



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:53 PM UTC

PDB ID : 8UP2 / pdb_00008up2
Title : Murine Fab JAR 4 bound to meningococcal Factor H binding protein
Authors : Beernink, P.T.; Beernink, B.P.
Deposited on : 2023-10-20
Resolution : 1.60 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
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)	:	2.49

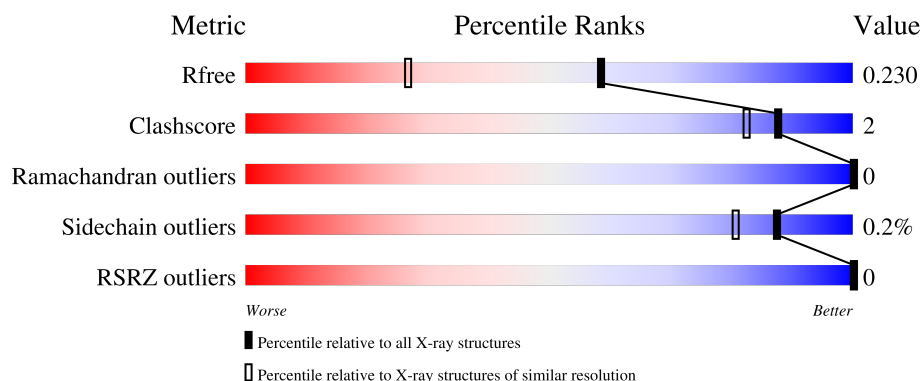
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

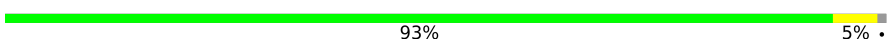
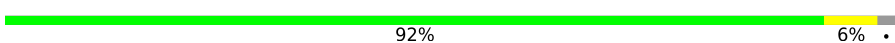
The reported resolution of this entry is 1.60 Å.

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}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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 $\leq 5\%$. 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	223	
1	D	223	
2	B	220	
2	E	220	
3	C	257	

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Mol	Chain	Length	Quality of chain
3	F	257	 87%6% • 6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21246 atoms, of which 10043 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 Human-mouse chimeric immunoglobulin heavy chain, Fd fragment.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	209	Total	C	H	N	O	S	0	2	0
			3150	1015	1559	260	309	7			
1	D	209	Total	C	H	N	O	S	0	2	0
			3155	1017	1563	260	308	7			

- Molecule 2 is a protein called Human-mouse chimeric immunoglobulin, kappa light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	217	Total	C	H	N	O	S	0	0	0
			3332	1063	1652	280	332	5			
2	E	216	Total	C	H	N	O	S	0	0	0
			3335	1061	1659	279	331	5			

- Molecule 3 is a protein called Factor H binding protein, sequence variant ID 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	241	Total	C	H	N	O	S	0	1	0
			3620	1131	1802	326	360	1			
3	F	241	Total	C	H	N	O	S	0	0	0
			3604	1129	1789	326	359	1			

There are 18 discrepancies between the modelled and reference sequences:

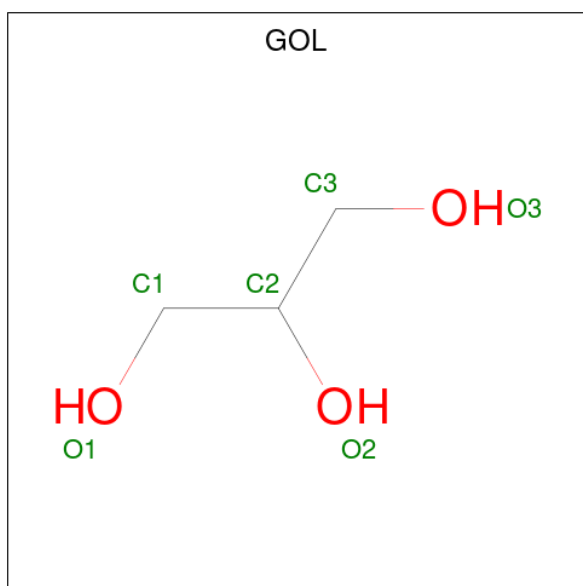
Chain	Residue	Modelled	Actual	Comment	Reference
C	7	MET	-	initiating methionine	UNP Q6VRZ6
C	256	LEU	-	expression tag	UNP Q6VRZ6
C	257	GLU	-	expression tag	UNP Q6VRZ6
C	258	HIS	-	expression tag	UNP Q6VRZ6
C	259	HIS	-	expression tag	UNP Q6VRZ6
C	260	HIS	-	expression tag	UNP Q6VRZ6
C	261	HIS	-	expression tag	UNP Q6VRZ6

