Full wwPDB X-ray Structure Validation Report (i)

Nov 30, 2022 – 12:32 am GMT

PDB ID	:	4CZS
Title	:	Discovery of Glycomimetic Ligands via Genetically-encoded Library of Phage displaying Mannose-peptides
Authors	:	Ng, S.; Lin, E.; Tjhung, K.F.; Gerlits, O.; Sood, A.; Kasper, B.; Deng, L.; Kitov, P.I.; Matochko, W.L.; Paschal, B.M.; Noren, C.J.; Klassen, J.; Mahal, L.K.; Coates, L.; Woods, R.J.; Derda, R.
Deposited on	:	2014-04-22
Resolution	:	1.73 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

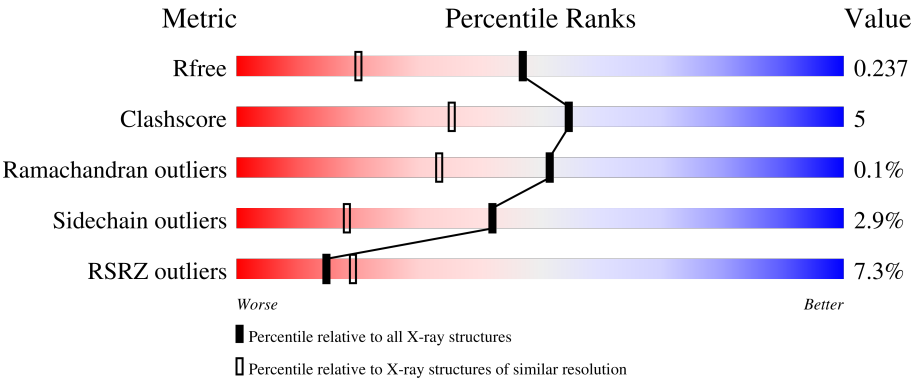
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 1.73 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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

Mol	Chain	Length	Quality of chain
1	A	237	5% 85% 14%
1	B	237	5% 92% 7%
1	C	237	8% 86% 14%
1	D	237	8% 84% 14%

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Mol	Chain	Length	Quality of chain
2	E	4	25% 25% 50% 25%
2	F	4	25% 25% 50% 25%
2	G	4	75% 75% 25%
2	H	4	75% 25% 50% 25%

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
2	XSN	G	5	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8528 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 Concanavalin V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	8	0
			1843	1168	305	368	2			
1	B	237	Total	C	N	O	S	0	3	0
			1819	1149	302	366	2			
1	C	237	Total	C	N	O	S	0	4	0
			1826	1154	304	366	2			
1	D	237	Total	C	N	O	S	0	4	0
			1824	1154	302	366	2			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	58	ASP	GLY	conflict	UNP C0HJY1
A	70	ALA	GLY	conflict	UNP C0HJY1
A	129	MET	VAL	conflict	UNP C0HJY1
A	192	GLU	ASP	conflict	UNP C0HJY1
B	58	ASP	GLY	conflict	UNP C0HJY1
B	70	ALA	GLY	conflict	UNP C0HJY1
B	129	MET	VAL	conflict	UNP C0HJY1
B	192	GLU	ASP	conflict	UNP C0HJY1
C	58	ASP	GLY	conflict	UNP C0HJY1
C	70	ALA	GLY	conflict	UNP C0HJY1
C	129	MET	VAL	conflict	UNP C0HJY1
C	192	GLU	ASP	conflict	UNP C0HJY1
D	58	ASP	GLY	conflict	UNP C0HJY1
D	70	ALA	GLY	conflict	UNP C0HJY1
D	129	MET	VAL	conflict	UNP C0HJY1
D	192	GLU	ASP	conflict	UNP C0HJY1

- Molecule 2 is a protein called MAN-WYD.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	E	4	Total C N O 39 26 6 7	0	0	0
2	F	4	Total C N O 39 26 6 7	0	0	0
2	G	4	Total C N O 39 26 6 7	0	0	0
2	H	4	Total C N O 39 26 6 7	0	0	0

