



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2025 – 12:11 pm GMT

PDB ID : 9I59 / pdb\_00009i59  
Title : RVFV GnH complexed with RVFV-379 Fab  
Authors : Paesen, G.C.; Bowden, T.A.  
Deposited on : 2025-01-27  
Resolution : 2.09 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](mailto: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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

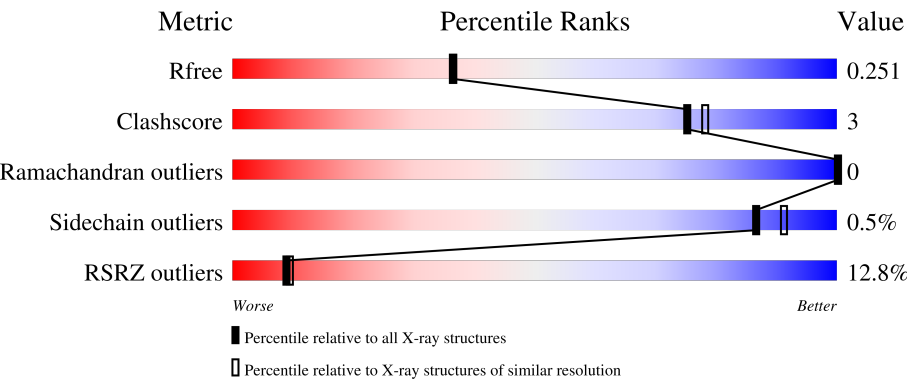
MolProbity : 4-5-2 with Phenix2.0  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.09 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))
$R_{free}$	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	345	<div><div>7%</div><div>81%5%14%</div></div>
1	B	345	<div><div>26%</div><div>73%8%19%</div></div>
2	H	223	<div><div>4%</div><div>93%. .</div></div>
2	X	223	<div><div>10%</div><div>81%12%6%</div></div>
3	L	215	<div><div>%</div><div>94%6%</div></div>

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Mol	Chain	Length	Quality of chain
3	Y	215	<div><div></div><div>15%</div><div>80%</div><div>5%</div><div>14%</div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11339 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 Envelopment polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2281	1431	391	435	24			
1	B	280	Total	C	N	O	S	0	0	0
			2178	1364	374	416	24			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	491	THR	-	expression tag	UNP A2T080
A	492	LYS	-	expression tag	UNP A2T080
A	493	HIS	-	expression tag	UNP A2T080
A	494	HIS	-	expression tag	UNP A2T080
A	495	HIS	-	expression tag	UNP A2T080
A	496	HIS	-	expression tag	UNP A2T080
A	497	HIS	-	expression tag	UNP A2T080
A	498	HIS	-	expression tag	UNP A2T080
B	491	THR	-	expression tag	UNP A2T080
B	492	LYS	-	expression tag	UNP A2T080
B	493	HIS	-	expression tag	UNP A2T080
B	494	HIS	-	expression tag	UNP A2T080
B	495	HIS	-	expression tag	UNP A2T080
B	496	HIS	-	expression tag	UNP A2T080
B	497	HIS	-	expression tag	UNP A2T080
B	498	HIS	-	expression tag	UNP A2T080

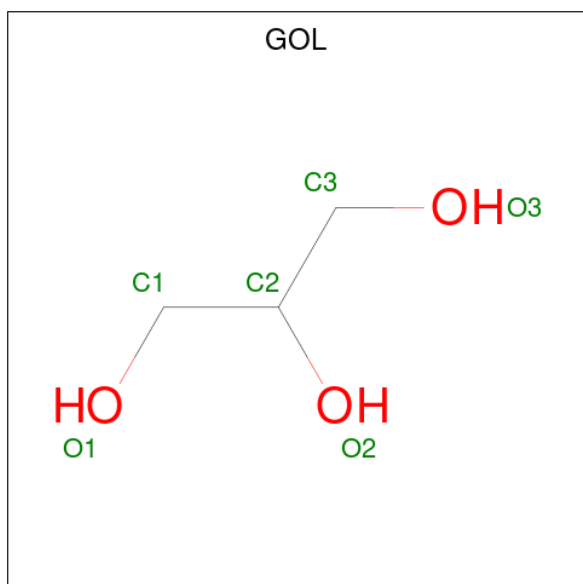
- Molecule 2 is a protein called Heavy chain of Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	216	Total	C	N	O	S	0	0	0
			1622	1026	270	320	6			
2	X	209	Total	C	N	O	S	0	0	0
			1576	998	262	311	5			

