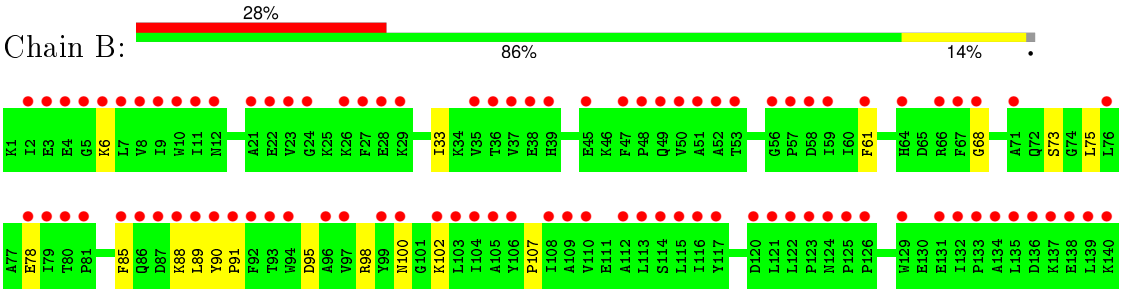
• Molecule 1: Maltose-binding periplasmic protein, Heparan sulfate 2-O-sulfotransferase 1 fusion

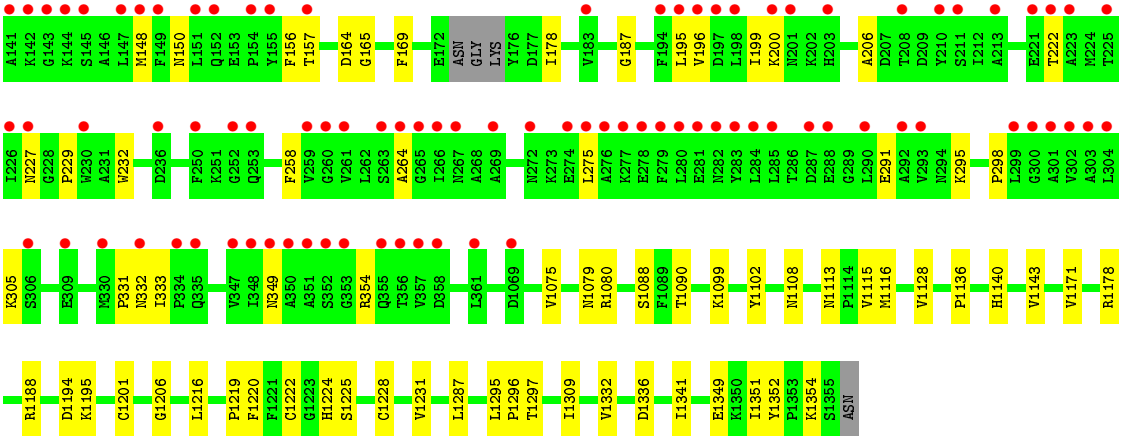
Chain A:



• Molecule 1: Maltose-binding periplasmic protein, Heparan sulfate 2-O-sulfotransferase 1 fusion

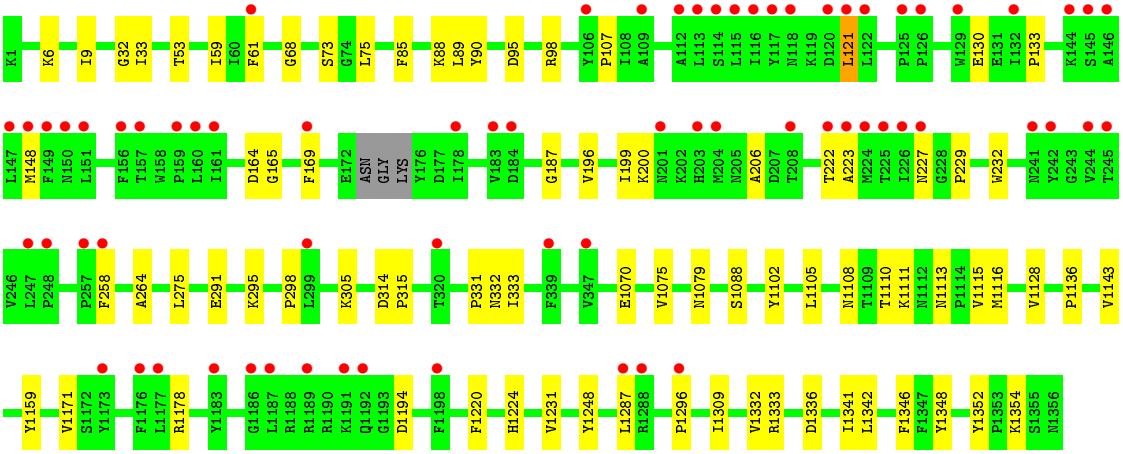
Chain B:





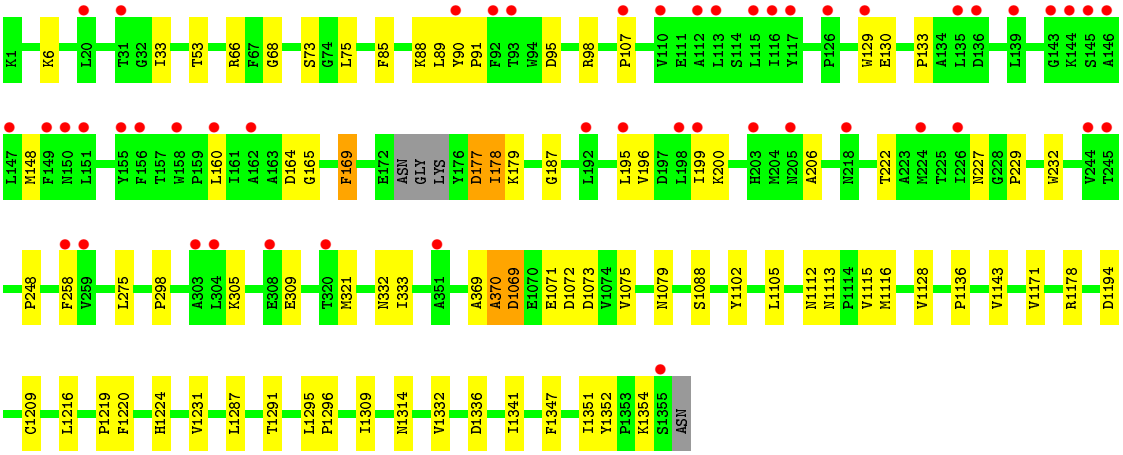
• Molecule 1: Maltose-binding periplasmic protein, Heparan sulfate 2-O-sulfotransferase 1 fusion

Chain C:



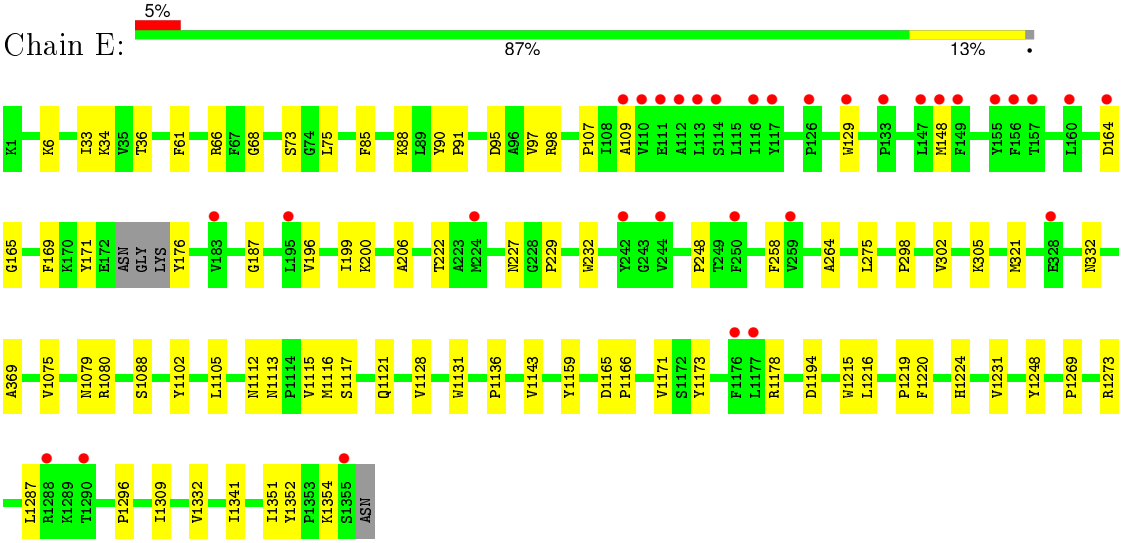
• Molecule 1: Maltose-binding periplasmic protein, Heparan sulfate 2-O-sulfotransferase 1 fusion

Chain D:



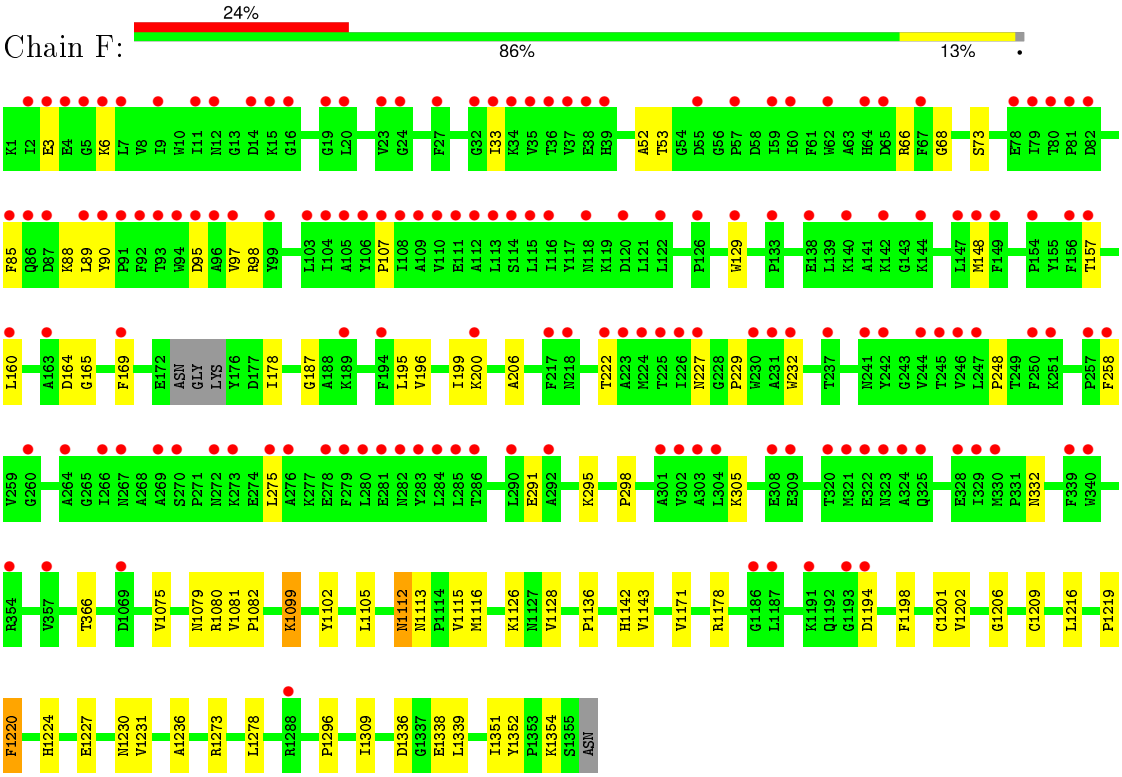
• Molecule 1: Maltose-binding periplasmic protein, Heparan sulfate 2-O-sulfotransferase 1 fusion