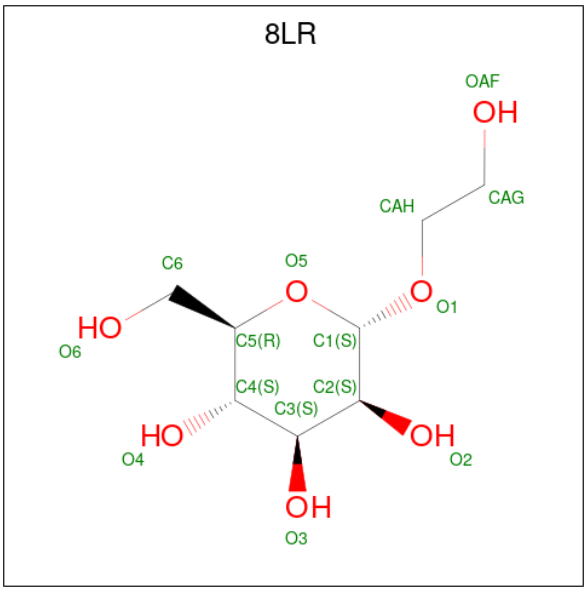
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mn 1 1	0	0
4	B	1	Total Mn 1 1	0	0
4	C	1	Total Mn 1 1	0	0
4	D	1	Total Mn 1 1	0	0

- Molecule 5 is 2-hydroxyethyl alpha-D-mannopyranoside (three-letter code: 8LR) (formula: $C_8H_{16}O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total C O 15 8 7	0	0
5	F	1	Total C O 15 8 7	0	0
5	G	1	Total C O 15 8 7	0	0
5	H	1	Total C O 15 8 7	0	0

- Molecule 6 is water.

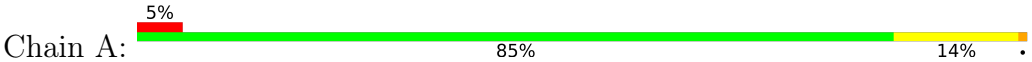
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	272	Total O 272 272	0	0
6	B	242	Total O 242 242	0	0
6	C	220	Total O 220 220	0	0
6	D	214	Total O 214 214	0	0
6	E	14	Total O 14 14	0	0
6	F	18	Total O 18 18	0	0
6	G	5	Total O 5 5	0	0
6	H	7	Total O 7 7	0	0

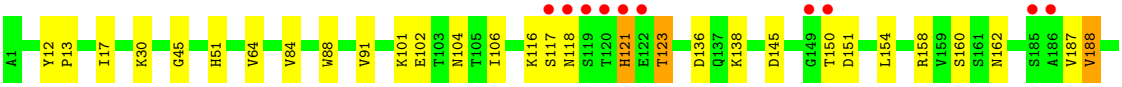
3 Residue-property plots (i)

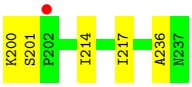
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Concanavalin V

Chain A:

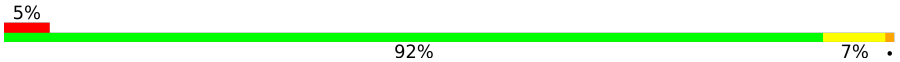






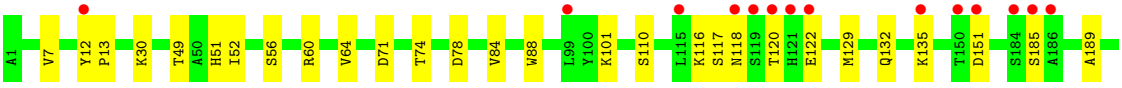
• Molecule 1: Concanavalin V

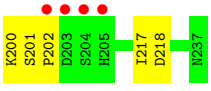
Chain B:



• Molecule 1: Concanavalin V

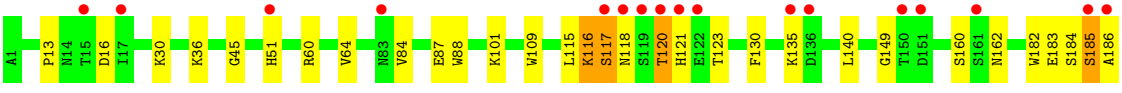
Chain C:

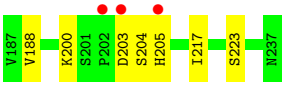




• Molecule 1: Concanavalin V

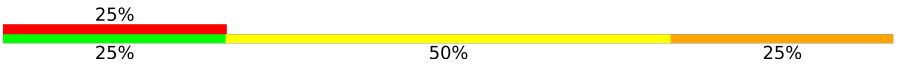
Chain D:





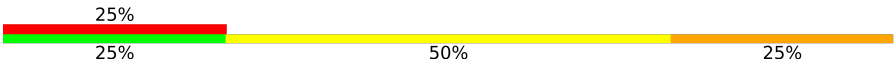
• Molecule 2: MAN-WYD

Chain E:



• Molecule 2: MAN-WYD

Chain F:

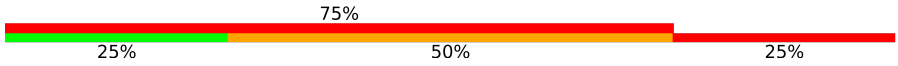


• Molecule 2: MAN-WYD

Chain G:

• Molecule 2: MAN-WYD

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	59.99Å 62.76Å 124.83Å 90.00° 96.10° 90.00°	Depositor
Resolution (Å)	45.49 – 1.73 45.49 – 1.73	Depositor EDS
% Data completeness (in resolution range)	98.4 (45.49-1.73) 98.4 (45.49-1.73)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 1.73Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.192 , 0.237 0.192 , 0.237	Depositor DCC
R_{free} test set	4660 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	19.3	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8528	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.08% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 8LR, CA, XSN, MN

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	0.41	0/1910	0.62	0/2601
1	B	0.39	0/1870	0.60	0/2548
1	C	0.40	0/1881	0.60	0/2563
1	D	0.38	0/1878	0.61	0/2559
2	E	2.08	1/32 (3.1%)	1.59	0/43
2	F	2.10	2/32 (6.2%)	1.19	0/43
2	G	2.20	2/32 (6.2%)	1.37	0/43
2	H	2.18	2/32 (6.2%)	1.68	0/43
All	All	0.48	7/7667 (0.1%)	0.63	0/10443

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	3	TRP	CB-CG	5.83	1.60	1.50
2	H	3	TRP	CB-CG	5.78	1.60	1.50
2	F	3	TRP	CB-CG	5.34	1.59	1.50
2	E	3	TRP	CB-CG	5.27	1.59	1.50
2	F	4	TYR	CZ-OH	5.16	1.46	1.37
2	G	4	TYR	CZ-OH	5.15	1.46	1.37
2	H	4	TYR	CZ-OH	5.01	1.46	1.37

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	1843	0	1815	22	0
1	B	1819	0	1773	12	0
1	C	1826	0	1781	20	0
1	D	1824	0	1784	22	0
2	E	39	0	26	1	0
2	F	39	0	26	1	0
2	G	39	0	26	1	0
2	H	39	0	26	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	E	15	0	15	0	0
5	F	15	0	15	0	0
5	G	15	0	15	0	0
5	H	15	0	15	0	0
6	A	272	0	0	0	0
6	B	242	0	0	5	0
6	C	220	0	0	3	2
6	D	214	0	0	5	2
6	E	14	0	0	0	0
6	F	18	0	0	1	0
6	G	5	0	0	0	0
6	H	7	0	0	1	0
All	All	8528	0	7317	77	2

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 5.