- Molecule 3 is a protein called Light chain of Fab.

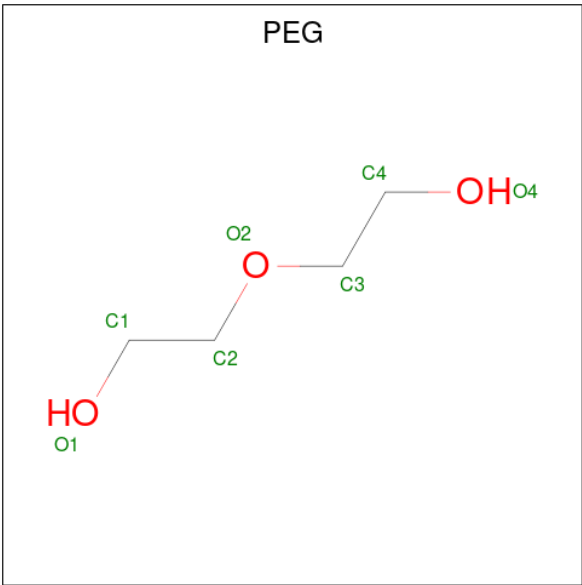
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	215	Total	C	N	O	S	0	0	0
			1668	1047	282	333	6			
3	Y	184	Total	C	N	O	S	0	0	0
			1431	901	240	286	4			

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		
4	X	1	Total	C	O	0	0
			6	3	3		
4	Y	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total	C	O	0	0
			7	4	3		

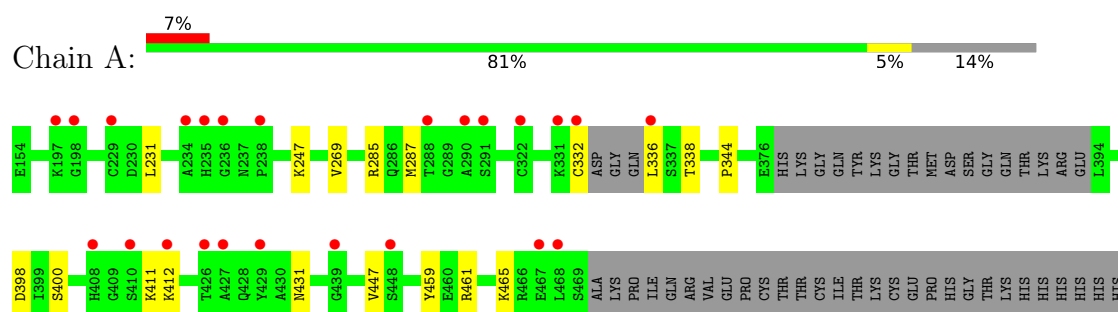
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	147	Total	O	0	0
			147	147		
6	B	47	Total	O	0	0
			47	47		
6	H	107	Total	O	0	0
			107	107		
6	L	123	Total	O	0	0
			123	123		
6	X	58	Total	O	0	0
			58	58		
6	Y	58	Total	O	0	0
			58	58		