Chain E:



• Molecule 1: Maltose-binding periplasmic protein, Heparan sulfate 2-O-sulfotransferase 1 fusion

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	155.72Å 170.69Å 183.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.66 – 3.45 49.80 – 3.45	Depositor EDS
% Data completeness (in resolution range)	98.5 (49.66-3.45) 91.1 (49.80-3.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	3.65 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.176 , 0.228 0.186 , 0.228	Depositor DCC
R_{free} test set	1962 reflections (3.41%)	DCC
Wilson B-factor (Å^2)	90.6	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 85.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 64251 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	28764	wwPDB-VP
Average B, all atoms (Å^2)	138.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% 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: GNS, NPO, A3P, GLC, IDR, NDG, BDP

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	0.38	0/2416	0.47	0/3270
1	B	0.30	0/5267	0.42	0/7153
1	C	0.29	0/5259	0.43	0/7144
1	D	0.30	0/5267	0.43	0/7152
1	E	0.30	0/5241	0.44	0/7123
1	F	0.29	0/5256	0.42	0/7142
All	All	0.30	0/28706	0.43	0/38984

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	2352	0	2265	21	0
1	B	5136	0	4988	49	0
1	C	5128	0	4973	41	0
1	D	5136	0	4988	45	0
1	E	5110	0	4933	47	0
1	F	5124	0	4950	48	0
2	A	27	0	11	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	27	0	11	0	0
2	C	27	0	11	0	0
2	D	27	0	11	0	0
2	E	27	0	11	0	0
2	F	27	0	11	0	0
3	A	92	0	59	0	0
3	B	92	0	59	2	0
3	D	92	0	59	0	0
3	E	92	0	59	2	0
3	F	93	0	61	2	0
4	A	10	0	4	0	0
4	B	10	0	4	0	0
4	D	10	0	4	0	0
4	E	10	0	4	0	0
5	B	23	0	21	0	0
5	C	23	0	21	0	0
5	D	23	0	21	1	0
5	E	23	0	21	1	0
5	F	23	0	21	1	0
All	All	28764	0	27581	239	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 (239) 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:D:369:ALA:O	1:D:1069:ASP:N	2.24	0.71
1:E:1131:TRP:NE1	1:F:366:THR:HG21	2.08	0.68
1:E:1131:TRP:CD1	1:F:366:THR:HG21	2.30	0.66
1:D:1071:GLU:O	1:D:1073:ASP:N	2.30	0.65
1:A:1120:ASP:OD1	1:A:1123:ARG:NH1	2.31	0.63
1:B:349:ASN:OD1	1:B:354:ARG:NH1	2.32	0.62
1:C:32:GLY:O	1:D:1291:THR:HG22	2.00	0.62
1:B:1075:VAL:HG11	1:B:1128:VAL:HG13	1.82	0.61
1:D:6:LYS:HA	1:D:33:ILE:HG23	1.82	0.61
1:F:6:LYS:HA	1:F:33:ILE:HG23	1.85	0.59
1:B:6:LYS:HA	1:B:33:ILE:HG23	1.85	0.58
1:D:1071:GLU:C	1:D:1073:ASP:H	2.07	0.57
1:F:1075:VAL:HG11	1:F:1128:VAL:HG13	1.87	0.57
1:A:1349:GLU:OE2	1:C:1108:ASN:ND2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1075:VAL:HG11	1:A:1128:VAL:HG13	1.87	0.56
1:E:1173:TYR:OH	3:E:2010:BDP:O6A	2.17	0.56
1:E:1075:VAL:HG11	1:E:1128:VAL:HG13	1.88	0.55
1:B:1352:TYR:CE1	1:B:1354:LYS:HE2	2.42	0.55
1:D:68:GLY:HA3	1:D:332:ASN:O	2.07	0.55
1:C:6:LYS:HA	1:C:33:ILE:HG23	1.87	0.55
1:F:68:GLY:HA3	1:F:332:ASN:O	2.08	0.54
1:B:1080:ARG:NH1	3:B:2007:GNS:O2S	2.40	0.54
1:C:95:ASP:OD1	1:C:98:ARG:NH1	2.41	0.54
1:E:68:GLY:HA3	1:E:332:ASN:O	2.08	0.53
1:B:68:GLY:HA3	1:B:332:ASN:O	2.08	0.53
1:D:1075:VAL:HG11	1:D:1128:VAL:HG13	1.89	0.53
1:F:232:TRP:HB2	1:F:298:PRO:HG2	1.91	0.53
1:E:196:VAL:HG12	1:E:200:LYS:HE2	1.91	0.53
1:C:121:LEU:HD22	1:C:223:ALA:HB2	1.90	0.53
1:D:1079:ASN:HB2	1:D:1143:VAL:O	2.09	0.53
1:C:199:ILE:HG21	1:C:206:ALA:HB2	1.91	0.53
1:D:232:TRP:HB2	1:D:298:PRO:HG2	1.91	0.52
1:C:1075:VAL:HG11	1:C:1128:VAL:HG13	1.90	0.52
1:E:6:LYS:HA	1:E:33:ILE:HG23	1.91	0.52
1:E:199:ILE:HG21	1:E:206:ALA:HB2	1.91	0.52
1:F:1338:GLU:HG2	1:F:1339:LEU:H	1.74	0.52
1:F:1352:TYR:CE1	1:F:1354:LYS:HE2	2.45	0.52
1:F:148:MET:HB2	1:F:222:THR:HG21	1.92	0.52
1:E:1352:TYR:CE1	1:E:1354:LYS:HE2	2.45	0.52
1:F:1079:ASN:HB2	1:F:1143:VAL:O	2.10	0.52
1:C:68:GLY:HA3	1:C:332:ASN:O	2.10	0.52
1:F:291:GLU:HG2	1:F:295:LYS:HE3	1.92	0.51
1:B:95:ASP:OD1	1:B:98:ARG:NH1	2.43	0.51
1:F:52:ALA:HA	1:F:1099:LYS:CD	2.40	0.51
1:C:1231:VAL:HG12	1:C:1309:ILE:HD12	1.91	0.51
1:E:95:ASP:OD1	1:E:98:ARG:NH1	2.42	0.51
1:C:1352:TYR:CE1	1:C:1354:LYS:HE2	2.45	0.51
1:B:1195:LYS:CB	1:F:1230:ASN:HA	2.41	0.51
1:A:1079:ASN:HB2	1:A:1143:VAL:O	2.11	0.51
1:B:232:TRP:HB2	1:B:298:PRO:HG2	1.91	0.51
1:D:95:ASP:OD1	1:D:98:ARG:NH1	2.44	0.51
1:A:1352:TYR:CE1	1:A:1354:LYS:HE2	2.46	0.51
1:B:199:ILE:HG21	1:B:206:ALA:HB2	1.92	0.51
1:E:148:MET:HB2	1:E:222:THR:HG21	1.92	0.51
1:C:232:TRP:HB2	1:C:298:PRO:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:THR:HG22	1:D:1347:PHE:CE2	2.46	0.51
1:D:196:VAL:HG12	1:D:200:LYS:HE2	1.93	0.51
1:F:73:SER:HB3	1:F:1273:ARG:HH22	1.76	0.50
1:E:232:TRP:HB2	1:E:298:PRO:HG2	1.93	0.50
1:E:1332:VAL:HG12	1:E:1341:ILE:HD12	1.94	0.50
1:E:90:TYR:CE1	1:E:305:LYS:HG2	2.47	0.50
1:D:1352:TYR:CE1	1:D:1354:LYS:HE2	2.47	0.50
1:F:1113:ASN:ND2	1:F:1115:VAL:O	2.44	0.50
1:A:1171:VAL:HG21	1:A:1296:PRO:HG3	1.94	0.50
1:B:196:VAL:HG12	1:B:200:LYS:HE2	1.94	0.50
1:B:1079:ASN:HB2	1:B:1143:VAL:O	2.12	0.50
1:F:199:ILE:HG21	1:F:206:ALA:HB2	1.93	0.50
1:F:1112:ASN:HB2	3:F:2010:BDP:H3	1.94	0.49
1:C:73:SER:HB2	1:C:75:LEU:HG	1.95	0.49
1:C:1079:ASN:HB2	1:C:1143:VAL:O	2.13	0.49
1:D:164:ASP:HB3	1:D:187:GLY:HA2	1.95	0.49
1:D:148:MET:HB2	1:D:222:THR:HG21	1.94	0.49
1:B:1116:MET:H	1:B:1224:HIS:CD2	2.31	0.49
1:B:85:PHE:HA	1:B:88:LYS:HE3	1.95	0.49
1:D:1113:ASN:ND2	1:D:1115:VAL:O	2.46	0.49
1:D:85:PHE:O	1:D:88:LYS:HG2	2.12	0.48
1:A:1351:ILE:HG23	1:C:1105:LEU:HG	1.95	0.48
1:D:199:ILE:HG21	1:D:206:ALA:HB2	1.94	0.48
1:B:33:ILE:HG12	1:B:275:LEU:HD13	1.95	0.48
1:F:196:VAL:HG12	1:F:200:LYS:HE2	1.95	0.48
1:E:1102:TYR:HB3	1:E:1136:PRO:HG2	1.96	0.48
1:B:164:ASP:HB3	1:B:187:GLY:HA2	1.95	0.48
1:B:1216:LEU:C	1:B:1219:PRO:HD2	2.34	0.48
1:E:1171:VAL:HG21	1:E:1296:PRO:HG3	1.95	0.48
1:D:179:LYS:HA	1:D:370:ALA:HB3	1.95	0.48
1:B:148:MET:HB2	1:B:222:THR:HG21	1.95	0.48
1:C:148:MET:HB2	1:C:222:THR:HG21	1.96	0.48
1:B:1332:VAL:HG12	1:B:1341:ILE:HD12	1.94	0.48
1:D:1332:VAL:HG12	1:D:1341:ILE:HD12	1.95	0.47
1:D:66:ARG:NH2	5:D:2001:GLC:O4	2.40	0.47
1:D:1178:ARG:HD2	1:D:1194:ASP:HB3	1.96	0.47
1:A:1216:LEU:C	1:A:1219:PRO:HD2	2.35	0.47
1:F:164:ASP:HB3	1:F:187:GLY:HA2	1.95	0.47
1:E:97:VAL:HG21	1:E:107:PRO:HD3	1.96	0.47
1:D:1171:VAL:HG21	1:D:1296:PRO:HG3	1.96	0.47
1:F:1171:VAL:HG21	1:F:1296:PRO:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:ASP:HB3	1:C:187:GLY:HA2	1.95	0.47
1:E:164:ASP:HB3	1:E:187:GLY:HA2	1.95	0.47
1:D:1351:ILE:HG23	1:F:1105:LEU:HG	1.97	0.47
1:E:34:LYS:NZ	1:E:36:THR:OG1	2.47	0.47
1:D:85:PHE:HA	1:D:88:LYS:HE3	1.97	0.47
1:C:291:GLU:O	1:C:295:LYS:HG3	2.14	0.47
1:B:73:SER:HB2	1:B:75:LEU:HG	1.96	0.47