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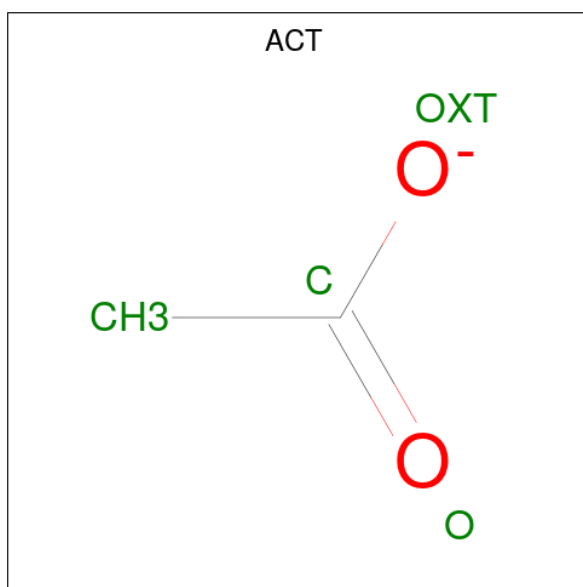
Chain	Residue	Modelled	Actual	Comment	Reference
C	262	HIS	-	expression tag	UNP Q6VRZ6
C	263	HIS	-	expression tag	UNP Q6VRZ6
F	7	MET	-	initiating methionine	UNP Q6VRZ6
F	256	LEU	-	expression tag	UNP Q6VRZ6
F	257	GLU	-	expression tag	UNP Q6VRZ6
F	258	HIS	-	expression tag	UNP Q6VRZ6
F	259	HIS	-	expression tag	UNP Q6VRZ6
F	260	HIS	-	expression tag	UNP Q6VRZ6
F	261	HIS	-	expression tag	UNP Q6VRZ6
F	262	HIS	-	expression tag	UNP Q6VRZ6
F	263	HIS	-	expression tag	UNP Q6VRZ6

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	H	O	0	0
			14	3	8	3		
4	F	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 6 is water.

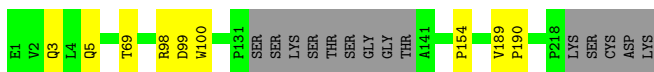
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	197	Total	O	0	0
			197	197		
6	B	152	Total	O	0	0
			152	152		
6	C	167	Total	O	0	0
			167	167		
6	D	190	Total	O	0	0
			190	190		
6	E	147	Total	O	0	0
			147	147		
6	F	162	Total	O	0	0
			162	162		

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.

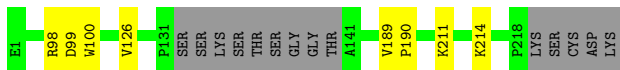
- Molecule 1: Human-mouse chimeric immunoglobulin heavy chain, Fd fragment

Chain A: 

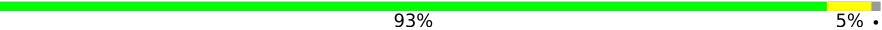


- Molecule 1: Human-mouse chimeric immunoglobulin heavy chain, Fd fragment

Chain D: 



- Molecule 2: Human-mouse chimeric immunoglobulin, kappa light chain

Chain B: 



- Molecule 2: Human-mouse chimeric immunoglobulin, kappa light chain

Chain E: 



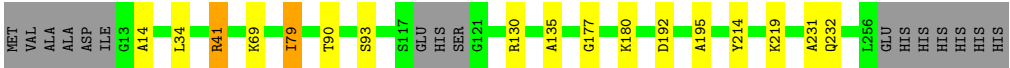
- Molecule 3: Factor H binding protein, sequence variant ID 1

Chain C: 



- Molecule 3: Factor H binding protein, sequence variant ID 1

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.43Å 67.44Å 168.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.43 – 1.60 74.43 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (74.43-1.60) 94.9 (74.43-1.60)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.187 , 0.212 (Not available) , 0.230	Depositor DCC
R_{free} test set	2014 reflections (0.92%)	wwPDB-VP
Wilson B-factor (Å ²)	17.6	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 23.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.400 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	21246	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% 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: GOL, ACT

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	0.54	1/1650 (0.1%)	0.67	0/2251
1	D	0.49	0/1651	0.65	0/2253
2	B	0.43	0/1717	0.61	2/2328 (0.1%)
2	E	0.48	0/1713	0.63	0/2323
3	C	0.54	1/1844 (0.1%)	0.69	0/2472
3	F	0.62	3/1838 (0.2%)	0.71	0/2464
All	All	0.52	5/10413 (0.0%)	0.66	2/14091 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	1
3	C	0	1
3	F	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	231	ALA	C-O	-8.32	1.13	1.23
3	C	40	VAL	C-O	-7.60	1.15	1.24
1	A	69	THR	C-O	-6.74	1.16	1.24
3	F	79	ILE	C-O	-6.28	1.17	1.24
3	F	232	GLN	C-O	-5.25	1.17	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	161	SER	CA-C-N	5.23	131.16	120.80
2	B	161	SER	C-N-CA	5.23	131.16	120.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	41	ARG	Sidechain
2	E	82	ARG	Sidechain
3	F	41	ARG	Sidechain

