



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:26 PM GMT

PDB ID : 4ETQ
Title : Vaccinia virus D8L IMV envelope protein in complex with Fab of murine IgG2a LA5
Authors : Matho, M.H.; Zajonc, D.M.
Deposited on : 2012-04-24
Resolution : 2.10 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 (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

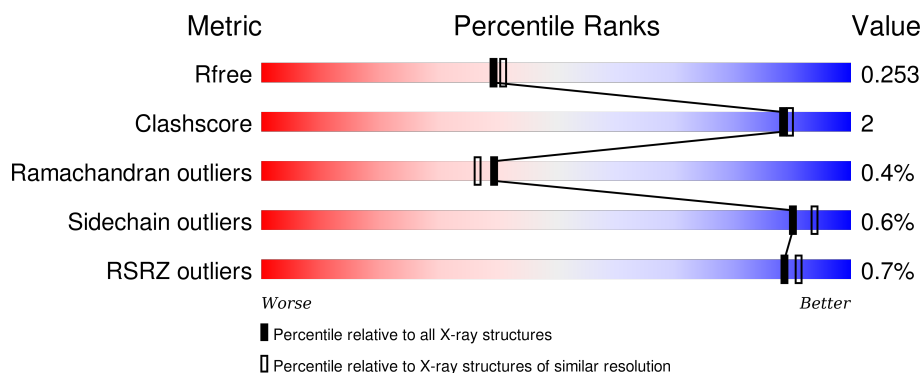
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	221	<div> <div>2%</div> <div>93%</div> <div>5%</div> <div>.</div> </div>
1	H	221	<div> <div>86%</div> <div>12%</div> <div>.</div> </div>
2	B	212	<div> <div>94%</div> <div>6%</div> </div>
2	L	212	<div> <div>98%</div> <div>.</div> </div>
3	C	269	<div> <div>2%</div> <div>78%</div> <div>6%</div> <div>16%</div> </div>

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Mol	Chain	Length	Quality of chain
3	X	269	 78% 6% 15%

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
4	SCN	A	303	-	-	X	-
6	GOL	A	301	-	-	-	X
6	GOL	B	301	-	-	-	X
6	GOL	L	301	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10798 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 anti-vaccinia D8L antigen murine monoclonal IgG2a antibody LA5, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	215	Total	C	N	O	S	0	2	0
			1651	1041	274	326	10			
1	A	217	Total	C	N	O	S	0	3	0
			1670	1053	278	329	10			

- Molecule 2 is a protein called anti-vaccinia D8L antigen murine monoclonal IgG2a antibody LA5, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	212	Total	C	N	O	S	0	3	0
			1647	1028	271	338	10			
2	B	212	Total	C	N	O	S	0	5	0
			1657	1035	272	340	10			

- Molecule 3 is a protein called IMV membrane protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	228	Total	C	N	O		0	0	0
			1842	1189	299	354				
3	C	225	Total	C	N	O		0	1	0
			1800	1164	295	341				

There are 16 discrepancies between the modelled and reference sequences:

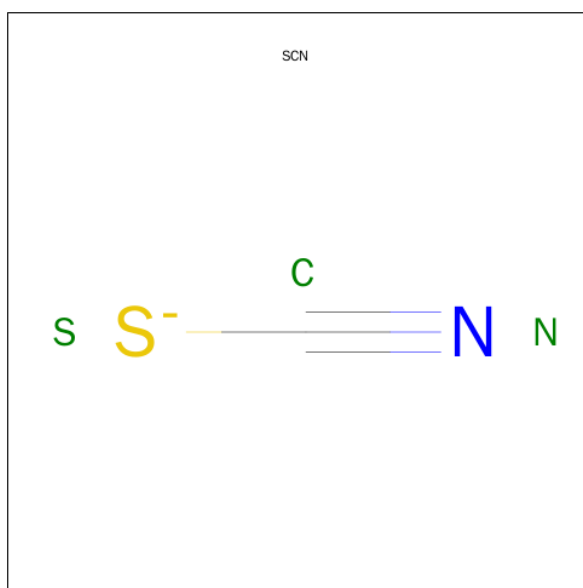
Chain	Residue	Modelled	Actual	Comment	Reference
X	262	LEU	-	EXPRESSION TAG	UNP Q1M1K6
X	263	GLU	-	EXPRESSION TAG	UNP Q1M1K6
X	264	HIS	-	EXPRESSION TAG	UNP Q1M1K6
X	265	HIS	-	EXPRESSION TAG	UNP Q1M1K6
X	266	HIS	-	EXPRESSION TAG	UNP Q1M1K6
X	267	HIS	-	EXPRESSION TAG	UNP Q1M1K6