1:B:1231:VAL:HG12	1:B:1309:ILE:HD12	1.97	0.47
1:F:1102:TYR:HB3	1:F:1136:PRO:HG2	1.98	0.46
1:A:1116:MET:H	1:A:1224:HIS:CD2	2.33	0.46
1:D:89:LEU:HD23	1:D:107:PRO:HG2	1.96	0.46
1:E:229:PRO:HA	1:E:232:TRP:CE2	2.49	0.46
1:D:73:SER:HB2	1:D:75:LEU:HG	1.97	0.46
1:E:1105:LEU:HG	1:F:1351:ILE:HG23	1.96	0.46
1:A:1105:LEU:HG	1:B:1351:ILE:HG23	1.97	0.46
1:E:1216:LEU:C	1:E:1219:PRO:HD2	2.35	0.46
1:E:1178:ARG:HD2	1:E:1194:ASP:HB3	1.97	0.46
1:A:1113:ASN:ND2	1:A:1115:VAL:O	2.48	0.46
1:D:1116:MET:H	1:D:1224:HIS:CD2	2.33	0.46
1:E:33:ILE:HG12	1:E:275:LEU:HD13	1.98	0.46
1:B:229:PRO:HA	1:B:232:TRP:CE2	2.50	0.46
1:D:169:PHE:CD2	1:D:333:ILE:HD11	2.50	0.46
1:E:66:ARG:NH2	5:E:2001:GLC:O4	2.44	0.46
1:E:1231:VAL:HG12	1:E:1309:ILE:HD12	1.97	0.46
1:C:1171:VAL:HG21	1:C:1296:PRO:HG3	1.96	0.46
1:C:85:PHE:HA	1:C:88:LYS:HE3	1.97	0.46
1:E:85:PHE:O	1:E:88:LYS:HG2	2.16	0.46
1:F:95:ASP:OD1	1:F:98:ARG:NH1	2.48	0.46
1:D:229:PRO:HA	1:D:232:TRP:CE2	2.51	0.46
1:C:1113:ASN:ND2	1:C:1115:VAL:O	2.49	0.46
1:D:129:TRP:CD1	1:D:248:PRO:HB2	2.51	0.45
1:E:1269:PRO:O	1:E:1273:ARG:HB2	2.15	0.45
1:C:1178:ARG:HD2	1:C:1194:ASP:HB3	1.98	0.45
1:F:1080:ARG:NH1	3:F:2007:GNS:O2S	2.50	0.45
1:E:1216:LEU:O	1:E:1219:PRO:HD2	2.17	0.45
1:A:1332:VAL:HG12	1:A:1341:ILE:HD12	1.98	0.45
1:B:85:PHE:O	1:B:88:LYS:HG2	2.16	0.45
1:F:97:VAL:HG21	1:F:107:PRO:HD3	1.99	0.45
1:E:1079:ASN:HB2	1:E:1143:VAL:O	2.17	0.45
1:B:1178:ARG:HD2	1:B:1194:ASP:HB3	1.98	0.45
1:C:130:GLU:O	1:C:133:PRO:HD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:PRO:HB2	1:C:333:ILE:HG12	1.99	0.45
1:D:1088:SER:HA	1:D:1287:LEU:HD12	1.99	0.45
1:C:1110:THR:HG22	1:C:1111:LYS:HG3	1.99	0.45
1:C:1116:MET:H	1:C:1224:HIS:CD2	2.35	0.45
1:F:90:TYR:CE1	1:F:305:LYS:HG2	2.52	0.45
1:C:90:TYR:CE1	1:C:305:LYS:HG2	2.52	0.45
1:B:157:THR:HG23	1:B:195:LEU:HD22	1.99	0.45
1:B:1201:CYS:SG	1:B:1206:GLY:HA3	2.56	0.44
1:F:1116:MET:H	1:F:1224:HIS:CD2	2.35	0.44
1:D:33:ILE:HG12	1:D:275:LEU:HD13	1.98	0.44
1:B:1108:ASN:O	1:C:1346:PHE:HA	2.17	0.44
1:C:1332:VAL:HG12	1:C:1341:ILE:HD12	2.00	0.44
1:B:89:LEU:HD23	1:B:107:PRO:HG2	1.99	0.44
1:C:33:ILE:HG12	1:C:275:LEU:HD13	2.00	0.44
1:E:1215:TRP:NE1	1:E:1219:PRO:HG3	2.33	0.44
1:F:85:PHE:HA	1:F:88:LYS:HE3	1.99	0.44
1:E:85:PHE:HA	1:E:88:LYS:HE3	1.99	0.44
1:F:1216:LEU:C	1:F:1219:PRO:HD2	2.38	0.44
1:D:1102:TYR:HB3	1:D:1136:PRO:HG2	2.00	0.44
1:B:1295:LEU:HA	1:B:1296:PRO:HD3	1.84	0.44
1:D:90:TYR:CE1	1:D:305:LYS:HG2	2.53	0.44
1:B:1113:ASN:ND2	1:B:1115:VAL:O	2.51	0.44
1:F:229:PRO:HA	1:F:232:TRP:CE2	2.52	0.44
1:C:229:PRO:HA	1:C:232:TRP:CE2	2.53	0.43
1:A:1295:LEU:HA	1:A:1296:PRO:HD3	1.85	0.43
1:F:85:PHE:O	1:F:88:LYS:HG2	2.18	0.43
1:A:1231:VAL:HG12	1:A:1309:ILE:HD12	1.99	0.43
1:E:1116:MET:H	1:E:1224:HIS:CD2	2.35	0.43
1:A:1216:LEU:O	1:A:1219:PRO:HD2	2.18	0.43
1:F:1178:ARG:HD2	1:F:1194:ASP:HB3	2.00	0.43
1:F:33:ILE:HG12	1:F:275:LEU:HD13	2.00	0.43
1:C:196:VAL:HG12	1:C:200:LYS:HE2	1.99	0.43
1:F:1201:CYS:SG	1:F:1206:GLY:HA3	2.58	0.43
1:B:1216:LEU:O	1:B:1219:PRO:HD2	2.19	0.43
1:E:129:TRP:CD1	1:E:248:PRO:HB2	2.54	0.43
1:B:291:GLU:O	1:B:295:LYS:HG3	2.19	0.43
1:A:1201:CYS:SG	1:A:1206:GLY:HA3	2.58	0.43
1:A:1269:PRO:O	1:A:1273:ARG:HB2	2.19	0.43
1:B:1188:ARG:NH2	1:D:1314:ASN:OD1	2.52	0.43
1:E:1080:ARG:HG2	1:E:1080:ARG:H	1.61	0.43
1:E:1080:ARG:NH1	3:E:2007:GNS:O2S	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:PHE:CE2	1:C:264:ALA:HB2	2.54	0.43
1:C:85:PHE:O	1:C:88:LYS:HG2	2.18	0.43
1:C:1102:TYR:HB3	1:C:1136:PRO:HG2	2.01	0.42
1:A:1264:LEU:HA	1:A:1264:LEU:HD23	1.90	0.42
1:C:1333:ARG:HB2	1:C:1342:LEU:HD21	2.01	0.42
1:B:1090:THR:HG21	1:B:1140:HIS:CE1	2.54	0.42
1:F:1216:LEU:O	1:F:1219:PRO:HD2	2.18	0.42
1:E:73:SER:HB2	1:E:75:LEU:HG	2.01	0.42
1:F:1231:VAL:HG12	1:F:1309:ILE:HD12	2.01	0.42
1:E:90:TYR:HA	1:E:91:PRO:HD3	1.87	0.42
1:F:1080:ARG:H	1:F:1080:ARG:HG2	1.57	0.42
1:B:291:GLU:HG2	1:B:295:LYS:HE3	2.01	0.42
1:E:1113:ASN:ND2	1:E:1115:VAL:O	2.52	0.42
1:E:1117:SER:O	1:E:1121:GLN:HG3	2.20	0.42
1:E:61:PHE:CE2	1:E:264:ALA:HB2	2.55	0.42
1:C:89:LEU:HD23	1:C:107:PRO:HG2	2.00	0.42
1:D:1216:LEU:C	1:D:1219:PRO:HD2	2.40	0.42
1:B:90:TYR:CE1	1:B:305:LYS:HG2	2.54	0.42
1:C:1159:TYR:HB3	1:C:1248:TYR:CD2	2.55	0.42
3:B:2005:NDG:O7	3:B:2005:NDG:O3	2.33	0.42
1:F:66:ARG:NH2	5:F:2001:GLC:O4	2.45	0.42
1:A:1181:ASP:OD2	1:A:1183:TYR:N	2.53	0.41
1:D:130:GLU:O	1:D:133:PRO:HD2	2.20	0.41
1:D:169:PHE:HB3	1:D:177:ASP:HB3	2.00	0.41
1:D:305:LYS:O	1:D:309:GLU:HG3	2.20	0.41
1:C:53:THR:HB	1:C:1348:TYR:CE2	2.55	0.41
1:F:1081:VAL:HA	1:F:1082:PRO:HD3	1.91	0.41
1:E:1088:SER:HA	1:E:1287:LEU:HD12	2.02	0.41
1:F:160:LEU:HD23	1:F:195:LEU:HB2	2.01	0.41
1:D:1295:LEU:HA	1:D:1296:PRO:HD3	1.88	0.41
1:C:314:ASP:HA	1:C:315:PRO:HD3	1.91	0.41
1:B:1352:TYR:HE1	1:B:1354:LYS:HE2	1.85	0.41
1:A:1108:ASN:ND2	1:B:1349:GLU:OE2	2.42	0.41
1:E:171:TYR:HA	1:E:176:TYR:O	2.21	0.41
1:B:1102:TYR:HB3	1:B:1136:PRO:HG2	2.03	0.41
1:B:90:TYR:HA	1:B:91:PRO:HD3	1.90	0.41
1:F:1198:PHE:O	1:F:1202:VAL:HG23	2.20	0.41
1:D:1105:LEU:HG	1:E:1351:ILE:HG23	2.02	0.41
1:D:160:LEU:HD23	1:D:195:LEU:HB2	2.03	0.41
1:C:1088:SER:HA	1:C:1287:LEU:HD12	2.03	0.41
1:F:1227:GLU:O	1:F:1236:ALA:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:109:ALA:HA	1:E:302:VAL:HA	2.03	0.41
1:B:61:PHE:CE2	1:B:264:ALA:HB2	2.56	0.41
1:F:1142[B]:HIS:CD2	1:F:1220:PHE:HZ	2.38	0.41
1:B:150:ASN:HB3	1:B:156:PHE:CD1	2.55	0.41
1:F:53:THR:HB	1:F:1278:LEU:HD13	2.03	0.41
1:B:331:PRO:HB2	1:B:333:ILE:HG12	2.03	0.41
1:B:1088:SER:HA	1:B:1287:LEU:HD12	2.02	0.40
1:F:129:TRP:CD1	1:F:248:PRO:HB2	2.57	0.40
1:B:1222:CYS:HB3	1:B:1228:CYS:HB3	2.02	0.40
1:D:1231:VAL:HG12	1:D:1309:ILE:HD12	2.02	0.40
1:F:89:LEU:HD23	1:F:107:PRO:HG2	2.03	0.40
1:B:1171:VAL:HG21	1:B:1296:PRO:HG3	2.03	0.40
1:D:90:TYR:HA	1:D:91:PRO:HD3	1.90	0.40
1:E:1165:ASP:OD2	1:E:1166:PRO:HD2	2.21	0.40
1:E:1159:TYR:HB3	1:E:1248:TYR:CD2	2.57	0.40
1:C:9:ILE:HG12	1:C:59:ILE:HB	2.03	0.40
1:F:157:THR:HG23	1:F:195:LEU:HD22	2.02	0.40
1:B:100:ASN:OD1	1:B:1099:LYS:HE2	2.22	0.40
1:B:78:GLU:HG3	1:B:102:LYS:HB3	2.04	0.40
1:A:1165:ASP:OD2	1:A:1166:PRO:HD2	2.22	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	285/658 (43%)	272 (95%)	13 (5%)	0	100	100
1	B	650/658 (99%)	616 (95%)	31 (5%)	3 (0%)	34	77
1	C	651/658 (99%)	619 (95%)	28 (4%)	4 (1%)	30	74
1	D	650/658 (99%)	614 (94%)	30 (5%)	6 (1%)	21	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	650/658 (99%)	619 (95%)	28 (4%)	3 (0%)	34 77
1	F	651/658 (99%)	619 (95%)	29 (4%)	3 (0%)	34 77
All	All	3537/3948 (90%)	3359 (95%)	159 (4%)	19 (0%)	34 77