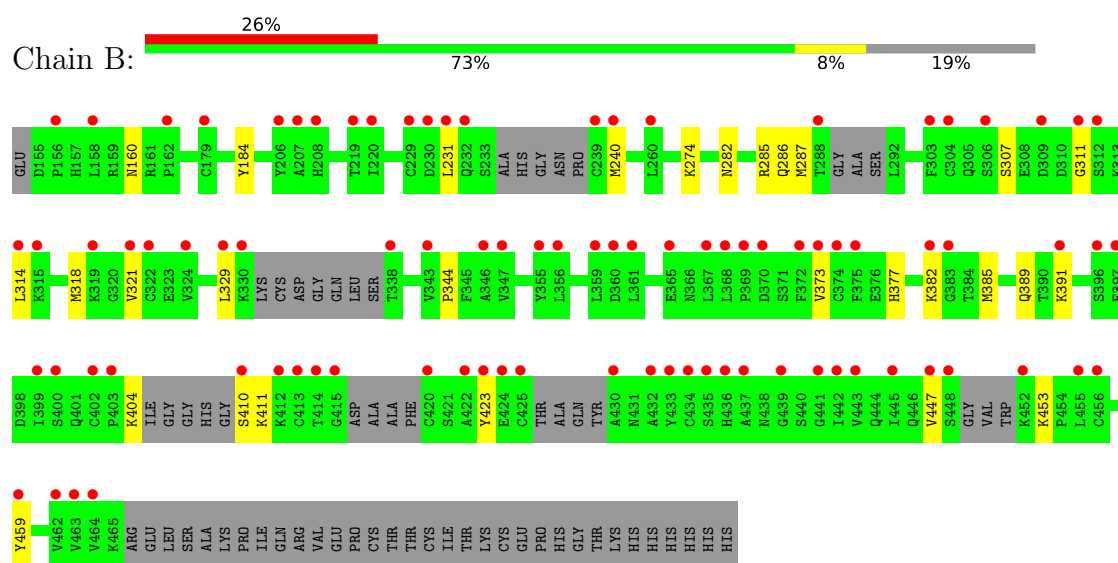
### 3 Residue-property plots [i](#)

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.

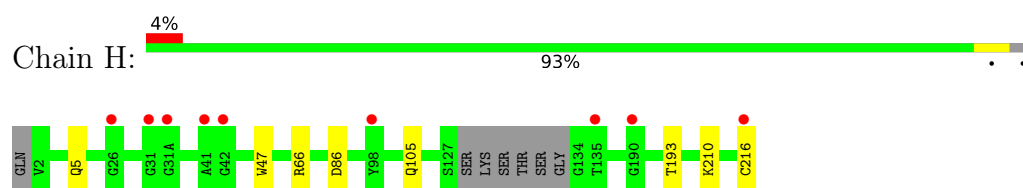
#### • Molecule 1: Envelopment polypeptide



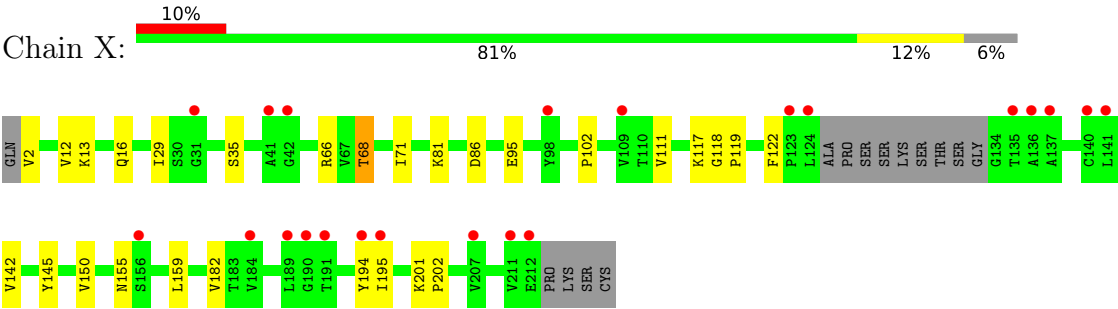
#### • Molecule 1: Envelopment polypeptide