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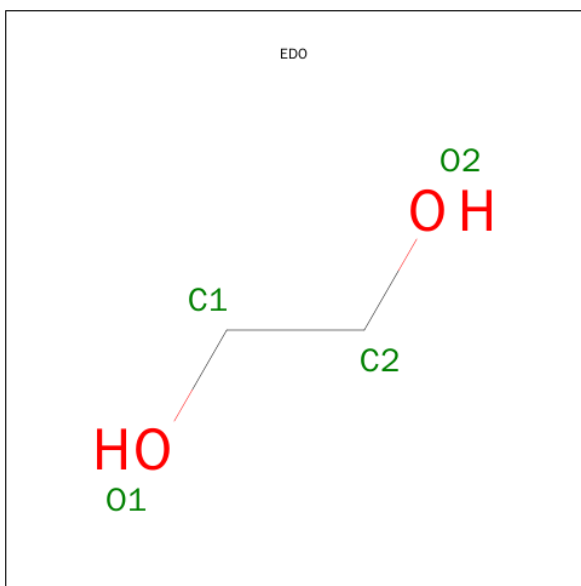
Chain	Residue	Modelled	Actual	Comment	Reference
X	268	HIS	-	EXPRESSION TAG	UNP Q1M1K6
X	269	HIS	-	EXPRESSION TAG	UNP Q1M1K6
C	262	LEU	-	EXPRESSION TAG	UNP Q1M1K6
C	263	GLU	-	EXPRESSION TAG	UNP Q1M1K6
C	264	HIS	-	EXPRESSION TAG	UNP Q1M1K6
C	265	HIS	-	EXPRESSION TAG	UNP Q1M1K6
C	266	HIS	-	EXPRESSION TAG	UNP Q1M1K6
C	267	HIS	-	EXPRESSION TAG	UNP Q1M1K6
C	268	HIS	-	EXPRESSION TAG	UNP Q1M1K6
C	269	HIS	-	EXPRESSION TAG	UNP Q1M1K6

- Molecule 4 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



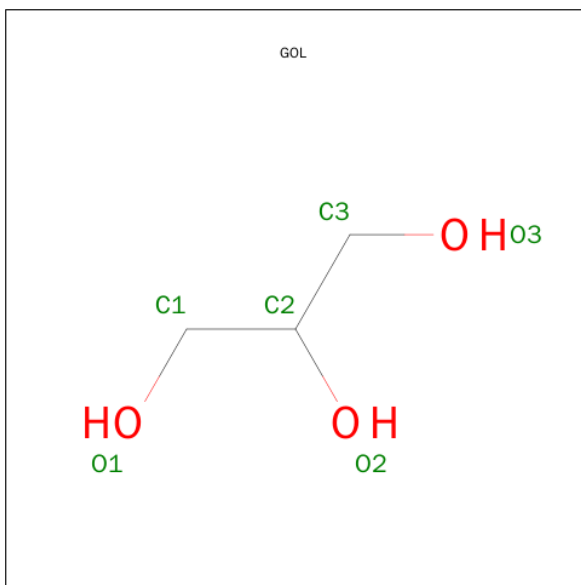
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	S	0	0
			3	1	1	1		
4	L	1	Total	C	N	S	0	0
			3	1	1	1		
4	A	1	Total	C	N	S	0	0
			3	1	1	1		
4	A	1	Total	S			0	0
			1	1				
4	B	1	Total	C	N	S	0	0
			3	1	1	1		
4	X	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Cl	0	0
			1	1		