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	370	ALA
1	D	1072	ASP
1	E	369	ALA
1	B	1336	ASP
1	B	169	PHE
1	D	1069	ASP
1	E	169	PHE
1	F	1336	ASP
1	C	1336	ASP
1	F	169	PHE
1	C	169	PHE
1	D	169	PHE
1	C	1070	GLU
1	B	165	GLY
1	C	165	GLY
1	F	165	GLY
1	D	165	GLY
1	E	165	GLY
1	D	178	ILE

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	245/548 (45%)	240 (98%)	5 (2%)	63 86
1	B	524/548 (96%)	518 (99%)	6 (1%)	80 92
1	C	522/548 (95%)	518 (99%)	4 (1%)	86 95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	524/548 (96%)	515 (98%)	9 (2%)	68 89
1	E	519/548 (95%)	514 (99%)	5 (1%)	82 93
1	F	521/548 (95%)	512 (98%)	9 (2%)	68 89
All	All	2855/3288 (87%)	2817 (99%)	38 (1%)	76 91

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1112	ASN
1	A	1133	GLU
1	A	1220	PHE
1	A	1225	SER
1	A	1297	THR
1	B	178	ILE
1	B	227	ASN
1	B	258	PHE
1	B	1220	PHE
1	B	1225	SER
1	B	1297	THR
1	C	121	LEU
1	C	227	ASN
1	C	258	PHE
1	C	1220	PHE
1	D	177	ASP
1	D	178	ILE
1	D	227	ASN
1	D	258	PHE
1	D	321	MET
1	D	1112	ASN
1	D	1209	CYS
1	D	1220	PHE
1	D	1336	ASP
1	E	227	ASN
1	E	258	PHE
1	E	321	MET
1	E	1112	ASN
1	E	1220	PHE
1	F	3	GLU
1	F	178	ILE
1	F	227	ASN
1	F	258	PHE

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Mol	Chain	Res	Type
1	F	1099	LYS
1	F	1112	ASN
1	F	1126	LYS
1	F	1209	CYS
1	F	1220	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1127	ASN
1	B	1127	ASN
1	C	1106	HIS
1	C	1127	ASN
1	D	1127	ASN
1	E	1127	ASN
1	F	1106	HIS
1	F	1127	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

45 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	$\#\|Z\| > 2$
3	BDP	A	2004	3	9,12,13	2.81	5 (55%)	13,17,19	1.25	2 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NDG	A	2005	3	14,14,15	0.59	1 (7%)	15,19,21	0.39	0
3	BDP	A	2006	3	9,12,13	2.67	3 (33%)	13,17,19	1.57	1 (7%)
3	GNS	A	2007	3	13,15,16	2.45	8 (61%)	14,22,24	1.86	3 (21%)
3	IDR	A	2008	3	9,12,13	2.65	4 (44%)	13,17,19	0.95	0
3	GNS	A	2009	3	13,15,16	2.57	7 (53%)	14,22,24	1.40	1 (7%)
3	BDP	A	2010	3,4	9,12,13	3.00	4 (44%)	13,17,19	1.65	2 (15%)
5	GLC	B	2001	5	11,11,12	0.60	0	14,15,17	0.70	0
5	GLC	B	2002	5	12,12,12	0.53	0	17,17,17	0.66	0
3	BDP	B	2004	3	9,12,13	2.88	4 (44%)	13,17,19	1.18	1 (7%)
3	NDG	B	2005	3	14,14,15	0.57	0	15,19,21	0.61	0
3	BDP	B	2006	3	9,12,13	2.67	4 (44%)	13,17,19	1.33	1 (7%)
3	GNS	B	2007	3	13,15,16	2.61	7 (53%)	14,22,24	1.85	2 (14%)
3	IDR	B	2008	3	9,12,13	2.62	5 (55%)	13,17,19	1.01	1 (7%)
3	GNS	B	2009	3	13,15,16	2.57	6 (46%)	14,22,24	1.36	1 (7%)
3	BDP	B	2010	3,4	9,12,13	3.00	5 (55%)	13,17,19	1.33	2 (15%)
5	GLC	C	2001	5	11,11,12	0.58	0	14,15,17	0.74	0
5	GLC	C	2002	5	12,12,12	0.53	0	17,17,17	0.64	0
5	GLC	D	2001	5	11,11,12	0.63	0	14,15,17	0.76	0
5	GLC	D	2002	5	12,12,12	0.53	0	17,17,17	0.65	0
3	BDP	D	2004	3	9,12,13	2.73	5 (55%)	13,17,19	1.26	2 (15%)
3	NDG	D	2005	3	14,14,15	0.48	0	15,19,21	0.61	0
3	BDP	D	2006	3	9,12,13	2.57	3 (33%)	13,17,19	1.39	1 (7%)
3	GNS	D	2007	3	13,15,16	2.56	6 (46%)	14,22,24	1.94	3 (21%)
3	IDR	D	2008	3	9,12,13	2.60	4 (44%)	13,17,19	0.64	0
3	GNS	D	2009	3	13,15,16	2.68	7 (53%)	14,22,24	1.42	3 (21%)
3	BDP	D	2010	3,4	9,12,13	2.67	5 (55%)	13,17,19	1.57	1 (7%)
5	GLC	E	2001	5	11,11,12	0.63	0	14,15,17	0.84	0
5	GLC	E	2002	5	12,12,12	0.53	0	17,17,17	0.73	1 (5%)
3	BDP	E	2004	3	9,12,13	2.83	5 (55%)	13,17,19	1.25	1 (7%)
3	NDG	E	2005	3	14,14,15	0.58	1 (7%)	15,19,21	0.39	0
3	BDP	E	2006	3	9,12,13	2.86	3 (33%)	13,17,19	0.95	1 (7%)
3	GNS	E	2007	3	13,15,16	2.40	6 (46%)	14,22,24	1.72	2 (14%)
3	IDR	E	2008	3	9,12,13	2.44	4 (44%)	13,17,19	0.91	0
3	GNS	E	2009	3	13,15,16	2.60	7 (53%)	14,22,24	1.63	1 (7%)
3	BDP	E	2010	3,4	9,12,13	2.92	4 (44%)	13,17,19	1.35	2 (15%)
5	GLC	F	2001	5	11,11,12	0.62	0	14,15,17	0.63	0
5	GLC	F	2002	5	12,12,12	0.51	0	17,17,17	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	BDP	F	2004	3	9,12,13	2.70	5 (55%)	13,17,19	1.29	2 (15%)
3	NDG	F	2005	3	14,14,15	0.56	0	15,19,21	0.40	0
3	BDP	F	2006	3	9,12,13	2.87	3 (33%)	13,17,19	1.22	1 (7%)
3	GNS	F	2007	3	13,15,16	2.42	7 (53%)	14,22,24	1.64	1 (7%)
3	IDR	F	2008	3	9,12,13	2.47	4 (44%)	13,17,19	0.85	0
3	GNS	F	2009	3	13,15,16	2.61	8 (61%)	14,22,24	1.32	1 (7%)
3	BDP	F	2010	3	10,13,13	1.98	3 (30%)	15,19,19	1.38	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	BDP	A	2004	3	-	0/0/21/24	0/1/1/1
3	NDG	A	2005	3	-	0/6/23/26	0/1/1/1
3	BDP	A	2006	3	-	0/0/21/24	0/1/1/1
3	GNS	A	2007	3	-	0/7/24/27	0/1/1/1
3	IDR	A	2008	3	-	0/0/21/24	0/1/1/1
3	GNS	A	2009	3	-	0/7/24/27	0/1/1/1
3	BDP	A	2010	3,4	-	0/0/21/24	0/1/1/1
5	GLC	B	2001	5	-	0/2/19/22	0/1/1/1
5	GLC	B	2002	5	-	0/2/22/22	0/1/1/1
3	BDP	B	2004	3	-	0/0/21/24	0/1/1/1
3	NDG	B	2005	3	-	0/6/23/26	0/1/1/1
3	BDP	B	2006	3	-	0/0/21/24	0/1/1/1
3	GNS	B	2007	3	-	0/7/24/27	0/1/1/1
3	IDR	B	2008	3	-	0/0/21/24	0/1/1/1
3	GNS	B	2009	3	-	0/7/24/27	0/1/1/1
3	BDP	B	2010	3,4	-	0/0/21/24	0/1/1/1
5	GLC	C	2001	5	-	0/2/19/22	0/1/1/1
5	GLC	C	2002	5	-	0/2/22/22	0/1/1/1
5	GLC	D	2001	5	-	0/2/19/22	0/1/1/1
5	GLC	D	2002	5	-	0/2/22/22	0/1/1/1
3	BDP	D	2004	3	-	0/0/21/24	0/1/1/1
3	NDG	D	2005	3	-	0/6/23/26	0/1/1/1
3	BDP	D	2006	3	-	0/0/21/24	0/1/1/1
3	GNS	D	2007	3	-	0/7/24/27	0/1/1/1
3	IDR	D	2008	3	-	0/0/21/24	0/1/1/1
3	GNS	D	2009	3	-	0/7/24/27	0/1/1/1
3	BDP	D	2010	3,4	-	0/0/21/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GLC	E	2001	5	-	0/2/19/22	0/1/1/1
5	GLC	E	2002	5	-	0/2/22/22	0/1/1/1
3	BDP	E	2004	3	-	0/0/21/24	0/1/1/1
3	NDG	E	2005	3	-	0/6/23/26	0/1/1/1
3	BDP	E	2006	3	-	0/0/21/24	0/1/1/1
3	GNS	E	2007	3	-	0/7/24/27	0/1/1/1
3	IDR	E	2008	3	-	0/0/21/24	0/1/1/1
3	GNS	E	2009	3	-	0/7/24/27	0/1/1/1
3	BDP	E	2010	3,4	-	0/0/21/24	0/1/1/1
5	GLC	F	2001	5	-	0/2/19/22	0/1/1/1
5	GLC	F	2002	5	-	0/2/22/22	0/1/1/1
3	BDP	F	2004	3	-	0/0/21/24	0/1/1/1
3	NDG	F	2005	3	-	0/6/23/26	0/1/1/1
3	BDP	F	2006	3	-	0/0/21/24	0/1/1/1
3	GNS	F	2007	3	-	0/7/24/27	0/1/1/1
3	IDR	F	2008	3	-	0/0/21/24	0/1/1/1
3	GNS	F	2009	3	-	0/7/24/27	0/1/1/1
3	BDP	F	2010	3	-	0/0/24/24	0/1/1/1