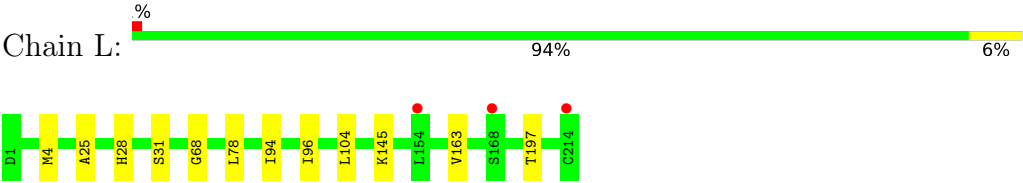
#### • Molecule 2: Heavy chain of Fab



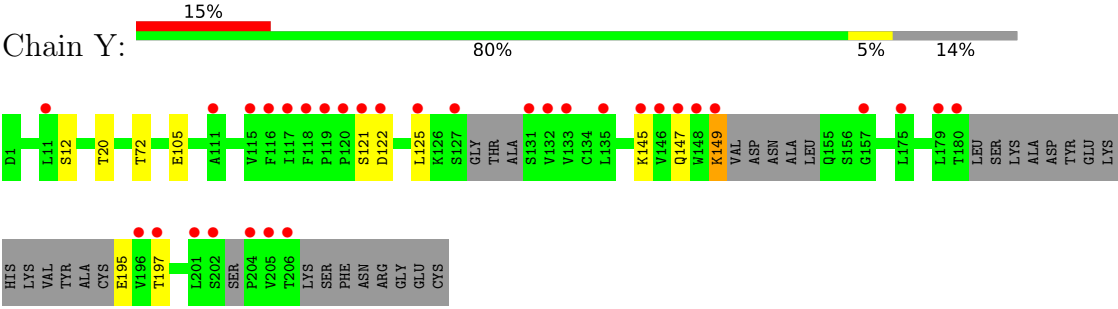
#### • Molecule 2: Heavy chain of Fab



• Molecule 3: Light chain of Fab



• Molecule 3: Light chain of Fab





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.09Å 187.37Å 157.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.47 – 2.09 39.47 – 2.09	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.47-2.09) 100.0 (39.47-2.09)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.23 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, $R_{free}$	0.212 , 0.251 0.212 , 0.251	Depositor DCC
$R_{free}$ test set	5257 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.4	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 49.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11339	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, PEG

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	0.17	0/2329	0.40	0/3137
1	B	0.15	0/2216	0.38	0/2970
2	H	0.18	0/1665	0.43	0/2277
2	X	0.15	0/1617	0.40	0/2211
3	L	0.18	0/1704	0.44	0/2312
3	Y	0.15	0/1459	0.41	0/1976
All	All	0.16	0/10990	0.41	0/14883

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 [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	2281	0	2225	11	0
1	B	2178	0	2136	16	0
2	H	1622	0	1574	4	0
2	X	1576	0	1528	17	0
3	L	1668	0	1628	7	0
3	Y	1431	0	1399	8	0
4	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	12	0	16	0	0
4	L	6	0	8	0	0
4	X	6	0	8	0	0
4	Y	6	0	8	0	0
5	L	7	0	10	0	0
6	A	147	0	0	0	0
6	B	47	0	0	0	0
6	H	107	0	0	0	0
6	L	123	0	0	1	0
6	X	58	0	0	0	0
6	Y	58	0	0	0	0
All	All	11339	0	10548	61	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 3.