All (77) 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:118:ASN:N	1:D:185:SER:O	2.12	0.82
1:D:45:GLY:HA2	1:D:200:LYS:HG2	1.63	0.79
1:D:130:PHE:HB2	6:D:406:HOH:O	1.81	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:5:XSN:N1	6:H:201:HOH:O	2.15	0.72
1:B:71:ASP:OD2	6:B:402:HOH:O	2.14	0.65
1:D:205:HIS:HD2	2:H:4:TYR:HB3	1.62	0.64
2:F:5:XSN:N1	6:F:201:HOH:O	2.30	0.64
1:A:116[A]:LYS:HE2	1:A:121:HIS:O	1.97	0.64
1:D:160:SER:OG	1:D:162:ASN:OD1	2.15	0.64
1:C:60:ARG:NH1	1:C:78:ASP:OD1	2.34	0.61
1:B:160:SER:OG	1:B:162:ASN:OD1	2.19	0.60
1:A:116[B]:LYS:HG3	1:A:123:THR:HB	1.82	0.60
1:A:116[B]:LYS:HD2	1:A:188:VAL:HG13	1.85	0.59
1:C:118:ASN:N	1:C:185:SER:O	2.27	0.59
1:D:109:TRP:HB3	6:D:406:HOH:O	2.03	0.58
1:D:117:SER:HA	1:D:186:ALA:HA	1.86	0.57
1:D:116:LYS:HG3	1:D:188:VAL:HG23	1.85	0.57
1:C:30:LYS:HD2	1:C:84:VAL:HG13	1.86	0.56
1:C:74:THR:OG1	6:C:401:HOH:O	2.12	0.55
1:D:109:TRP:N	6:D:406:HOH:O	2.38	0.55
1:B:60:ARG:NH1	6:B:409:HOH:O	2.39	0.55
1:C:117:SER:OG	1:C:120:THR:OG1	2.16	0.53
1:D:203:ASP:O	1:D:205:HIS:ND1	2.39	0.51
1:D:115:LEU:HD21	1:D:183:GLU:HB2	1.93	0.51
1:A:88:TRP:HB3	1:A:217[A]:ILE:HD11	1.94	0.50
1:A:118:ASN:HA	1:A:187:VAL:HG23	1.92	0.50
1:D:101:LYS:NZ	6:D:407:HOH:O	2.40	0.49
1:A:51[A]:HIS:CE1	1:C:116:LYS:HE2	2.47	0.49
1:A:102:GLU:OE2	1:A:104:ASN:ND2	2.34	0.48
1:B:132:GLN:NE2	6:B:415:HOH:O	2.47	0.48
1:A:145:ASP:HB3	1:A:158:ARG:HG2	1.95	0.48
1:C:110:SER:HB3	1:C:129:MET:HG3	1.95	0.47
1:B:118:ASN:N	1:B:185:SER:O	2.38	0.47
1:B:150:THR:HG22	6:B:468:HOH:O	2.14	0.47
1:C:51[A]:HIS:HB2	1:C:64[A]:VAL:HG13	1.96	0.47
1:C:120:THR:OG1	1:C:122:GLU:HG2	2.15	0.47
1:D:16:ASP:OD1	1:D:16:ASP:N	2.48	0.47
1:D:30:LYS:HD2	1:D:84:VAL:HG13	1.98	0.46
1:A:17:ILE:HG21	1:A:236:ALA:HB1	1.96	0.46
1:B:16:ASP:OD2	6:B:404:HOH:O	2.20	0.46
1:A:51[A]:HIS:HB2	1:A:64[A]:VAL:CG1	2.46	0.46
1:B:116:LYS:O	1:B:187:VAL:N	2.47	0.46
1:B:51:HIS:HB2	1:B:64[A]:VAL:HG13	1.99	0.45
1:D:51:HIS:HB2	1:D:64[A]:VAL:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2:GLY:O	2:G:5:XSN:HB	2.16	0.45
1:A:30:LYS:HD2	1:A:84:VAL:HG13	1.98	0.45
1:D:117:SER:HB3	1:D:120:THR:HG23	1.97	0.45
1:C:218:ASP:HB3	6:C:594:HOH:O	2.17	0.44
2:E:4:TYR:O	2:E:5:XSN:HBA	2.16	0.44
1:A:45:GLY:CA	1:A:200:LYS:HD3	2.48	0.44
1:A:160:SER:OG	1:A:162:ASN:OD1	2.36	0.44
1:D:135:LYS:HD2	1:D:149:GLY:HA3	1.99	0.44
1:D:13:PRO:HG2	2:H:3:TRP:CZ2	2.52	0.43
1:A:51[A]:HIS:HB2	1:A:64[A]:VAL:HG13	1.99	0.43
1:C:88:TRP:HB3	1:C:217:ILE:HD11	1.99	0.43
1:C:200:LYS:HB2	1:C:200:LYS:HE3	1.84	0.43
1:A:91:VAL:HG12	1:A:214:ILE:HG12	2.00	0.43
1:B:51:HIS:HB2	1:B:64[A]:VAL:CG1	2.49	0.43
1:A:136:ASP:OD1	1:A:138:LYS:NZ	2.46	0.42
1:B:207:ALA:HA	1:B:208:ASP:HA	1.91	0.42
1:C:135:LYS:HD2	1:C:135:LYS:HA	1.84	0.42
1:D:140:LEU:HD23	1:D:140:LEU:HA	1.83	0.42
1:A:116[A]:LYS:HD3	1:C:51[A]:HIS:CE1	2.55	0.42
1:D:88:TRP:HB3	1:D:217[A]:ILE:HD11	2.01	0.42
1:A:106:ILE:HB	1:A:154:LEU:HB3	2.01	0.42
1:C:56:SER:HB3	1:C:189:ALA:HB3	2.01	0.41
1:A:12:TYR:HA	1:A:13:PRO:HD3	1.82	0.41
1:C:7:VAL:HG21	1:C:52:ILE:HG12	2.02	0.41
1:D:223:SER:O	6:D:401:HOH:O	2.21	0.41
1:B:201:SER:HA	1:B:202:PRO:HD2	1.83	0.41
1:A:121:HIS:HD2	1:C:49:THR:OG1	2.02	0.41
1:C:71:ASP:HB3	6:C:446:HOH:O	2.20	0.41
1:D:87:GLU:HG3	1:D:182:TRP:O	2.21	0.41
1:C:201:SER:HA	1:C:202:PRO:HD3	1.91	0.40
1:C:12:TYR:HA	1:C:13:PRO:HD3	1.90	0.40
1:A:200:LYS:HD2	1:A:201:SER:N	2.37	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:582:HOH:O	6:D:508:HOH:O[2_355]	2.17	0.03
6:C:606:HOH:O	6:D:527:HOH:O[2_355]	2.19	0.01

