



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:59 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

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

with specific help available everywhere you see the ⓘ symbol.

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

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

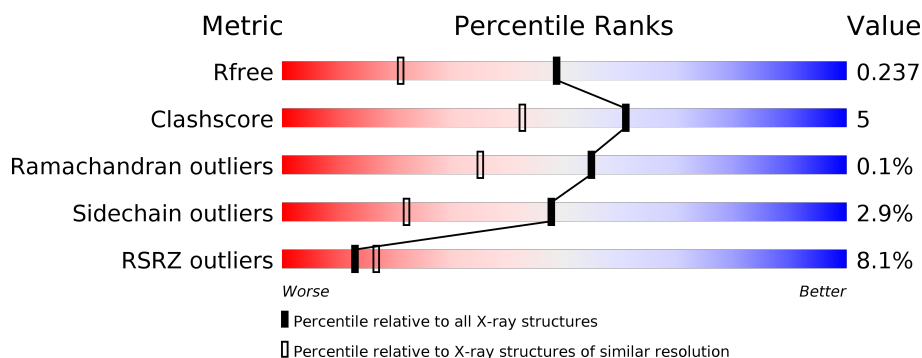
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	100719	2694 (1.76-1.72)
Clashscore	112137	2854 (1.76-1.72)
Ramachandran outliers	110173	2824 (1.76-1.72)
Sidechain outliers	110143	2824 (1.76-1.72)
RSRZ outliers	101464	2705 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	237	<div> <div>5%</div> <div>85%</div> <div>14%</div> <div>•</div> </div>
1	B	237	<div> <div>7%</div> <div>92%</div> <div>7%</div> <div>•</div> </div>
1	C	237	<div> <div>8%</div> <div>86%</div> <div>14%</div> </div>
1	D	237	<div> <div>9%</div> <div>84%</div> <div>14%</div> <div>•</div> </div>
2	E	5	<div> <div>20%</div> <div>40%</div> <div>60%</div> </div>
2	F	5	<div> <div>20%</div> <div>40%</div> <div>60%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	5	
2	H	5	

2 Entry composition

There are 5 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 CONCANAVALLIN-A.

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 P81461
A	70	ALA	GLY	CONFLICT	UNP P81461
A	168	SER	ASN	CONFLICT	UNP P81461
A	192	GLU	ASP	CONFLICT	UNP P81461
B	58	ASP	GLY	CONFLICT	UNP P81461
B	70	ALA	GLY	CONFLICT	UNP P81461
B	168	SER	ASN	CONFLICT	UNP P81461
B	192	GLU	ASP	CONFLICT	UNP P81461
C	58	ASP	GLY	CONFLICT	UNP P81461
C	70	ALA	GLY	CONFLICT	UNP P81461
C	168	SER	ASN	CONFLICT	UNP P81461
C	192	GLU	ASP	CONFLICT	UNP P81461
D	58	ASP	GLY	CONFLICT	UNP P81461
D	70	ALA	GLY	CONFLICT	UNP P81461
D	168	SER	ASN	CONFLICT	UNP P81461
D	192	GLU	ASP	CONFLICT	UNP P81461

- Molecule 2 is a protein called MAN-WYD.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	5	Total	C	N	O	0	0	0
			54	34	6	14			
2	F	5	Total	C	N	O	0	0	0
			54	34	6	14			
2	G	5	Total	C	N	O	0	0	0
			54	34	6	14			
2	H	5	Total	C	N	O	0	0	0
			54	34	6	14			

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

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

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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	298	Total	O	0	0
			298	298		
5	B	256	Total	O	0	0
			256	256		
5	C	236	Total	O	0	0
			236	236		

Continued on next page...