All (61) 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:X:201:LYS:HG2	2:X:202:PRO:HD3	1.71	0.72
1:B:318:MET:HB2	1:B:321:VAL:HG21	1.74	0.70
2:X:68:THR:HG23	2:X:81:LYS:HB3	1.80	0.63
3:Y:145:LYS:HB3	3:Y:197:THR:HB	1.82	0.62
2:H:193:THR:HG23	2:H:210:LYS:HE3	1.83	0.59
1:B:321:VAL:HG23	1:B:329:LEU:HD12	1.84	0.59
1:B:285:ARG:HD2	1:B:287:MET:SD	2.43	0.58
2:H:5:GLN:HA	2:H:105:GLN:HE22	1.68	0.58
1:B:404:LYS:HA	1:B:423:TYR:HA	1.86	0.57
1:A:412:LYS:H	1:A:431:ASN:HD22	1.53	0.57
3:L:94:ILE:HG22	3:L:96:ILE:HD11	1.88	0.56
2:X:66:ARG:NH2	2:X:86:ASP:OD2	2.39	0.55
1:B:344:PRO:HB3	1:B:459:TYR:CE2	2.44	0.53
2:X:13:LYS:O	2:X:16:GLN:HB2	2.09	0.52
1:A:411:LYS:HB3	1:A:431:ASN:HD22	1.74	0.52
1:B:318:MET:HB2	1:B:321:VAL:CG2	2.40	0.49
1:B:377:HIS:CG	1:B:382:LYS:HG2	2.48	0.49
2:X:155:ASN:ND2	2:X:195:ILE:H	2.11	0.49
3:Y:149:LYS:HB2	3:Y:149:LYS:HE3	1.64	0.48
2:X:12:VAL:O	2:X:111:VAL:HA	2.14	0.48
1:A:412:LYS:HA	1:A:412:LYS:HD2	1.59	0.48
1:B:410:SER:O	1:B:411:LYS:HD3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:MET:HB3	1:B:389:GLN:HB3	1.96	0.47
2:H:47:TRP:CE2	3:L:96:ILE:HD12	2.50	0.47
2:H:66:ARG:NH2	2:H:86:ASP:OD2	2.48	0.47
1:A:338:THR:OG1	1:A:465:LYS:HG2	2.16	0.46
1:A:344:PRO:HB3	1:A:459:TYR:CE1	2.50	0.46
3:L:145:LYS:HB3	3:L:197:THR:HB	1.97	0.46
1:B:231:LEU:HD13	1:B:282:ASN:C	2.41	0.46
1:A:398:ASP:OD2	1:A:400:SER:OG	2.26	0.45
1:A:412:LYS:H	1:A:431:ASN:ND2	2.14	0.45
3:Y:147:GLN:HB3	3:Y:195:GLU:HB3	1.97	0.45
2:X:35:SER:OG	2:X:95:GLU:OE2	2.29	0.45
1:A:285:ARG:HD2	1:A:287:MET:SD	2.57	0.44
2:X:159:LEU:HD21	2:X:182:VAL:HG21	1.99	0.44
3:Y:12:SER:HA	3:Y:105:GLU:O	2.18	0.44
2:X:13:LYS:HB2	2:X:16:GLN:CD	2.43	0.44
1:B:307:SER:HA	1:B:453:LYS:HE2	1.99	0.44
3:L:78:LEU:HD11	3:L:104:LEU:HD21	2.00	0.44
2:X:2:VAL:HG13	2:X:102:PRO:HG3	1.99	0.44
3:Y:147:GLN:O	3:Y:195:GLU:N	2.51	0.44
1:A:231:LEU:HD11	1:A:269:VAL:HB	2.00	0.43
2:X:155:ASN:HD21	2:X:194:TYR:HA	1.83	0.43
1:B:311:GLY:HA2	1:B:314:LEU:HD23	2.00	0.43
3:L:28:HIS:CE1	3:L:68:GLY:HA2	2.54	0.43
3:Y:20:THR:HG23	3:Y:72:THR:HG23	2.00	0.43
3:Y:122:ASP:HA	3:Y:125:LEU:HD23	2.01	0.43
3:L:31:SER:OG	6:L:401:HOH:O	2.21	0.43
1:B:274:LYS:HB3	1:B:286:GLN:NE2	2.33	0.42
2:X:119:PRO:HB3	2:X:145:TYR:HB3	2.01	0.42
1:B:184:TYR:O	1:B:391:LYS:HG2	2.19	0.42
2:X:142:VAL:HG11	2:X:150:VAL:HG11	2.02	0.42
2:X:117:LYS:HD3	2:X:118:GLY:O	2.19	0.42
1:B:160:ASN:CG	1:B:373:VAL:HG23	2.45	0.42
2:X:29:ILE:HG21	2:X:71:ILE:HD11	2.02	0.42
1:A:247:LYS:HG2	1:A:461:ARG:HD2	2.02	0.41
2:X:13:LYS:HD3	2:X:16:GLN:OE1	2.20	0.41
1:A:332:CYS:HB3	1:A:336:LEU:HD11	2.03	0.41
1:B:240:MET:HE2	1:B:240:MET:HB2	1.79	0.40
3:L:4:MET:HE1	3:L:25:ALA:HB2	2.02	0.40
2:X:122:PHE:HB3	3:Y:121:SER:OG	2.21	0.40