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	243/237 (102%)	236 (97%)	7 (3%)	0	100 100
1	B	238/237 (100%)	233 (98%)	5 (2%)	0	100 100
1	C	239/237 (101%)	233 (98%)	6 (2%)	0	100 100
1	D	239/237 (101%)	234 (98%)	5 (2%)	0	100 100
2	E	2/4 (50%)	2 (100%)	0	0	100 100
2	F	2/4 (50%)	2 (100%)	0	0	100 100
2	G	2/4 (50%)	2 (100%)	0	0	100 100
2	H	2/4 (50%)	1 (50%)	0	1 (50%)	0 0
All	All	967/964 (100%)	943 (98%)	23 (2%)	1 (0%)	51 33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	4	TYR

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	211/203 (104%)	204 (97%)	7 (3%)	38 14
1	B	206/203 (102%)	202 (98%)	4 (2%)	57 36
1	C	207/203 (102%)	204 (99%)	3 (1%)	67 50
1	D	207/203 (102%)	197 (95%)	10 (5%)	25 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	E	2/2 (100%)	2 (100%)	0	100 100
2	F	2/2 (100%)	2 (100%)	0	100 100
2	G	2/2 (100%)	2 (100%)	0	100 100
2	H	2/2 (100%)	2 (100%)	0	100 100
All	All	839/820 (102%)	815 (97%)	24 (3%)	42 18