All (153) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2010	BDP	O5-C5	-6.77	1.36	1.43
3	B	2010	BDP	O5-C5	-6.45	1.37	1.43
3	E	2010	BDP	O5-C5	-6.44	1.37	1.43
3	F	2006	BDP	O5-C5	-6.40	1.37	1.43
3	B	2004	BDP	O5-C5	-6.35	1.37	1.43
3	E	2006	BDP	O5-C5	-6.23	1.37	1.43
3	E	2004	BDP	O5-C5	-6.05	1.37	1.43
3	A	2004	BDP	O5-C5	-5.96	1.37	1.43
3	B	2006	BDP	O5-C5	-5.78	1.37	1.43
3	A	2006	BDP	O5-C5	-5.75	1.37	1.43
3	D	2004	BDP	O5-C5	-5.74	1.37	1.43
3	D	2006	BDP	O5-C5	-5.66	1.38	1.43
3	D	2010	BDP	O5-C5	-5.65	1.38	1.43
3	F	2004	BDP	O5-C5	-5.63	1.38	1.43
3	D	2008	IDR	O5-C5	-5.30	1.38	1.43
3	B	2008	IDR	O5-C5	-5.18	1.38	1.43
3	A	2008	IDR	O5-C5	-5.18	1.38	1.43
3	F	2008	IDR	O5-C5	-4.92	1.38	1.43
3	E	2008	IDR	O5-C5	-4.84	1.38	1.43
3	F	2010	BDP	O5-C5	-4.24	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2009	GNS	O5-C1	-4.05	1.36	1.43
3	F	2006	BDP	O5-C1	-4.03	1.37	1.43
3	B	2009	GNS	O5-C1	-4.02	1.37	1.43
3	E	2006	BDP	O5-C1	-3.99	1.37	1.43
3	E	2010	BDP	O5-C1	-3.90	1.37	1.43
3	D	2009	GNS	O5-C1	-3.82	1.37	1.43
3	B	2004	BDP	O5-C1	-3.79	1.37	1.43
3	F	2009	GNS	O5-C1	-3.75	1.37	1.43
3	B	2010	BDP	O5-C1	-3.71	1.37	1.43
3	E	2004	BDP	O5-C1	-3.70	1.37	1.43
3	A	2008	IDR	O5-C1	-3.69	1.37	1.43
3	A	2004	BDP	O5-C1	-3.68	1.37	1.43
3	A	2006	BDP	O5-C1	-3.64	1.37	1.43
3	D	2004	BDP	O5-C1	-3.61	1.37	1.43
3	D	2007	GNS	O5-C1	-3.60	1.37	1.43
3	B	2006	BDP	O5-C1	-3.56	1.37	1.43
3	A	2010	BDP	O5-C1	-3.55	1.37	1.43
3	F	2007	GNS	O5-C1	-3.54	1.37	1.43
3	F	2004	BDP	O5-C1	-3.52	1.37	1.43
3	D	2006	BDP	O5-C1	-3.52	1.37	1.43
3	B	2007	GNS	O5-C1	-3.48	1.37	1.43
3	E	2009	GNS	O5-C1	-3.48	1.37	1.43
3	B	2008	IDR	O5-C1	-3.47	1.37	1.43
3	D	2008	IDR	O5-C1	-3.43	1.38	1.43
3	E	2007	GNS	O5-C1	-3.40	1.38	1.43
3	E	2008	IDR	O5-C1	-3.35	1.38	1.43
3	A	2007	GNS	O5-C1	-3.22	1.38	1.43
3	F	2008	IDR	O5-C1	-3.22	1.38	1.43
3	D	2010	BDP	O5-C1	-3.17	1.38	1.43
3	A	2009	GNS	O5-C5	-2.77	1.37	1.43
3	B	2009	GNS	O5-C5	-2.73	1.37	1.43
3	D	2007	GNS	O5-C5	-2.57	1.37	1.43
3	A	2010	BDP	O2-C2	-2.54	1.37	1.43
3	A	2007	GNS	O5-C5	-2.53	1.37	1.43
3	B	2007	GNS	O5-C5	-2.52	1.37	1.43
3	D	2009	GNS	O5-C5	-2.52	1.37	1.43
3	A	2006	BDP	O2-C2	-2.52	1.37	1.43
3	B	2010	BDP	O2-C2	-2.50	1.37	1.43
3	E	2006	BDP	O2-C2	-2.48	1.37	1.43
3	A	2008	IDR	O2-C2	-2.44	1.37	1.43
3	D	2010	BDP	O2-C2	-2.44	1.37	1.43
3	E	2009	GNS	O5-C5	-2.42	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2008	IDR	O2-C2	-2.42	1.37	1.43
3	A	2004	BDP	O2-C2	-2.42	1.37	1.43
3	D	2004	BDP	O2-C2	-2.41	1.37	1.43
3	F	2010	BDP	O5-C1	-2.41	1.38	1.43
3	F	2004	BDP	O2-C2	-2.40	1.38	1.43
3	A	2007	GNS	C2-N	-2.38	1.43	1.47
3	E	2010	BDP	O2-C2	-2.38	1.38	1.43
3	B	2010	BDP	O3-C3	-2.37	1.37	1.43
3	E	2009	GNS	C2-N	-2.37	1.43	1.47
3	D	2009	GNS	C2-N	-2.37	1.43	1.47
3	B	2004	BDP	O2-C2	-2.35	1.38	1.43
3	F	2008	IDR	O2-C2	-2.34	1.38	1.43
3	E	2008	IDR	O2-C2	-2.34	1.38	1.43
3	F	2009	GNS	O5-C5	-2.34	1.38	1.43
3	E	2004	BDP	O2-C2	-2.31	1.38	1.43
3	D	2008	IDR	O2-C2	-2.31	1.38	1.43
3	F	2006	BDP	O2-C2	-2.31	1.38	1.43
3	D	2006	BDP	O2-C2	-2.29	1.38	1.43
3	A	2008	IDR	O3-C3	-2.28	1.37	1.43
3	B	2006	BDP	O2-C2	-2.28	1.38	1.43
3	F	2008	IDR	O3-C3	-2.27	1.37	1.43
3	F	2009	GNS	C2-N	-2.27	1.43	1.47
3	B	2007	GNS	C2-N	-2.27	1.43	1.47
3	B	2008	IDR	O3-C3	-2.26	1.37	1.43
3	E	2007	GNS	O5-C5	-2.26	1.38	1.43
3	A	2010	BDP	O3-C3	-2.26	1.37	1.43
3	B	2009	GNS	C2-N	-2.26	1.43	1.47
3	A	2009	GNS	C2-N	-2.24	1.43	1.47
3	D	2007	GNS	C2-N	-2.24	1.43	1.47
3	D	2008	IDR	O3-C3	-2.20	1.37	1.43
3	F	2007	GNS	O5-C5	-2.20	1.38	1.43
3	F	2010	BDP	O3-C3	-2.19	1.37	1.43
3	A	2009	GNS	C1-C2	-2.16	1.49	1.52
3	A	2007	GNS	O4-C4	-2.16	1.37	1.43
3	E	2009	GNS	O3-C3	-2.15	1.37	1.43
3	B	2007	GNS	O3-C3	-2.15	1.37	1.43
3	E	2004	BDP	O4-C4	-2.14	1.37	1.43
3	D	2009	GNS	O4-C4	-2.13	1.37	1.43
3	A	2004	BDP	O4-C4	-2.13	1.37	1.43
3	B	2006	BDP	O3-C3	-2.13	1.37	1.43
3	E	2010	BDP	O3-C3	-2.13	1.37	1.43
3	E	2008	IDR	O3-C3	-2.13	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2009	GNS	O3-C3	-2.12	1.37	1.43
3	B	2010	BDP	C4-C5	-2.12	1.48	1.53
3	E	2007	GNS	O3-C3	-2.11	1.37	1.43
3	F	2009	GNS	C1-C2	-2.11	1.49	1.52
3	A	2009	GNS	O3-C3	-2.11	1.37	1.43
3	F	2007	GNS	O3-C3	-2.10	1.37	1.43
3	D	2009	GNS	O3-C3	-2.09	1.38	1.43
3	F	2004	BDP	O4-C4	-2.08	1.38	1.43
3	B	2007	GNS	O4-C4	-2.07	1.38	1.43
3	A	2004	BDP	O3-C3	-2.07	1.38	1.43
3	D	2007	GNS	O3-C3	-2.07	1.38	1.43
3	D	2004	BDP	O3-C3	-2.07	1.38	1.43
3	E	2009	GNS	C1-C2	-2.07	1.49	1.52
3	E	2004	BDP	O3-C3	-2.06	1.38	1.43
3	F	2007	GNS	O4-C4	-2.06	1.38	1.43
3	B	2004	BDP	O4-C4	-2.06	1.38	1.43
3	E	2007	GNS	O4-C4	-2.06	1.38	1.43
3	A	2007	GNS	O3-C3	-2.06	1.38	1.43
3	F	2007	GNS	C2-N	-2.04	1.44	1.47
3	D	2010	BDP	O3-C3	-2.04	1.38	1.43
3	A	2007	GNS	C4-C5	-2.04	1.48	1.53
3	D	2010	BDP	C2-C3	-2.04	1.49	1.52
3	D	2004	BDP	O4-C4	-2.04	1.38	1.43
3	B	2009	GNS	O3-C3	-2.03	1.38	1.43
3	A	2005	NDG	O-C1	-2.02	1.40	1.43
3	F	2009	GNS	O4-C4	-2.01	1.38	1.43
3	B	2008	IDR	C2-C3	-2.01	1.49	1.52
3	F	2004	BDP	O3-C3	-2.01	1.38	1.43
3	E	2005	NDG	O-C1	-2.00	1.40	1.43
3	A	2007	GNS	O2S-S1	3.79	1.46	1.42
3	F	2007	GNS	O2S-S1	3.94	1.46	1.42
3	B	2009	GNS	O2S-S1	3.99	1.46	1.42
3	E	2007	GNS	O2S-S1	3.99	1.46	1.42
3	A	2009	GNS	O2S-S1	4.04	1.46	1.42
3	D	2007	GNS	O2S-S1	4.40	1.46	1.42
3	A	2009	GNS	O3S-S1	4.50	1.46	1.42
3	F	2009	GNS	O2S-S1	4.59	1.46	1.42
3	E	2007	GNS	O3S-S1	4.62	1.46	1.42
3	A	2007	GNS	O3S-S1	4.63	1.46	1.42
3	E	2009	GNS	O2S-S1	4.66	1.46	1.42
3	F	2007	GNS	O3S-S1	4.73	1.46	1.42
3	B	2007	GNS	O2S-S1	4.73	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2007	GNS	O3S-S1	4.75	1.47	1.42
3	D	2009	GNS	O2S-S1	4.76	1.47	1.42
3	B	2007	GNS	O3S-S1	4.82	1.47	1.42
3	B	2009	GNS	O3S-S1	4.87	1.47	1.42
3	E	2009	GNS	O3S-S1	4.89	1.47	1.42
3	F	2009	GNS	O3S-S1	4.92	1.47	1.42
3	D	2009	GNS	O3S-S1	5.02	1.47	1.42