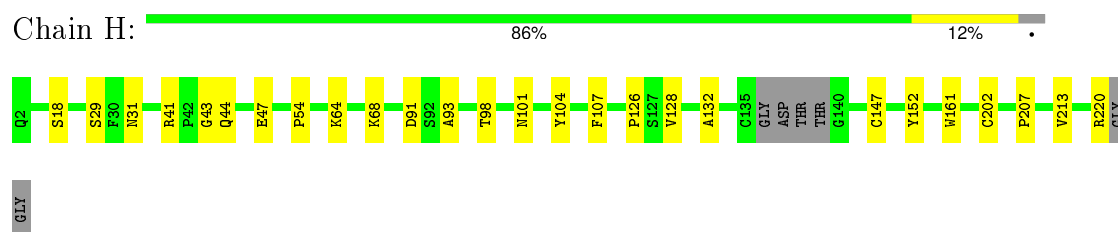
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	90	Total	O	0	0
			90	90		
8	L	76	Total	O	0	0
			76	76		
8	A	122	Total	O	0	0
			122	122		
8	B	135	Total	O	0	0
			135	135		
8	X	43	Total	O	0	0
			43	43		
8	C	26	Total	O	0	0
			26	26		

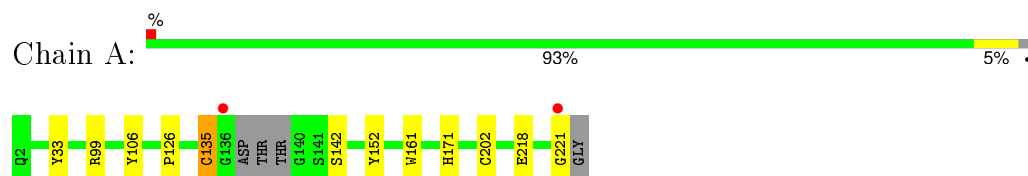
3 Residue-property plots [i](#)

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.

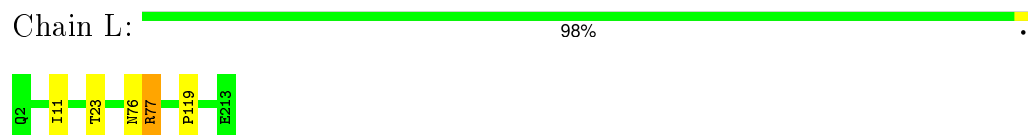
- Molecule 1: anti-vaccinia D8L antigen murine monoclonal IgG2a antibody LA5, heavy chain



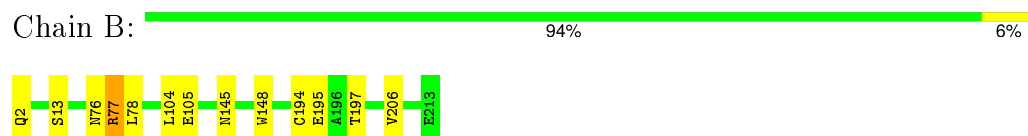
- Molecule 1: anti-vaccinia D8L antigen murine monoclonal IgG2a antibody LA5, heavy chain



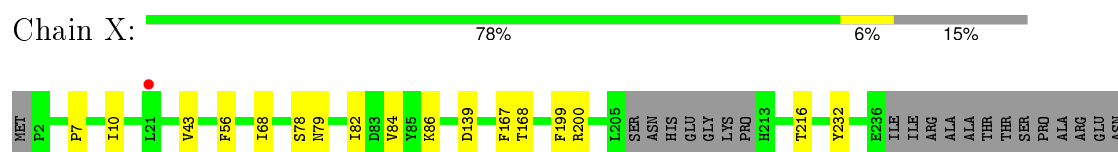
- Molecule 2: anti-vaccinia D8L antigen murine monoclonal IgG2a antibody LA5, light chain



- Molecule 2: anti-vaccinia D8L antigen murine monoclonal IgG2a antibody LA5, light chain