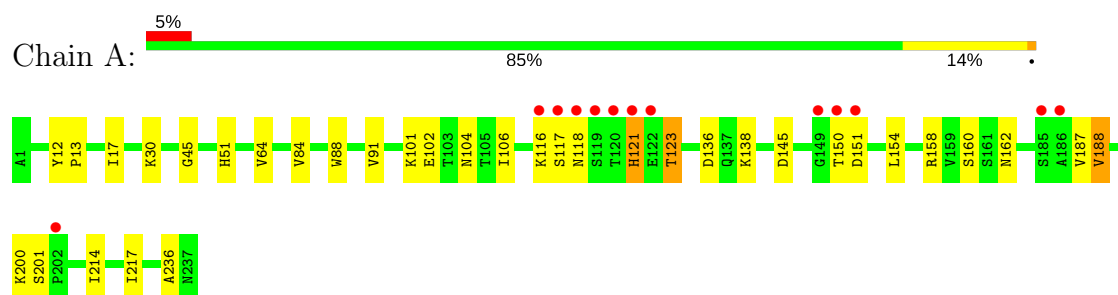
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	202	Total 202	O 202	0	0

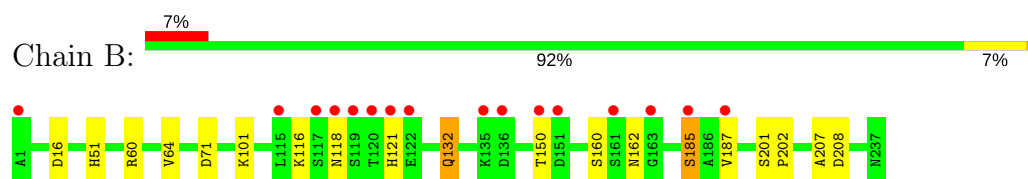
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