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2010	BDP	O5-C1-C2	-2.74	106.41	110.86
3	D	2004	BDP	O5-C1-C2	-2.53	106.76	110.86
3	E	2010	BDP	O5-C1-C2	-2.38	107.00	110.86
3	B	2010	BDP	O5-C1-C2	-2.21	107.28	110.86
3	A	2007	GNS	C3-C4-C5	-2.20	106.36	110.20
3	F	2004	BDP	O5-C1-C2	-2.18	107.31	110.86
3	D	2009	GNS	O4-C4-C5	-2.17	103.49	109.24
3	B	2007	GNS	C3-C4-C5	-2.08	106.57	110.20
3	A	2004	BDP	O5-C1-C2	-2.07	107.51	110.86
3	D	2007	GNS	C3-C4-C5	-2.02	106.67	110.20
5	E	2002	GLC	C1-C2-C3	2.01	113.42	110.43
3	B	2008	IDR	C1-C2-C3	2.05	111.97	109.54
3	E	2006	BDP	C1-O5-C5	2.08	115.05	111.84
3	D	2009	GNS	O5-C5-C6	2.10	111.90	107.35
3	E	2007	GNS	O3S-S1-N	2.44	111.76	108.50
3	A	2007	GNS	O3S-S1-N	2.48	111.80	108.50
3	D	2004	BDP	C1-O5-C5	2.83	116.20	111.84
3	D	2007	GNS	O3S-S1-N	2.94	112.42	108.50
3	D	2009	GNS	C1-O5-C5	2.96	116.00	112.25
3	F	2006	BDP	C1-O5-C5	3.08	116.58	111.84
3	B	2010	BDP	C1-O5-C5	3.31	116.93	111.84
3	E	2010	BDP	C1-O5-C5	3.33	116.98	111.84
3	B	2006	BDP	C1-O5-C5	3.40	117.08	111.84
3	A	2004	BDP	C1-O5-C5	3.50	117.24	111.84
3	F	2009	GNS	C1-O5-C5	3.53	116.73	112.25
3	B	2009	GNS	C1-O5-C5	3.59	116.81	112.25
3	B	2004	BDP	C1-O5-C5	3.60	117.39	111.84
3	F	2004	BDP	C1-O5-C5	3.66	117.47	111.84
3	E	2004	BDP	C1-O5-C5	3.78	117.66	111.84
3	A	2009	GNS	C1-O5-C5	3.89	117.19	112.25
3	D	2006	BDP	C1-O5-C5	4.05	118.09	111.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	2010	BDP	C1-O5-C5	4.09	118.25	112.22
3	A	2006	BDP	C1-O5-C5	4.44	118.68	111.84
3	A	2010	BDP	C1-O5-C5	4.48	118.74	111.84
3	D	2010	BDP	C1-O5-C5	4.56	118.87	111.84
3	E	2009	GNS	C1-O5-C5	4.94	118.52	112.25
3	F	2007	GNS	C1-O5-C5	4.97	118.56	112.25
3	E	2007	GNS	C1-O5-C5	5.39	119.09	112.25
3	A	2007	GNS	C1-O5-C5	5.43	119.14	112.25
3	B	2007	GNS	C1-O5-C5	5.60	119.36	112.25
3	D	2007	GNS	C1-O5-C5	5.76	119.56	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2005	NDG	1	0
3	B	2007	GNS	1	0
5	D	2001	GLC	1	0
5	E	2001	GLC	1	0
3	E	2007	GNS	1	0
3	E	2010	BDP	1	0
5	F	2001	GLC	1	0
3	F	2007	GNS	1	0
3	F	2010	BDP	1	0

5.6 Ligand geometry (i)

10 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	$\#\|Z\|>2$

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	A3P	A	2003	-	24,29,29	2.69	11 (45%)	28,45,45	1.96	2 (7%)
4	NPO	A	2011	3	8,10,10	0.44	0	11,13,13	0.86	1 (9%)
2	A3P	B	2003	-	24,29,29	2.65	11 (45%)	28,45,45	2.04	1 (3%)
4	NPO	B	2011	3	8,10,10	0.34	0	11,13,13	0.71	0
2	A3P	C	2003	-	24,29,29	2.71	11 (45%)	28,45,45	2.01	2 (7%)
2	A3P	D	2003	-	24,29,29	2.68	11 (45%)	28,45,45	2.01	2 (7%)
4	NPO	D	2011	3	8,10,10	0.30	0	11,13,13	0.53	0
2	A3P	E	2003	-	24,29,29	2.72	11 (45%)	28,45,45	2.10	2 (7%)
4	NPO	E	2011	3	8,10,10	0.33	0	11,13,13	0.49	0
2	A3P	F	2003	-	24,29,29	2.75	11 (45%)	28,45,45	2.00	2 (7%)

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
2	A3P	A	2003	-	-	0/11/31/31	0/3/3/3
4	NPO	A	2011	3	-	0/4/4/4	0/1/1/1
2	A3P	B	2003	-	-	0/11/31/31	0/3/3/3
4	NPO	B	2011	3	-	0/4/4/4	0/1/1/1
2	A3P	C	2003	-	-	0/11/31/31	0/3/3/3
2	A3P	D	2003	-	-	0/11/31/31	0/3/3/3
4	NPO	D	2011	3	-	0/4/4/4	0/1/1/1
2	A3P	E	2003	-	-	0/11/31/31	0/3/3/3
4	NPO	E	2011	3	-	0/4/4/4	0/1/1/1
2	A3P	F	2003	-	-	0/11/31/31	0/3/3/3

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2003	A3P	O4'-C4'	-3.23	1.37	1.45
2	A	2003	A3P	O4'-C4'	-3.19	1.37	1.45
2	C	2003	A3P	O4'-C4'	-3.03	1.38	1.45
2	F	2003	A3P	O4'-C4'	-3.03	1.38	1.45
2	D	2003	A3P	O4'-C4'	-3.01	1.38	1.45
2	E	2003	A3P	O4'-C4'	-2.93	1.38	1.45
2	D	2003	A3P	O4'-C1'	-2.60	1.37	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2003	A3P	O4'-C1'	-2.58	1.38	1.41
2	A	2003	A3P	O4'-C1'	-2.43	1.38	1.41
2	E	2003	A3P	O2'-C2'	-2.41	1.37	1.43
2	B	2003	A3P	O4'-C1'	-2.38	1.38	1.41
2	D	2003	A3P	O2'-C2'	-2.33	1.37	1.43
2	C	2003	A3P	O2'-C2'	-2.28	1.37	1.43
2	C	2003	A3P	O4'-C1'	-2.28	1.38	1.41
2	F	2003	A3P	O2'-C2'	-2.28	1.37	1.43
2	A	2003	A3P	O2'-C2'	-2.27	1.37	1.43
2	A	2003	A3P	C2'-C3'	-2.27	1.47	1.53
2	E	2003	A3P	C2'-C3'	-2.24	1.48	1.53
2	A	2003	A3P	O3'-C3'	-2.23	1.37	1.44
2	F	2003	A3P	C2'-C3'	-2.20	1.48	1.53
2	F	2003	A3P	O3'-C3'	-2.17	1.37	1.44
2	B	2003	A3P	C2'-C3'	-2.17	1.48	1.53
2	C	2003	A3P	C2'-C3'	-2.16	1.48	1.53
2	E	2003	A3P	O4'-C1'	-2.16	1.38	1.41
2	B	2003	A3P	O2'-C2'	-2.13	1.37	1.43
2	D	2003	A3P	C2'-C3'	-2.09	1.48	1.53
2	C	2003	A3P	O3'-C3'	-2.06	1.37	1.44
2	E	2003	A3P	O3'-C3'	-2.05	1.37	1.44
2	B	2003	A3P	O3'-C3'	-2.02	1.37	1.44
2	D	2003	A3P	O3'-C3'	-2.01	1.37	1.44
2	A	2003	A3P	C6-N6	2.55	1.42	1.34
2	D	2003	A3P	C6-N6	2.61	1.43	1.34
2	B	2003	A3P	C6-N6	2.63	1.43	1.34
2	C	2003	A3P	C6-N6	2.67	1.43	1.34
2	E	2003	A3P	C6-N6	2.70	1.43	1.34
2	F	2003	A3P	C6-N6	2.71	1.43	1.34
2	D	2003	A3P	C5-C4	3.38	1.48	1.40
2	B	2003	A3P	C5-C4	3.44	1.48	1.40
2	A	2003	A3P	C5-C4	3.51	1.48	1.40
2	C	2003	A3P	C5-C4	3.52	1.48	1.40
2	E	2003	A3P	C5-C4	3.56	1.48	1.40
2	F	2003	A3P	C5-C4	3.57	1.48	1.40
2	D	2003	A3P	C8-N7	4.51	1.43	1.34
2	F	2003	A3P	C8-N7	4.53	1.43	1.34
2	B	2003	A3P	C8-N7	4.58	1.43	1.34
2	A	2003	A3P	C8-N7	4.61	1.43	1.34
2	E	2003	A3P	C8-N7	4.62	1.43	1.34
2	C	2003	A3P	C8-N7	4.64	1.43	1.34
2	D	2003	A3P	C4-N3	4.83	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2003	A3P	C4-N3	4.92	1.42	1.35
2	A	2003	A3P	C4-N3	4.92	1.42	1.35
2	B	2003	A3P	C2-N1	4.94	1.43	1.33
2	A	2003	A3P	C2-N1	4.97	1.43	1.33
2	C	2003	A3P	C2-N1	5.02	1.43	1.33
2	F	2003	A3P	C4-N3	5.06	1.43	1.35
2	E	2003	A3P	C2-N1	5.08	1.43	1.33
2	C	2003	A3P	C4-N3	5.11	1.43	1.35
2	D	2003	A3P	C2-N1	5.13	1.43	1.33
2	F	2003	A3P	C2-N1	5.14	1.43	1.33
2	E	2003	A3P	C4-N3	5.15	1.43	1.35
2	B	2003	A3P	C2-N3	6.16	1.43	1.32
2	A	2003	A3P	C2-N3	6.29	1.43	1.32
2	C	2003	A3P	C2-N3	6.35	1.43	1.32
2	D	2003	A3P	C2-N3	6.43	1.43	1.32
2	E	2003	A3P	C2-N3	6.49	1.43	1.32
2	F	2003	A3P	C2-N3	6.58	1.43	1.32