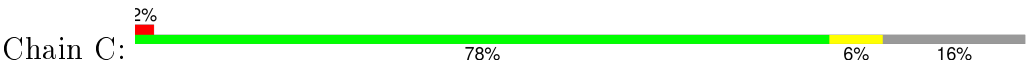


- Molecule 3: IMV membrane protein



TYR
PHE
MET
ARG
TRP
LEU
SER
ASP
LEU
ARG
GLU
THR
LEU
GLU
HIS
HIS
HIS
HIS
HIS

● Molecule 3: IMV membrane protein



MET	PRO	Q3	A19	K41	I45	S53	L57	P56	L66	S78	V84	Y89	K86	I115	L138	A144	D151	V181	T201	L202	L205	SER	ASN	HIS	GLU	GLY	LYS	PRO	HIS	Y214	I215	G235	GLU	ILE	ARG	ALA	ALA	THR	THR	SER	PRO	ALA
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ARG
GLU
ASN
TYR
PHE
MET
ARG
TRP
LEU
SER
ASP
LEU
ARG
GLU
THR
GLU
HIS
HIS
HIS
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.02Å 91.16Å 103.77Å 90.00° 107.32° 90.00°	Depositor
Resolution (Å)	36.20 – 2.10 36.20 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.7 (36.20-2.10) 97.7 (36.20-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.202 , 0.252 0.202 , 0.253	Depositor DCC
R_{free} test set	1533 reflections (2.03%)	DCC
Wilson B-factor (Å ²)	34.9	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 77145 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10798	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.47 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.9679e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: GOL, SCN, EDO, CL

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	0.52	0/1720	0.59	0/2345
1	H	0.45	0/1695	0.56	0/2314
2	B	0.47	0/1708	0.57	0/2324
2	L	0.42	0/1689	0.55	0/2299
3	C	0.38	0/1850	0.51	0/2518
3	X	0.41	0/1891	0.53	0/2576
All	All	0.44	0/10553	0.55	0/14376

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	1670	0	1618	6	0
1	H	1651	0	1586	15	0
2	B	1657	0	1584	9	0
2	L	1647	0	1565	4	0
3	C	1800	0	1716	10	0
3	X	1842	0	1758	8	0
4	A	4	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	3	0	0	0	0
4	H	3	0	0	0	0
4	L	3	0	0	0	0
4	X	3	0	0	0	0
5	H	4	0	6	1	0
6	A	6	0	8	0	0
6	B	6	0	8	1	0
6	L	6	0	8	0	0
7	C	1	0	0	0	0
8	A	122	0	0	0	0
8	B	135	0	0	2	0
8	C	26	0	0	0	0
8	H	90	0	0	1	0
8	L	76	0	0	1	0
8	X	43	0	0	0	0
All	All	10798	0	9857	50	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 2.