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	290/345 (84%)	283 (98%)	7 (2%)	0	100	100
1	B	264/345 (76%)	261 (99%)	3 (1%)	0	100	100
2	H	212/223 (95%)	208 (98%)	4 (2%)	0	100	100
2	X	205/223 (92%)	202 (98%)	3 (2%)	0	100	100
3	L	213/215 (99%)	206 (97%)	7 (3%)	0	100	100
3	Y	174/215 (81%)	166 (95%)	8 (5%)	0	100	100
All	All	1358/1566 (87%)	1326 (98%)	32 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	255/298 (86%)	254 (100%)	1 (0%)	89	93
1	B	247/298 (83%)	246 (100%)	1 (0%)	89	93
2	H	184/190 (97%)	183 (100%)	1 (0%)	86	91
2	X	178/190 (94%)	177 (99%)	1 (1%)	84	89
3	L	190/190 (100%)	189 (100%)	1 (0%)	86	91
3	Y	165/190 (87%)	164 (99%)	1 (1%)	84	89
All	All	1219/1356 (90%)	1213 (100%)	6 (0%)	86	91

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	447	VAL
1	B	447	VAL
2	H	216	CYS
3	L	163	VAL
2	X	68	THR
3	Y	149	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	286	GLN
1	A	350	ASN
1	A	431	ASN
1	A	444	GLN
1	A	446	GLN
1	B	208	HIS
1	B	286	GLN
1	B	401	GLN
1	B	436	HIS
2	H	105	GLN
2	H	171	GLN
2	H	192	GLN
3	L	37	GLN
3	L	38	GLN
2	X	5	GLN
2	X	155	ASN
2	X	192	GLN
3	Y	147	GLN

### 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

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

7 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	$\# Z  > 2$
4	GOL	A	501	-	5,5,5	0.28	0	5,5,5	0.36	0
4	GOL	H	302	-	5,5,5	0.32	0	5,5,5	0.46	0
4	GOL	L	301	-	5,5,5	0.35	0	5,5,5	0.45	0
4	GOL	H	301	-	5,5,5	0.32	0	5,5,5	0.55	0
4	GOL	X	301	-	5,5,5	0.34	0	5,5,5	0.39	0
5	PEG	L	302	-	6,6,6	0.24	0	5,5,5	0.28	0
4	GOL	Y	301	-	5,5,5	0.31	0	5,5,5	0.48	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	501	-	-	1/4/4/4	-
4	GOL	H	302	-	-	0/4/4/4	-
4	GOL	L	301	-	-	0/4/4/4	-
4	GOL	H	301	-	-	4/4/4/4	-
4	GOL	X	301	-	-	4/4/4/4	-
5	PEG	L	302	-	-	3/4/4/4	-
4	GOL	Y	301	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	301	GOL	O1-C1-C2-O2
4	H	301	GOL	O1-C1-C2-C3
4	H	301	GOL	C1-C2-C3-O3
4	X	301	GOL	O1-C1-C2-O2
4	X	301	GOL	O1-C1-C2-C3
5	L	302	PEG	O1-C1-C2-O2
4	X	301	GOL	C1-C2-C3-O3
4	H	301	GOL	O2-C2-C3-O3
4	X	301	GOL	O2-C2-C3-O3
5	L	302	PEG	C1-C2-O2-C3
5	L	302	PEG	C4-C3-O2-C2
4	A	501	GOL	O2-C2-C3-O3