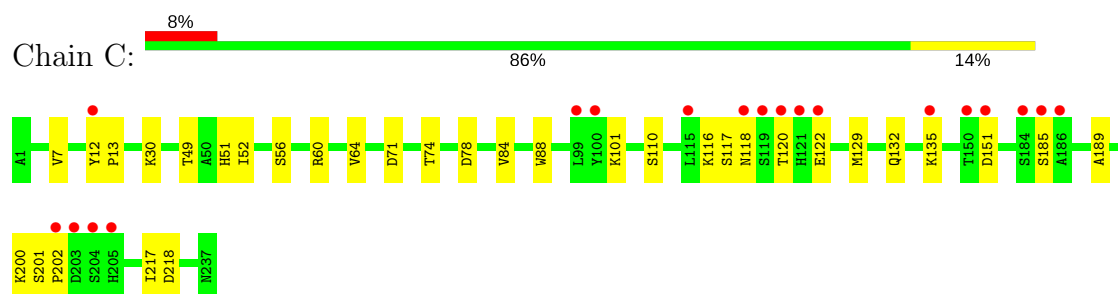
- Molecule 1: CONCANAVALIN-A



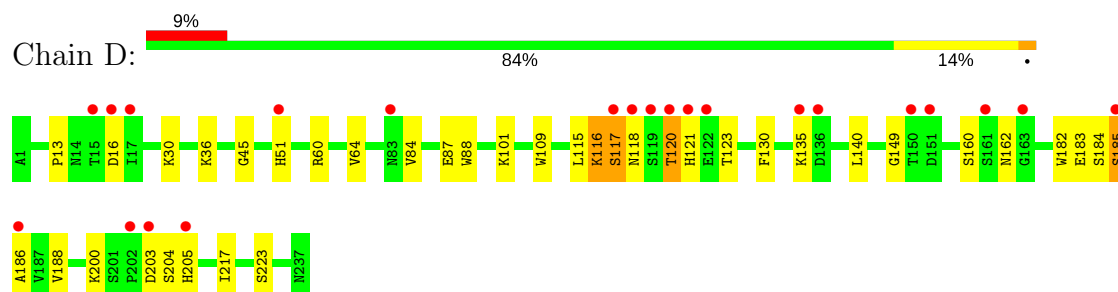
- Molecule 1: CONCANAVALIN-A



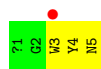
- Molecule 1: CONCANAVALIN-A



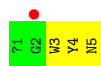
- Molecule 1: CONCANAVALIN-A



● Molecule 2: MAN-WYD



● Molecule 2: MAN-WYD



● Molecule 2: MAN-WYD



● Molecule 2: MAN-WYD



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 1.73Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.192 , 0.237 0.190 , 0.237	Depositor DCC
R_{free} test set	4659 reflections (4.91%)	DCC
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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	54	0	41	1	0
2	F	54	0	41	1	0
2	G	54	0	41	1	0
2	H	54	0	41	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	A	298	0	0	1	0
5	B	256	0	0	5	0
5	C	236	0	0	3	2
5	D	202	0	0	6	2
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	5:D:2122:HOH:O	1.81	0.78
5:D:2200:HOH:O	2:H:5:XSN:N1	2.15	0.72
1:B:71:ASP:OD2	5:B:2114:HOH:O	2.14	0.65
1:D:205:HIS:HD2	2:H:4:TYR:HB3	1.62	0.64
5:B:2220:HOH:O	2:F:5:XSN:N1	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	5:D:2122: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	5:C:2104:HOH:O	2.12	0.55
1:D:109:TRP:N	5:D:2122:HOH:O	2.38	0.55
1:B:60:ARG:NH1	5:B:2103: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:118:ASN:HA	1:A:187:VAL:HG23	1.92	0.50
1:A:88:TRP:HB3	1:A:217[A]:ILE:HD11	1.94	0.50
1:D:101:LYS:NZ	5:D:2114: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
5:A:2184:HOH:O	1:B:132:GLN:NE2	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	5:B:2183: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	5:B:2030: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
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	5:C:2215:HOH:O	2.17	0.44
2:E:4:TYR:O	2:E:5:XSN:HBA	2.16	0.44
1:A:160:SER:OG	1:A:162:ASN:OD1	2.36	0.44
1:A:45:GLY:CA	1:A:200:LYS:HD3	2.48	0.44
1:D:135:LYS:HD2	1:D:149:GLY:HA3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:C:135:LYS:HD2	1.84	0.42
1:D:140:LEU:HA	1:D:140:LEU:HD23	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	5:D:2182: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	5:C:2102: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)
5:C:2089:HOH:O	5:D:2179:HOH:O[2_355]	2.17	0.03
5:C:2114:HOH:O	5:D:2151:HOH:O[2_355]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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	2/5 (40%)	2 (100%)	0	0	100	100
2	F	2/5 (40%)	2 (100%)	0	0	100	100
2	G	2/5 (40%)	2 (100%)	0	0	100	100
2	H	2/5 (40%)	1 (50%)	0	1 (50%)	0	0
All	All	967/968 (100%)	943 (98%)	23 (2%)	1 (0%)	55	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	4	TYR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	211/203 (104%)	204 (97%)	7 (3%)	43	17
1	B	206/203 (102%)	202 (98%)	4 (2%)	62	41
1	C	207/203 (102%)	204 (99%)	3 (1%)	71	55
1	D	207/203 (102%)	197 (95%)	10 (5%)	30	8
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%)	48	22

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

Some 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	E	5	2	5,8,8	3.07	1 (20%)	6,10,10	1.28	0
2	XSN	F	5	2	5,8,8	2.89	1 (20%)	6,10,10	1.49	1 (16%)
2	XSN	G	5	2	5,8,8	3.03	1 (20%)	6,10,10	1.42	1 (16%)
2	XSN	H	5	2	5,8,8	2.94	1 (20%)	6,10,10	1.53	2 (33%)

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	E	5	2	-	0/5/8/8	0/0/0/0
2	XSN	F	5	2	-	0/5/8/8	0/0/0/0
2	XSN	G	5	2	-	0/5/8/8	0/0/0/0
2	XSN	H	5	2	-	0/5/8/8	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	5	XSN	C-N1	6.41	1.45	1.32
2	H	5	XSN	C-N1	6.48	1.45	1.32
2	G	5	XSN	C-N1	6.66	1.45	1.32
2	E	5	XSN	C-N1	6.77	1.45	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	5	XSN	CB-CA-C	-2.78	103.24	108.57
2	G	5	XSN	O-C-N1	-2.37	119.43	123.06
2	H	5	XSN	O-C-N1	-2.01	119.99	123.06
2	F	5	XSN	CA-C-N1	2.22	121.03	116.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