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	LYS
1	A	117	SER
1	A	121	HIS
1	A	123	THR
1	A	150	THR
1	A	151	ASP
1	A	188	VAL
1	B	101	LYS
1	B	121	HIS
1	B	132	GLN
1	B	185	SER
1	C	101	LYS
1	C	132	GLN
1	C	151	ASP
1	D	36	LYS
1	D	60	ARG
1	D	116	LYS
1	D	117	SER
1	D	120	THR
1	D	121	HIS
1	D	123	THR
1	D	184	SER
1	D	185	SER
1	D	204	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	132	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
2	XSN	G	5	2	7,8,8	2.15	2 (28%)	9,10,10	1.32	1 (11%)
2	XSN	F	5	2	7,8,8	1.99	1 (14%)	9,10,10	1.26	1 (11%)
2	XSN	H	5	2	7,8,8	2.09	2 (28%)	9,10,10	1.46	2 (22%)
2	XSN	E	5	2	7,8,8	2.12	1 (14%)	9,10,10	1.17	1 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	XSN	G	5	2	-	6/8/8/8	-
2	XSN	F	5	2	-	3/8/8/8	-
2	XSN	H	5	2	-	1/8/8/8	-
2	XSN	E	5	2	-	5/8/8/8	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	5	XSN	C-N1	5.13	1.45	1.32
2	G	5	XSN	C-N1	5.05	1.45	1.32
2	H	5	XSN	C-N1	4.92	1.45	1.32
2	F	5	XSN	C-N1	4.86	1.45	1.32
2	G	5	XSN	OD2-CG	2.15	1.29	1.22
2	H	5	XSN	OD2-CG	2.13	1.29	1.22

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	5	XSN	CA-C-N1	2.54	121.03	116.68
2	H	5	XSN	CB-CA-C	-2.51	103.24	109.09
2	E	5	XSN	CA-C-N1	2.08	120.25	116.68
2	G	5	XSN	O-C-N1	-2.05	119.43	123.00
2	H	5	XSN	OD1-CG-CB	2.03	120.59	114.07

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	5	XSN	O-C-CA-CB
2	E	5	XSN	N1-C-CA-CB
2	F	5	XSN	N-CA-CB-CG
2	G	5	XSN	N1-C-CA-N
2	G	5	XSN	N-CA-CB-CG
2	H	5	XSN	N1-C-CA-N
2	E	5	XSN	CA-CB-CG-OD1
2	E	5	XSN	CA-CB-CG-OD2
2	F	5	XSN	C-CA-CB-CG
2	G	5	XSN	C-CA-CB-CG
2	E	5	XSN	N-CA-CB-CG
2	G	5	XSN	CA-CB-CG-OD2
2	G	5	XSN	O-C-CA-N
2	G	5	XSN	CA-CB-CG-OD1
2	F	5	XSN	O-C-CA-N

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	5	XSN	1	0
2	F	5	XSN	1	0
2	H	5	XSN	1	0
2	E	5	XSN	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	8LR	F	101	2	15,15,15	1.25	3 (20%)	20,20,20	0.79	0
5	8LR	G	101	2	15,15,15	1.36	2 (13%)	20,20,20	0.79	0
5	8LR	E	101	2	15,15,15	1.27	1 (6%)	20,20,20	0.78	0
5	8LR	H	101	2	15,15,15	1.28	3 (20%)	20,20,20	0.94	1 (5%)

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
5	8LR	F	101	2	-	0/6/26/26	0/1/1/1
5	8LR	G	101	2	-	1/6/26/26	0/1/1/1
5	8LR	E	101	2	-	0/6/26/26	0/1/1/1
5	8LR	H	101	2	-	1/6/26/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	101	8LR	O5-C1	3.01	1.49	1.41
5	H	101	8LR	O5-C1	2.82	1.49	1.41
5	F	101	8LR	O5-C1	2.66	1.48	1.41
5	E	101	8LR	O5-C1	2.66	1.48	1.41
5	G	101	8LR	C2-C3	-2.37	1.46	1.52
5	H	101	8LR	O3-C3	2.15	1.48	1.43
5	F	101	8LR	C2-C3	-2.13	1.46	1.52
5	H	101	8LR	C2-C3	-2.08	1.47	1.52
5	F	101	8LR	O3-C3	2.07	1.47	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	101	8LR	CAH-O1-C1	-2.01	110.51	113.84

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	101	8LR	O5-C1-O1-CAH
5	H	101	8LR	OAF-CAG-CAH-O1