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	296/345 (85%)	0.31	24 (8%) 19 21	21, 37, 75, 104	0
1	B	280/345 (81%)	1.46	89 (31%) 1 1	32, 63, 90, 99	0
2	H	216/223 (96%)	0.22	9 (4%) 41 43	21, 35, 61, 90	0
2	X	209/223 (93%)	0.80	22 (10%) 13 14	27, 50, 90, 104	0
3	L	215/215 (100%)	0.04	3 (1%) 73 74	21, 34, 53, 68	0
3	Y	184/215 (85%)	0.84	32 (17%) 5 5	26, 42, 92, 104	0
All	All	1400/1566 (89%)	0.63	179 (12%) 9 9	21, 43, 87, 104	0

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	372	PHE	5.9
3	Y	204	PRO	4.6
1	B	425	CYS	4.5
3	Y	179	LEU	4.3
1	B	442	ILE	4.3
3	Y	132	VAL	4.2
3	Y	196	VAL	4.2
3	Y	148	TRP	4.1
3	Y	205	VAL	4.1
1	B	439	GLY	4.0
3	Y	146	VAL	4.0
1	B	343	VAL	4.0
3	Y	111	ALA	3.9
1	A	429	TYR	3.8
2	X	194	TYR	3.8
3	Y	206	THR	3.8
1	B	423	TYR	3.8
1	A	336	LEU	3.6
3	Y	149	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	415	GLY	3.6
1	B	314	LEU	3.6
3	Y	117	ILE	3.5
1	B	288	THR	3.5
1	B	447	VAL	3.5
2	X	41	ALA	3.5
1	A	427	ALA	3.5
1	A	410	SER	3.5
1	B	367	LEU	3.5
2	H	41	ALA	3.4
1	B	420	CYS	3.4
1	B	455	LEU	3.4
1	B	368	LEU	3.4
1	B	373	VAL	3.4
1	B	239	CYS	3.3
2	X	124	LEU	3.3
3	L	154	LEU	3.3
1	B	311	GLY	3.3
1	B	397	PHE	3.3
1	B	321	VAL	3.3
3	L	168	SER	3.3
3	Y	116	PHE	3.2
3	Y	197	THR	3.2
1	B	399	ILE	3.2
2	X	211	VAL	3.2
1	B	463	VAL	3.2
2	X	191	THR	3.2
2	X	31	GLY	3.2
3	Y	157	GLY	3.2
1	B	374	CYS	3.1
2	X	140	CYS	3.1
1	B	370	ASP	3.1
1	B	435	SER	3.1
1	A	468	LEU	3.1
2	X	42	GLY	3.1
3	Y	180	THR	3.1
3	Y	118	PHE	3.0
1	A	235	HIS	3.0
1	B	231	LEU	3.0
1	B	422	ALA	3.0
1	B	433	TYR	3.0
3	Y	202	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	445	ILE	2.9
1	B	459	TYR	2.9
2	X	189	LEU	2.9
1	B	414	THR	2.9
1	B	306	SER	2.9
2	X	195	ILE	2.9
1	B	356	LEU	2.8
2	X	207	VAL	2.8
1	B	206	TYR	2.8
2	X	123	PRO	2.8
1	A	322	CYS	2.8
1	B	441	GLY	2.8
1	A	332	CYS	2.8
3	Y	115	VAL	2.8
1	A	234	ALA	2.7
1	B	383	GLY	2.7
1	B	359	LEU	2.7
3	Y	135	LEU	2.7
3	Y	127	SER	2.7
1	B	360	ASP	2.7
1	B	443	VAL	2.7
1	A	467	GLU	2.7
3	Y	125	LEU	2.6
3	Y	201	LEU	2.6
2	H	31	GLY	2.6
1	B	240	MET	2.6
2	H	42	GLY	2.6
2	X	190	GLY	2.6
1	B	347	VAL	2.6