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2003	A3P	N3-C2-N1	-10.11	121.16	128.89
2	B	2003	A3P	N3-C2-N1	-9.86	121.34	128.89
2	D	2003	A3P	N3-C2-N1	-9.76	121.42	128.89
2	C	2003	A3P	N3-C2-N1	-9.64	121.52	128.89
2	F	2003	A3P	N3-C2-N1	-9.45	121.66	128.89
2	A	2003	A3P	N3-C2-N1	-9.07	121.95	128.89
2	C	2003	A3P	C4-C5-N7	-2.87	106.84	109.48
2	A	2003	A3P	C4-C5-N7	-2.68	107.02	109.48
2	F	2003	A3P	C4-C5-N7	-2.44	107.23	109.48
2	D	2003	A3P	C4-C5-N7	-2.34	107.32	109.48
2	E	2003	A3P	C4-C5-N7	-2.31	107.35	109.48
4	A	2011	NPO	C2-C1-N1	2.26	121.31	119.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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	287/658 (43%)	-0.07	2 (0%) 89 84	48, 83, 133, 185	0
1	B	654/658 (99%)	1.47	182 (27%) 1 1	54, 196, 294, 399	0
1	C	655/658 (99%)	0.50	69 (10%) 8 9	63, 129, 207, 293	0
1	D	654/658 (99%)	0.38	49 (7%) 17 16	54, 128, 195, 252	0
1	E	654/658 (99%)	0.28	32 (4%) 33 28	58, 122, 191, 274	0
1	F	654/658 (99%)	1.11	156 (23%) 1 1	57, 170, 263, 333	0
All	All	3558/3948 (90%)	0.68	490 (13%) 4 5	48, 127, 250, 399	0

All (490) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	266	ILE	25.3
1	B	7	LEU	17.8
1	B	51	ALA	16.3
1	B	35	VAL	11.8
1	F	111	GLU	10.0
1	B	148	MET	9.7
1	F	94	TRP	9.7
1	B	50	VAL	9.7
1	B	52	ALA	9.3
1	B	48	PRO	9.2
1	F	285	LEU	9.1
1	B	64	HIS	8.9
1	B	11	ILE	8.8
1	B	5	GLY	8.8
1	B	59	ILE	8.6
1	B	67	PHE	8.4
1	B	104	ILE	8.4
1	F	110	VAL	8.2
1	F	113	LEU	7.9

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Mol	Chain	Res	Type	RSRZ
1	B	269	ALA	7.8
1	B	284	LEU	7.6
1	B	6	LYS	7.6
1	B	38	GLU	7.5
1	B	267	ASN	7.4
1	B	56	GLY	7.1
1	B	303	ALA	7.0
1	B	304	LEU	7.0
1	F	225	THR	6.9
1	B	227	ASN	6.7
1	F	276	ALA	6.7
1	B	103	LEU	6.7
1	F	37	VAL	6.7
1	B	47	PHE	6.6
1	F	106	TYR	6.6
1	B	114	SER	6.3
1	B	226	ILE	6.3
1	B	351	ALA	6.2
1	F	244	VAL	6.2
1	F	280	LEU	6.2
1	F	104	ILE	6.2
1	B	94	TRP	6.2
1	B	358	ASP	6.1
1	B	285	LEU	6.0
1	B	149	PHE	6.0
1	B	281	GLU	6.0
1	C	1189	ARG	5.9
1	B	306	SER	5.8
1	F	92	PHE	5.7
1	B	87	ASP	5.7
1	B	4	GLU	5.7
1	F	226	ILE	5.6
1	F	93	THR	5.6
1	B	9	ILE	5.5
1	B	124	ASN	5.5
1	F	91	PRO	5.5
1	F	301	ALA	5.5
1	D	146	ALA	5.5
1	B	141	ALA	5.4
1	B	280	LEU	5.4
1	B	302	VAL	5.4
1	B	225	THR	5.4

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Mol	Chain	Res	Type	RSRZ
1	B	265	GLY	5.3
1	B	282	ASN	5.3
1	B	80	THR	5.3
1	B	8	VAL	5.2
1	B	143	GLY	5.2
1	B	99	TYR	5.2
1	B	122	LEU	5.2
1	B	97	VAL	5.2
1	F	245	THR	5.2
1	F	279	PHE	5.1
1	D	112	ALA	5.1
1	F	112	ALA	5.1
1	B	299	LEU	5.1
1	F	304	LEU	5.0
1	B	78	GLU	5.0
1	B	134	ALA	5.0
1	B	350	ALA	5.0
1	F	324	ALA	4.9
1	F	284	LEU	4.9
1	B	61	PHE	4.8
1	F	35	VAL	4.8
1	F	224	MET	4.8
1	B	106	TYR	4.8
1	B	10	TRP	4.7
1	F	115	LEU	4.7
1	F	103	LEU	4.7
1	F	105	ALA	4.7
1	B	352	SER	4.7
1	B	37	VAL	4.6
1	F	258	PHE	4.6
1	B	133	PRO	4.6
1	B	105	ALA	4.6
1	C	257	PRO	4.5
1	B	49	GLN	4.5
1	C	226	ILE	4.5
1	F	80	THR	4.5
1	C	116	ILE	4.5
1	F	33	ILE	4.5
1	F	81	PRO	4.5
1	C	160	LEU	4.5
1	C	1177	LEU	4.5
1	B	123	PRO	4.4