All (50) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145[B]:ASN:HB3	2:B:197[B]:THR:OG1	1.78	0.83
3:C:115:ILE:HG12	3:C:181:VAL:CG1	2.15	0.76
1:H:29:SER:HA	3:C:205:LEU:HD13	1.71	0.72
1:H:207:PRO:HB2	5:H:302:EDO:H21	1.74	0.69
3:C:202:LEU:O	3:C:215:ILE:HG22	1.94	0.67
3:X:200:ARG:HG3	3:X:216:THR:HA	1.77	0.67
1:H:43:GLY:HA2	8:H:451:HOH:O	1.99	0.62
1:H:132:ALA:O	1:H:220:ARG:NH1	2.37	0.58
1:H:220:ARG:NH1	2:L:119:PRO:HD2	2.19	0.57
2:B:2:GLN:HB2	8:B:493:HOH:O	2.03	0.57
2:B:195:GLU:HG3	2:B:206:VAL:HG22	1.87	0.57
1:H:68:LYS:HE2	1:H:91:ASP:OD2	2.04	0.56
1:A:135:CYS:HB3	4:A:303:SCN:S	2.45	0.56
3:C:115:ILE:HG12	3:C:181:VAL:HG13	1.87	0.56
3:X:56:PHE:CE2	3:X:168:THR:HG21	2.41	0.56
3:C:45:ILE:HD12	3:C:66:LEU:HD22	1.89	0.53
3:C:41:LYS:O	3:C:215:ILE:HD11	2.08	0.52
1:A:126:PRO:HB3	1:A:152:TYR:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:138:LEU:HG	3:C:202:LEU:HD21	1.91	0.51
1:A:171:HIS:CE1	6:B:301:GOL:H31	2.46	0.50
2:L:76:ASN:O	2:L:77:ARG:HB2	2.12	0.48
1:H:126:PRO:HB3	1:H:152:TYR:HB3	1.95	0.48
3:C:78:SER:O	3:C:86:LYS:HE3	2.14	0.48
1:A:221:GLY:HA3	4:A:303:SCN:S	2.54	0.47
2:B:148:TRP:CH2	2:B:194[B]:CYS:SG	3.07	0.47
3:X:7:PRO:HG3	3:X:79:ASN:HB3	1.97	0.47
1:H:128:VAL:HG21	1:H:213:VAL:CG1	2.45	0.47
3:X:43:VAL:HG21	3:X:199:PHE:HE1	1.80	0.47
1:H:31:ASN:HA	1:H:54:PRO:HB2	1.96	0.46
2:B:145[A]:ASN:HB3	2:B:197[A]:THR:HB	1.97	0.46
2:B:13:SER:HA	2:B:105:GLU:O	2.16	0.46
2:B:2:GLN:N	8:B:523:HOH:O	2.49	0.46
3:X:43:VAL:CG2	3:X:68:ILE:HB	2.46	0.45
2:L:11:ILE:O	2:L:11:ILE:HG13	2.15	0.45
3:C:215:ILE:HG23	3:C:215:ILE:O	2.16	0.44
3:C:57:LEU:HA	3:C:58:PRO:HD3	1.88	0.44
1:H:98:THR:OG1	1:H:107:PHE:HB3	2.18	0.44
1:H:101:ASN:HB3	1:H:104:TYR:O	2.17	0.43
1:H:161:TRP:CZ3	1:H:202[A]:CYS:HB3	2.53	0.43
2:B:78:LEU:HD11	2:B:104:LEU:HD21	2.01	0.43
1:H:41:ARG:HB2	1:H:44:GLN:HB2	2.00	0.42
3:X:167:PHE:HA	3:X:232:TYR:O	2.18	0.42
2:L:23:THR:HG23	8:L:459:HOH:O	2.19	0.42
2:B:76:ASN:O	2:B:77:ARG:HB2	2.20	0.42
1:A:33:TYR:HB3	1:A:99:ARG:HG3	2.01	0.42
1:A:161:TRP:CZ3	1:A:202[B]:CYS:HB3	2.56	0.41
3:X:78:SER:OG	3:X:86:LYS:HG3	2.21	0.41
1:H:47:GLU:OE2	1:H:64:LYS:HE2	2.21	0.41
3:X:10:ILE:HB	3:X:82:ILE:HD13	2.03	0.41
1:H:41:ARG:HG3	1:H:93:ALA:HB2	2.01	0.41

There are no symmetry-related clashes.

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	216/221 (98%)	212 (98%)	3 (1%)	1 (0%)	34	30
1	H	213/221 (96%)	209 (98%)	4 (2%)	0	100	100
2	B	215/212 (101%)	209 (97%)	5 (2%)	1 (0%)	34	30
2	L	213/212 (100%)	210 (99%)	2 (1%)	1 (0%)	34	30
3	C	222/269 (82%)	207 (93%)	14 (6%)	1 (0%)	34	30
3	X	224/269 (83%)	212 (95%)	11 (5%)	1 (0%)	39	37
All	All	1303/1404 (93%)	1259 (97%)	39 (3%)	5 (0%)	39	37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	77	ARG
1	A	135	CYS
2	B	77	ARG
3	X	84	VAL
3	C	84	VAL

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	193/193 (100%)	190 (98%)	3 (2%)	70	76
1	H	190/193 (98%)	187 (98%)	3 (2%)	70	76
2	B	192/187 (103%)	192 (100%)	0	100	100
2	L	189/187 (101%)	189 (100%)	0	100	100
3	C	194/247 (78%)	193 (100%)	1 (0%)	92	95
3	X	203/247 (82%)	202 (100%)	1 (0%)	92	95
All	All	1161/1254 (93%)	1153 (99%)	8 (1%)	90	92