3	Y	145	LYS	2.6
1	B	322	CYS	2.6
1	B	456	CYS	2.6
1	A	439	GLY	2.5
1	B	432	ALA	2.5
1	A	408	HIS	2.5
1	A	448	SER	2.5
1	B	365	GLU	2.5
1	B	400	SER	2.5
1	B	158	LEU	2.5
1	B	361	LEU	2.5
2	X	184	VAL	2.5
2	H	26	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	309	ASP	2.5
1	B	424	GLU	2.4
1	B	156	PRO	2.4
3	Y	121	SER	2.4
1	B	430	ALA	2.4
1	B	329	LEU	2.4
1	B	434	CYS	2.4
1	B	179	CYS	2.4
1	B	208	HIS	2.4
2	X	135	THR	2.4
1	B	403	PRO	2.4
2	X	212	GLU	2.3
1	B	437	ALA	2.3
1	A	426	THR	2.3
1	B	219	THR	2.3
1	B	304	CYS	2.3
3	L	214	CYS	2.3
1	A	291	SER	2.3
3	Y	133	VAL	2.3
2	H	190	GLY	2.3
1	B	452	LYS	2.3
2	X	141	LEU	2.3
1	B	162	PRO	2.3
3	Y	120	PRO	2.3
1	B	462	VAL	2.3
1	A	288	THR	2.3
1	B	338	THR	2.3
1	B	410	SER	2.3
1	B	448	SER	2.3
2	X	156	SER	2.3
1	A	198	GLY	2.3
1	A	236	GLY	2.3
1	A	331	LYS	2.3
1	B	355	TYR	2.3
1	A	290	ALA	2.3
3	Y	119	PRO	2.2
1	B	391	LYS	2.2
1	B	375	PHE	2.2
1	B	260	LEU	2.2
1	B	346	ALA	2.2
2	X	137	ALA	2.2
1	B	229	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	230	ASP	2.2
1	B	402	CYS	2.2
1	B	330	LYS	2.2
1	B	464	VAL	2.2
3	Y	11	LEU	2.2
1	B	413	CYS	2.2
2	X	109	VAL	2.2
1	B	303	PHE	2.2
1	B	324	VAL	2.2
1	B	220	ILE	2.1
2	H	31(A)	GLY	2.1
1	A	229	CYS	2.1
3	Y	147	GLN	2.1
1	B	382	LYS	2.1
1	B	312	SER	2.1
3	Y	131	SER	2.1
1	A	238	PRO	2.1
1	B	369	PRO	2.1
1	B	315	LYS	2.1
1	B	396	SER	2.1
1	B	436	HIS	2.1
2	X	98	TYR	2.1
1	A	197	LYS	2.1
1	B	319	LYS	2.1
2	X	136	ALA	2.0
1	A	412	LYS	2.0
1	B	412	LYS	2.0
2	H	216	CYS	2.0
3	Y	122	ASP	2.0
1	B	232	GLN	2.0
2	H	135	THR	2.0
3	Y	175	LEU	2.0
1	B	207	ALA	2.0
2	H	98	TYR	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides 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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	GOL	L	301	6/6	0.78	0.15	31,42,49,53	0
5	PEG	L	302	7/7	0.81	0.16	36,51,56,57	0
4	GOL	A	501	6/6	0.87	0.13	32,46,48,58	0
4	GOL	Y	301	6/6	0.90	0.13	34,50,58,63	0
4	GOL	H	301	6/6	0.91	0.12	31,39,45,51	0
4	GOL	X	301	6/6	0.91	0.09	30,34,40,42	0
4	GOL	H	302	6/6	0.94	0.07	24,28,35,49	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.