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.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	237/237 (100%)	0.50	13 (5%)	26 31	10, 17, 40, 46	0
1	B	237/237 (100%)	0.53	16 (6%)	18 23	10, 18, 39, 52	0
1	C	237/237 (100%)	0.60	19 (8%)	13 17	12, 20, 42, 52	0
1	D	237/237 (100%)	0.79	22 (9%)	9 12	11, 22, 46, 61	0
2	E	3/5 (60%)	1.60	1 (33%)	0 1	23, 23, 25, 28	0
2	F	3/5 (60%)	1.68	1 (33%)	0 1	25, 25, 25, 27	0
2	G	3/5 (60%)	4.41	3 (100%)	0 0	39, 39, 40, 45	0
2	H	3/5 (60%)	6.91	3 (100%)	0 0	51, 51, 52, 64	0
All	All	960/968 (99%)	0.64	78 (8%)	13 17	10, 19, 42, 64	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	3	TRP	7.4
2	H	2	GLY	7.0
2	H	4	TYR	6.4
1	C	150	THR	6.0
2	G	3	TRP	5.9
1	D	205	HIS	5.4
2	G	4	TYR	4.8
1	D	117	SER	4.6
1	C	120	THR	4.5
1	A	122	GLU	4.3
1	D	202	PRO	4.1
1	A	186	ALA	4.0
1	D	118	ASN	3.9
1	B	118	ASN	3.9
1	B	119	SER	3.9
1	A	120	THR	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	185	SER	3.8
1	D	121	HIS	3.8
1	A	150	THR	3.7
1	A	118	ASN	3.6
1	C	202	PRO	3.5
1	C	118	ASN	3.5
1	D	185	SER	3.5
1	C	151	ASP	3.4
1	C	122	GLU	3.4
1	C	186	ALA	3.4
1	B	120	THR	3.4
1	B	121	HIS	3.3
1	C	121	HIS	3.2
1	D	122	GLU	3.2
1	A	121	HIS	3.2
1	C	203	ASP	3.1
1	A	185	SER	3.0
1	B	185	SER	3.0
1	D	120	THR	3.0
1	C	204	SER	3.0
1	D	203	ASP	2.9
1	D	119	SER	2.9
1	D	150	THR	2.9
1	D	151	ASP	2.9
1	D	161	SER	2.9
1	B	122	GLU	2.8
1	C	205	HIS	2.8
1	B	187	VAL	2.8
1	D	135	LYS	2.8
1	D	136	ASP	2.7
1	B	150	THR	2.7
1	D	17	ILE	2.7
1	B	151	ASP	2.6
1	B	117	SER	2.6
2	G	2	GLY	2.6
1	B	1	ALA	2.5
1	A	117	SER	2.5
1	C	12	TYR	2.5
1	A	202	PRO	2.5
2	E	3	TRP	2.5
1	B	136	ASP	2.4
1	A	119	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	83	ASN	2.3
1	A	149	GLY	2.3
2	F	2	GLY	2.3
1	C	135	LYS	2.3
1	D	163	GLY	2.3
1	D	51	HIS	2.2
1	C	115	LEU	2.2
1	C	99	LEU	2.2
1	A	116[A]	LYS	2.2
1	B	161	SER	2.1
1	B	163	GLY	2.1
1	D	16	ASP	2.1
1	B	115	LEU	2.1
1	D	15	THR	2.1
1	C	100	TYR	2.1
1	D	186	ALA	2.0
1	C	119	SER	2.0
1	C	184	SER	2.0
1	A	151	ASP	2.0
1	B	135	LYS	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	XSN	H	5	9/9	0.54	0.35	-	48,60,68,68	0
2	XSN	F	5	9/9	0.80	0.24	-	31,38,41,46	0
2	XSN	G	5	9/9	0.65	0.47	-	56,59,63,75	0
2	XSN	E	5	9/9	0.78	0.25	-	25,31,42,45	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	CA	B	1239	1/1	0.98	0.07	-1.91	14,14,14,14	0
3	CA	C	1239	1/1	0.98	0.06	-1.93	17,17,17,17	0
3	CA	D	1239	1/1	0.98	0.07	-2.08	19,19,19,19	0
3	CA	A	1239	1/1	1.00	0.06	-2.72	13,13,13,13	0
4	MN	C	1240	1/1	0.98	0.07	-3.29	17,17,17,17	0
4	MN	B	1240	1/1	0.99	0.07	-3.47	14,14,14,14	0
4	MN	A	1240	1/1	0.99	0.06	-3.58	13,13,13,13	0
4	MN	D	1240	1/1	0.97	0.07	-4.08	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.