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Mol	Chain	Res	Type	RSRZ
1	F	302	VAL	4.4
1	F	16	GLY	4.4
1	B	132	ILE	4.4
1	F	15	LYS	4.3
1	C	224	MET	4.3
1	E	244	VAL	4.3
1	B	135	LEU	4.2
1	B	93	THR	4.2
1	F	67	PHE	4.2
1	F	4	GLU	4.2
1	B	195	LEU	4.2
1	F	118	ASN	4.2
1	C	114	SER	4.2
1	B	39	HIS	4.2
1	C	1173	TYR	4.2
1	B	142	LYS	4.1
1	B	100	ASN	4.1
1	C	113	LEU	4.1
1	C	157	THR	4.1
1	F	275	LEU	4.0
1	C	129	TRP	4.0
1	F	330	MET	4.0
1	E	112	ALA	4.0
1	C	225	THR	4.0
1	D	156	PHE	4.0
1	F	140	LYS	4.0
1	F	232	TRP	4.0
1	B	27	PHE	3.9
1	B	68	GLY	3.9
1	C	120	ASP	3.9
1	B	348	ILE	3.9
1	B	139	LEU	3.9
1	C	121	LEU	3.9
1	B	279	PHE	3.9
1	B	126	PRO	3.9
1	F	60	ILE	3.9
1	F	309	GLU	3.9
1	B	58	ASP	3.9
1	F	20	LEU	3.9
1	B	277	LYS	3.8
1	B	292	ALA	3.8
1	F	109	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	1355	SER	3.8
1	B	198	LEU	3.8
1	B	29	LYS	3.8
1	C	147	LEU	3.8
1	F	231	ALA	3.8
1	C	126	PRO	3.8
1	B	272	ASN	3.8
1	C	1187	LEU	3.8
1	D	226	ILE	3.8
1	D	113	LEU	3.8
1	B	129	TRP	3.7
1	F	122	LEU	3.7
1	B	131	GLU	3.7
1	B	278	GLU	3.7
1	F	59	ILE	3.7
1	F	323	ASN	3.7
1	F	329	ILE	3.7
1	F	247	LEU	3.7
1	C	149	PHE	3.7
1	C	115	LEU	3.7
1	F	281	GLU	3.7
1	F	129	TRP	3.6
1	B	293	VAL	3.6
1	F	90	TYR	3.6
1	B	102	LYS	3.6
1	B	355	GLN	3.6
1	B	194	PHE	3.6
1	F	230	TRP	3.6
1	B	221	GLU	3.6
1	C	148	MET	3.5
1	B	208	THR	3.5
1	B	140	LYS	3.5
1	F	149	PHE	3.5
1	F	1187	LEU	3.5
1	D	198	LEU	3.5
1	B	3	GLU	3.5
1	B	332	ASN	3.5
1	D	143	GLY	3.5
1	C	183	VAL	3.5
1	D	126	PRO	3.5
1	F	160	LEU	3.5
1	B	203	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	107	PRO	3.5
1	F	147	LEU	3.5
1	B	144	LYS	3.5
1	B	89	LEU	3.5
1	B	26	LYS	3.5
1	F	267	ASN	3.5
1	B	276	ALA	3.5
1	F	142	LYS	3.5
1	F	241	ASN	3.5
1	F	108	ILE	3.5
1	B	283	TYR	3.4
1	C	242	TYR	3.4
1	F	79	ILE	3.4
1	E	1288	ARG	3.4
1	E	224	MET	3.4
1	F	1186	GLY	3.4
1	B	79	ILE	3.4
1	F	278	GLU	3.4
1	B	125	PRO	3.4
1	B	357	VAL	3.4
1	B	138	GLU	3.4
1	B	86	GLN	3.4
1	F	36	THR	3.4
1	B	250	PHE	3.4
1	B	92	PHE	3.4
1	B	113	LEU	3.4
1	E	113	LEU	3.4
1	F	19	GLY	3.3
1	C	145	SER	3.3
1	F	96	ALA	3.3
1	B	330	MET	3.3
1	F	7	LEU	3.3
1	F	114	SER	3.3
1	B	24	GLY	3.3
1	D	244	VAL	3.3
1	E	129	TRP	3.3
1	B	121	LEU	3.3
1	D	144	LYS	3.2
1	E	147	LEU	3.2
1	F	163	ALA	3.2
1	B	147	LEU	3.2
1	E	114	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	1191	LYS	3.2
1	C	112	ALA	3.2
1	F	227	ASN	3.2
1	B	137	LYS	3.2
1	D	203	HIS	3.2
1	B	210	TYR	3.2
1	B	222	THR	3.2
1	B	108	ILE	3.2
1	B	211	SER	3.2
1	D	129	TRP	3.1
1	F	273	LYS	3.1
1	B	309	GLU	3.1
1	F	250	PHE	3.1
1	C	223	ALA	3.1
1	E	117	TYR	3.1
1	F	2	ILE	3.1
1	F	246	VAL	3.1
1	F	322	GLU	3.1
1	B	36	THR	3.1
1	B	300	GLY	3.1
1	F	272	ASN	3.1
1	B	109	ALA	3.1
1	C	241	ASN	3.1
1	B	145	SER	3.1
1	F	97	VAL	3.1
1	F	257	PRO	3.1
1	D	303	ALA	3.1
1	F	340	TRP	3.0
1	B	261	VAL	3.0
1	F	82	ASP	3.0
1	F	95	ASP	3.0
1	C	244	VAL	3.0
1	F	200	LYS	3.0
1	D	92	PHE	3.0
1	D	135	LEU	3.0
1	B	81	PRO	3.0
1	B	259	VAL	3.0
1	F	290	LEU	3.0
1	F	242	TYR	3.0
1	B	290	LEU	3.0
1	F	217	PHE	3.0
1	D	205	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	258	PHE	2.9
1	E	156	PHE	2.9
1	D	150	ASN	2.9
1	C	247	LEU	2.9
1	C	201	ASN	2.9
1	F	12	ASN	2.9
1	F	64	HIS	2.9
1	B	183	VAL	2.9
1	E	250	PHE	2.9
1	C	122	LEU	2.9
1	B	110	VAL	2.9
1	E	183	VAL	2.9
1	F	62	TRP	2.9
1	D	245	THR	2.9
1	B	223	ALA	2.9
1	B	66	ARG	2.9
1	B	353	GLY	2.9
1	D	199	ILE	2.9
1	C	227	ASN	2.9
1	B	112	ALA	2.9
1	B	356	THR	2.8
1	F	320	THR	2.8
1	F	27	PHE	2.8
1	B	2	ILE	2.8
1	E	1290	THR	2.8
1	F	144	LYS	2.8
1	F	189	LYS	2.8
1	F	1194	ASP	2.8
1	B	196	VAL	2.8
1	F	6	LYS	2.8
1	D	115	LEU	2.8
1	B	347	VAL	2.8
1	C	118	ASN	2.8
1	F	303	ALA	2.7
1	C	151	LEU	2.7
1	F	65	ASP	2.7
1	B	57	PRO	2.7
1	D	117	TYR	2.7
1	C	146	ALA	2.7
1	C	159	PRO	2.7
1	B	275	LEU	2.7
1	C	169	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	116	ILE	2.7
1	F	11	ILE	2.7
1	B	334	PRO	2.7
1	E	126	PRO	2.7
1	C	156	PHE	2.6
1	B	301	ALA	2.6
1	C	144	LYS	2.6
1	F	126	PRO	2.6
1	B	45	GLU	2.6
1	E	242	TYR	2.6
1	D	162	ALA	2.6
1	C	222	THR	2.6
1	C	109	ALA	2.6
1	B	335	GLN	2.6
1	D	107	PRO	2.6
1	F	3	GLU	2.6
1	F	85	PHE	2.6
1	E	1355	SER	2.6
1	B	201	ASN	2.6
1	B	85	PHE	2.6
1	D	195	LEU	2.6
1	B	23	VAL	2.6
1	F	14	ASP	2.6
1	B	22	GLU	2.6
1	F	89	LEU	2.6
1	B	151	LEU	2.5
1	F	38	GLU	2.6
1	A	1069	ASP	2.5
1	D	259	VAL	2.5
1	C	1183	TYR	2.5
1	B	91	PRO	2.5
1	C	125	PRO	2.5
1	C	245	THR	2.5
1	F	57	PRO	2.5
1	F	260	GLY	2.5
1	B	197	ASP	2.5
1	F	120	ASP	2.5
1	B	136	ASP	2.5
1	F	1069	ASP	2.5
1	F	354	ARG	2.5
1	C	248	PRO	2.5
1	F	34	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	152	GLN	2.5
1	C	178	ILE	2.5
1	F	116	ILE	2.5
1	F	169	PHE	2.5
1	C	208	THR	2.5
1	F	270	SER	2.5
1	F	148	MET	2.5
1	F	218	ASN	2.5
1	B	274	GLU	2.4
1	D	147	LEU	2.4
1	B	96	ALA	2.4
1	C	117	TYR	2.4
1	B	200	LYS	2.4
1	B	263	SER	2.4
1	F	308	GLU	2.4
1	D	192	LEU	2.4
1	F	5	GLY	2.4
1	E	116	ILE	2.4
1	C	203	HIS	2.4
1	F	24	GLY	2.4
1	D	224	MET	2.4
1	E	160	LEU	2.4
1	F	222	THR	2.4
1	E	259	VAL	2.4
1	F	269	ALA	2.4
1	C	184	ASP	2.4
1	E	328	GLU	2.4
1	F	133	PRO	2.4
1	B	21	ALA	2.4
1	E	148	MET	2.4
1	B	12	ASN	2.4
1	C	1186	GLY	2.4
1	F	32	GLY	2.4
1	C	132	ILE	2.4
1	D	151	LEU	2.4
1	E	195	LEU	2.4
1	B	154	PRO	2.3
1	C	1296	PRO	2.3
1	F	325	GLN	2.3
1	B	53	THR	2.3
1	E	111	GLU	2.3
1	B	71	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	133	PRO	2.3
1	B	361	LEU	2.3
1	C	1198	PHE	2.3
1	F	339	PHE	2.3
1	F	328	GLU	2.3
1	B	76	LEU	2.3
1	D	149	PHE	2.3
1	C	320	THR	2.3
1	F	321	MET	2.3
1	B	116	ILE	2.3
1	B	1069	ASP	2.3
1	E	1177	LEU	2.3
1	D	218	ASN	2.3
1	F	292	ALA	2.3
1	C	204	MET	2.3
1	C	299	LEU	2.3
1	F	237	THR	2.3
1	B	155	TYR	2.3
1	B	236	ASP	2.3
1	F	283	TYR	2.3
1	F	86	GLN	2.3
1	E	157	THR	2.3
1	F	9	ILE	2.3
1	F	223	ALA	2.2
1	F	282	ASN	2.2
1	B	230	TRP	2.2
1	D	139	LEU	2.2
1	B	252	GLY	2.2
1	E	1176	PHE	2.2
1	C	1288	ARG	2.2
1	B	157	THR	2.2
1	F	78	GLU	2.2
1	B	120	ASP	2.2
1	F	87	ASP	2.2
1	F	264	ALA	2.2
1	D	136	ASP	2.2
1	C	1176	PHE	2.2
1	E	164	ASP	2.2
1	E	109	ALA	2.2
1	C	61	PHE	2.2
1	F	23	VAL	2.2
1	C	106	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	213	ALA	2.2
1	B	264	ALA	2.1
1	B	260	GLY	2.1
1	F	39	HIS	2.1
1	E	149	PHE	2.1
1	F	1288	ARG	2.1
1	F	156	PHE	2.1
1	B	253	GLN	2.1
1	C	1192	GLN	2.1
1	B	115	LEU	2.1
1	C	1287	LEU	2.1
1	D	320	THR	2.1
1	F	55	ASP	2.1
1	F	1193	GLY	2.1
1	C	161	ILE	2.1
1	B	117	TYR	2.1
1	D	145	SER	2.1
1	D	155	TYR	2.1
1	D	160	LEU	2.1
1	D	304	LEU	2.1
1	C	150	ASN	2.1
1	D	93	THR	2.1
1	D	158	TRP	2.1
1	B	90	TYR	2.1
1	B	28	GLU	2.1
1	C	347	VAL	2.1
1	F	357	VAL	2.1
1	F	1191	LYS	2.1
1	D	308	GLU	2.1
1	B	349	ASN	2.1
1	F	266	ILE	2.1
1	F	286	THR	2.1
1	E	155	TYR	2.1
1	B	88	LYS	2.1
1	B	287	ASP	2.1
1	F	157	THR	2.1
1	F	194	PHE	2.1
1	D	90	TYR	2.1
1	D	31	THR	2.0
1	D	258	PHE	2.0
1	F	138	GLU	2.0
1	D	351	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	1101	ARG	2.0
1	F	99	TYR	2.0
1	F	154	PRO	2.0
1	C	339	PHE	2.0
1	D	110	VAL	2.0
1	B	288	GLU	2.0
1	E	110	VAL	2.0
1	F	251	LYS	2.0
1	D	20	LEU	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
3	GNS	F	2009	15/16	0.91	0.52	1.73	177,183,197,203	0
3	BDP	D	2004	12/13	0.81	0.25	0.89	172,199,213,219	0
3	GNS	F	2007	15/16	0.90	0.28	0.24	112,150,186,198	0
5	GLC	E	2002	12/12	0.96	0.33	-0.22	88,98,112,113	0
3	IDR	A	2008	12/13	0.97	0.24	-0.24	68,88,103,113	0
3	IDR	E	2008	12/13	0.95	0.31	-0.31	128,148,209,213	0
5	GLC	C	2002	12/12	0.96	0.30	-0.33	95,124,137,149	0
3	GNS	E	2007	15/16	0.96	0.24	-0.50	123,144,168,187	0
5	GLC	D	2002	12/12	0.90	0.28	-0.52	135,142,153,154	0
5	GLC	B	2001	11/12	0.72	0.35	-0.53	218,235,256,257	0
3	GNS	E	2009	15/16	0.94	0.27	-0.56	150,164,191,196	0
5	GLC	D	2001	11/12	0.93	0.24	-0.65	92,109,127,127	0
3	IDR	F	2008	12/13	0.87	0.23	-0.80	142,162,187,200	0
3	IDR	B	2008	12/13	0.94	0.20	-0.82	100,112,121,124	0
3	GNS	A	2007	15/16	0.98	0.20	-1.03	72,78,98,101	0
3	BDP	E	2010	12/13	0.85	0.18	-1.11	146,191,216,218	0
5	GLC	F	2001	11/12	0.89	0.31	-1.12	149,166,181,185	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	GNS	A	2009	15/16	0.97	0.17	-1.17	63,75,99,100	0
3	GNS	D	2009	15/16	0.94	0.18	-1.22	100,120,139,152	0
3	GNS	B	2007	15/16	0.98	0.18	-1.24	79,93,110,133	0
5	GLC	F	2002	12/12	0.91	0.24	-1.32	165,176,181,186	0
5	GLC	B	2002	12/12	0.78	0.27	-1.34	197,218,230,239	0
3	IDR	D	2008	12/13	0.97	0.19	-1.42	103,126,151,165	0
5	GLC	E	2001	11/12	0.98	0.20	-1.57	79,95,124,133	0
3	GNS	D	2007	15/16	0.96	0.19	-1.77	88,117,142,145	0
3	GNS	B	2009	15/16	0.96	0.18	-1.83	84,89,108,118	0
5	GLC	C	2001	11/12	0.98	0.13	-2.03	93,97,110,112	0
3	NDG	E	2005	14/15	0.87	0.29	-	139,188,202,212	0
3	BDP	A	2006	12/13	0.88	0.15	-	95,130,153,167	0
3	BDP	F	2010	13/13	0.69	0.39	-	120,143,173,179	0
3	BDP	D	2006	12/13	0.83	0.20	-	126,144,163,173	0
3	BDP	A	2010	12/13	0.96	0.15	-	68,93,105,108	0
3	BDP	F	2004	12/13	0.72	0.40	-	195,218,230,230	0
3	BDP	F	2006	12/13	0.68	0.24	-	136,206,212,214	0
3	BDP	B	2010	12/13	0.97	0.18	-	77,94,107,109	0
3	BDP	D	2010	12/13	0.93	0.14	-	103,127,150,155	0
3	BDP	B	2004	12/13	0.88	0.16	-	148,161,172,176	0
3	BDP	E	2004	12/13	0.77	0.45	-	186,205,213,218	0
3	NDG	B	2005	14/15	0.93	0.13	-	109,128,158,160	0
3	NDG	A	2005	14/15	0.92	0.17	-	107,132,150,170	0
3	NDG	F	2005	14/15	0.83	0.22	-	145,173,202,210	0
3	BDP	A	2004	12/13	0.78	0.38	-	179,197,225,229	0
3	BDP	B	2006	12/13	0.91	0.14	-	108,137,152,153	0
3	BDP	E	2006	12/13	0.75	0.44	-	145,194,213,217	0
3	NDG	D	2005	14/15	0.90	0.18	-	104,145,162,178	0

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, 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
4	NPO	E	2011	10/10	0.73	0.37	7.26	157,172,185,189	0
4	NPO	A	2011	10/10	0.92	0.32	2.12	103,138,146,154	0
4	NPO	B	2011	10/10	0.96	0.30	1.71	105,120,169,173	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	NPO	D	2011	10/10	0.89	0.28	0.53	159,170,199,200	0
2	A3P	E	2003	27/27	0.94	0.27	-0.51	80,104,114,119	0
2	A3P	D	2003	27/27	0.97	0.20	-0.89	57,83,108,112	0
2	A3P	B	2003	27/27	0.97	0.18	-0.94	66,80,103,148	0
2	A3P	C	2003	27/27	0.93	0.21	-0.95	74,106,135,145	0
2	A3P	F	2003	27/27	0.96	0.20	-0.99	67,89,104,115	0
2	A3P	A	2003	27/27	0.97	0.19	-1.02	53,68,87,93	0

6.5 Other polymers (i)

There are no such residues in this entry.