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	18	SER
1	H	147[A]	CYS
1	H	147[B]	CYS
1	A	106	TYR
1	A	142	SER
1	A	218	GLU
3	X	139	ASP
3	C	53	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 1 is monoatomic and 1 is modelled with single atom - leaving 9 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	$\# Z > 2$
6	GOL	A	301	-	5,5,5	0.41	0	5,5,5	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SCN	A	302	-	2,2,2	1.70	1 (50%)	1,1,1	0.48	0
6	GOL	B	301	-	5,5,5	0.48	0	5,5,5	1.12	0
4	SCN	B	302	-	2,2,2	1.96	1 (50%)	1,1,1	0.50	0
4	SCN	H	301	-	2,2,2	1.90	1 (50%)	1,1,1	0.31	0
5	EDO	H	302	-	3,3,3	0.53	0	2,2,2	0.26	0
6	GOL	L	301	-	5,5,5	0.30	0	5,5,5	0.75	0
4	SCN	L	302	-	2,2,2	1.90	1 (50%)	1,1,1	0.23	0
4	SCN	X	301	-	2,2,2	1.78	1 (50%)	1,1,1	0.25	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	301	-	-	0/4/4/4	0/0/0/0
4	SCN	A	302	-	-	0/0/0/0	0/0/0/0
6	GOL	B	301	-	-	0/4/4/4	0/0/0/0
4	SCN	B	302	-	-	0/0/0/0	0/0/0/0
4	SCN	H	301	-	-	0/0/0/0	0/0/0/0
5	EDO	H	302	-	-	0/1/1/1	0/0/0/0
6	GOL	L	301	-	-	0/4/4/4	0/0/0/0
4	SCN	L	302	-	-	0/0/0/0	0/0/0/0
4	SCN	X	301	-	-	0/0/0/0	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	302	SCN	C-S	2.38	1.79	1.63
4	X	301	SCN	C-S	2.48	1.79	1.63
4	H	301	SCN	C-S	2.61	1.80	1.63
4	L	302	SCN	C-S	2.62	1.80	1.63
4	B	302	SCN	C-S	2.72	1.81	1.63

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	301	GOL	1	0
5	H	302	EDO	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	217/221 (98%)	-0.51	2 (0%) 85 88	22, 33, 54, 70	0
1	H	215/221 (97%)	-0.47	0 100 100	23, 39, 55, 65	0
2	B	212/212 (100%)	-0.60	0 100 100	21, 30, 47, 56	0
2	L	212/212 (100%)	-0.49	0 100 100	25, 35, 66, 78	0
3	C	225/269 (83%)	-0.01	6 (2%) 58 65	33, 56, 91, 107	0
3	X	228/269 (84%)	-0.32	1 (0%) 93 94	29, 49, 67, 75	0
All	All	1309/1404 (93%)	-0.39	9 (0%) 89 91	21, 39, 71, 107	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	19	ALA	4.5
3	X	21	LEU	3.0
3	C	144	ALA	2.6
3	C	201	THR	2.5
3	C	151	ASP	2.3
1	A	221	GLY	2.2
3	C	205	LEU	2.2
1	A	136	GLY	2.2
3	C	138	LEU	2.1

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

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

6.3 Carbohydrates [i](#)

There are no 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
6	GOL	B	301	6/6	0.79	0.18	8.06	33,36,38,40	0
6	GOL	L	301	6/6	0.75	0.15	6.71	36,40,42,43	0
6	GOL	A	301	6/6	0.94	0.10	3.03	45,46,47,47	0
4	SCN	L	302	3/3	0.92	0.10	1.78	68,68,68,68	0
4	SCN	A	302	3/3	0.96	0.11	1.35	30,30,30,31	0
4	SCN	H	301	3/3	0.97	0.13	0.63	40,40,40,40	0
4	SCN	X	301	3/3	0.73	0.13	0.23	66,66,67,67	0
4	SCN	B	302	3/3	0.95	0.08	-0.47	56,56,56,56	0
7	CL	C	301	1/1	0.95	0.05	-	62,62,62,62	0
4	SCN	A	303	1/3	0.32	0.15	-	90,90,90,90	0
5	EDO	H	302	4/4	0.88	0.15	-	54,54,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.