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	237/237 (100%)	0.45	11 (4%)	32	38	10, 17, 40, 46	0
1	B	237/237 (100%)	0.46	13 (5%)	25	30	10, 18, 39, 52	0
1	C	237/237 (100%)	0.56	18 (7%)	13	18	12, 20, 42, 52	0
1	D	237/237 (100%)	0.74	20 (8%)	11	14	11, 22, 46, 61	0
2	E	3/4 (75%)	1.54	1 (33%)	0	0	23, 23, 25, 28	0
2	F	3/4 (75%)	1.55	1 (33%)	0	0	25, 25, 25, 27	0
2	G	3/4 (75%)	4.43	3 (100%)	0	0	39, 39, 40, 45	0
2	H	3/4 (75%)	6.67	3 (100%)	0	0	51, 51, 52, 64	0
All	All	960/964 (99%)	0.59	70 (7%)	15	19	10, 19, 42, 64	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	3	TRP	7.2
2	H	2	GLY	6.5
2	H	4	TYR	6.3
1	C	150	THR	5.9
2	G	3	TRP	5.6
1	D	205	HIS	5.1
2	G	4	TYR	5.0
1	A	186	ALA	4.2
1	C	120	THR	4.2
1	A	122	GLU	4.2
1	D	202	PRO	4.2
1	B	118	ASN	4.1
1	C	185	SER	4.1
1	D	117	SER	4.0
1	D	121	HIS	4.0
1	D	118	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	150	THR	3.8
1	C	122	GLU	3.5
1	B	120	THR	3.5
1	A	120	THR	3.5
1	D	185	SER	3.4
1	B	121	HIS	3.4
1	C	202	PRO	3.4
1	B	119	SER	3.4
1	C	186	ALA	3.4
1	A	121	HIS	3.3
1	C	118	ASN	3.3
1	C	151	ASP	3.3
1	C	203	ASP	3.3
1	A	118	ASN	3.2
1	C	121	HIS	3.2
1	D	122	GLU	3.1
1	C	205	HIS	3.0
1	D	120	THR	2.9
1	C	204	SER	2.9
1	D	203	ASP	2.8
1	B	187	VAL	2.8
1	A	185	SER	2.8
1	D	150	THR	2.7
2	G	2	GLY	2.7
1	B	1	ALA	2.7
1	B	122	GLU	2.7
1	D	135	LYS	2.7
1	B	185	SER	2.7
1	D	161	SER	2.7
1	A	149	GLY	2.7
1	D	151	ASP	2.6
1	C	12	TYR	2.6
1	D	119	SER	2.6
1	D	17	ILE	2.5
1	B	150	THR	2.5
1	B	117	SER	2.5
1	D	136	ASP	2.4
1	A	202	PRO	2.4
1	C	184	SER	2.4
1	B	136	ASP	2.3
2	E	3	TRP	2.3
1	A	117	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	115	LEU	2.2
1	B	151	ASP	2.2
1	A	119	SER	2.2
2	F	2	GLY	2.2
1	C	135	LYS	2.1
1	C	99	LEU	2.1
1	C	119	SER	2.1
1	D	186	ALA	2.1
1	C	115	LEU	2.1
1	D	51	HIS	2.1
1	D	15	THR	2.0
1	D	83	ASN	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	XSN	H	5	9/9	0.54	0.36	48,60,68,68	0
2	XSN	G	5	9/9	0.65	0.46	56,59,63,75	0
2	XSN	E	5	9/9	0.80	0.23	25,31,42,45	0
2	XSN	F	5	9/9	0.80	0.23	31,38,41,46	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	8LR	H	101	15/15	0.86	0.17	20,25,46,62	0
5	8LR	G	101	15/15	0.89	0.16	15,19,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	8LR	E	101	15/15	0.92	0.13	13,16,29,36	0
5	8LR	F	101	15/15	0.93	0.10	13,17,28,39	0
4	MN	D	302	1/1	0.97	0.07	19,19,19,19	0
3	CA	D	301	1/1	0.98	0.07	19,19,19,19	0
3	CA	B	301	1/1	0.98	0.07	14,14,14,14	0
3	CA	C	301	1/1	0.98	0.06	17,17,17,17	0
4	MN	C	302	1/1	0.99	0.06	17,17,17,17	0
4	MN	A	302	1/1	0.99	0.06	13,13,13,13	0
4	MN	B	302	1/1	0.99	0.06	14,14,14,14	0
3	CA	A	301	1/1	1.00	0.06	13,13,13,13	0

6.5 Other polymers (i)

There are no such residues in this entry.