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	1591	1559	1550	4	0
1	D	1592	1563	1554	5	0
2	B	1680	1652	1662	6	0
2	E	1676	1659	1659	9	0
3	C	1818	1802	1819	7	0
3	F	1815	1789	1814	11	0
4	C	6	8	8	0	0
4	F	6	8	8	0	0
5	D	4	3	3	0	0
6	A	197	0	0	0	0
6	B	152	0	0	0	0
6	C	167	0	0	0	0
6	D	190	0	0	0	0
6	E	147	0	0	0	0
6	F	162	0	0	1	0
All	All	11203	10043	10077	40	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 (40) 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)
3:F:34:LEU:CD1	3:F:135:ALA:HB3	2.05	0.87
3:C:34:LEU:CD1	3:C:135:ALA:HB3	2.10	0.81
3:F:34:LEU:HD11	3:F:135:ALA:HB3	1.73	0.69
2:B:4:MET:HE3	2:B:23:CYS:SG	2.33	0.69
3:F:34:LEU:HD12	3:F:135:ALA:HB3	1.75	0.69
3:C:92:GLU:OE2	3:C:111:THR:OG1	2.13	0.65
3:F:79:ILE:HD13	3:F:93:SER:HB3	1.80	0.63
3:C:34:LEU:HD11	3:C:135:ALA:HB3	1.84	0.59
2:E:4:MET:HE3	2:E:23:CYS:SG	2.43	0.58
3:C:34:LEU:HD12	3:C:135:ALA:HB3	1.84	0.58
3:F:79:ILE:HG23	3:F:90:THR:HG23	1.87	0.57
2:B:130:LEU:O	2:B:188:LYS:HD2	2.12	0.49
2:E:13:VAL:HG11	2:E:83:VAL:HG21	1.96	0.47
3:F:180:LYS:HD3	3:F:192:ASP:OD1	2.14	0.47
3:C:79:ILE:HG23	3:C:90:THR:HG23	1.96	0.47
3:F:14:ALA:HA	3:F:69:LYS:HE3	1.97	0.47
2:B:81:SER:OG	2:B:82:ARG:NH1	2.48	0.46
2:E:82:ARG:O	2:E:82:ARG:HG3	2.17	0.45
2:E:88:LEU:HD12	2:E:171:GLN:HB3	1.99	0.45
2:E:188:LYS:O	2:E:192:GLU:HG3	2.17	0.44
1:A:98:ARG:O	1:A:99:ASP:C	2.60	0.44
1:A:3:GLN:NE2	1:A:5:GLN:OE1	2.50	0.44
1:D:211:LYS:HA	1:D:211:LYS:HD2	1.86	0.43
3:F:214:TYR:CB	3:F:219:LYS:HE2	2.48	0.43
1:D:100:TRP:CE2	2:E:94:LEU:HD21	2.53	0.43
3:F:130:ARG:NH1	6:F:403:HOH:O	2.49	0.43
1:D:126:VAL:O	1:D:214:LYS:HE3	2.19	0.43
3:C:177:GLY:O	3:C:195:ALA:HA	2.19	0.42
1:D:98:ARG:O	1:D:99:ASP:C	2.62	0.42
3:F:214:TYR:HB2	3:F:219:LYS:HE2	2.01	0.42
2:B:24:LYS:HG2	2:B:75:ASP:OD1	2.20	0.42
1:A:100:TRP:CE2	2:B:94:LEU:HD21	2.55	0.42
1:A:189:VAL:HB	1:A:190:PRO:HD2	2.02	0.41
2:E:4:MET:HE3	2:E:4:MET:HB3	1.87	0.41
2:E:24:LYS:HA	2:E:74:THR:O	2.20	0.41
3:C:13:GLY:C	3:C:69:LYS:HE3	2.45	0.41
3:F:177:GLY:O	3:F:195:ALA:HA	2.21	0.41
1:D:189:VAL:HB	1:D:190:PRO:HD2	2.03	0.40
2:E:152:GLN:NE2	2:E:159:LEU:HG	2.36	0.40
2:B:164:SER:HA	2:B:183:THR:O	2.22	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	207/223 (93%)	202 (98%)	5 (2%)	0	100	100
1	D	207/223 (93%)	203 (98%)	4 (2%)	0	100	100
2	B	215/220 (98%)	212 (99%)	3 (1%)	0	100	100
2	E	214/220 (97%)	211 (99%)	3 (1%)	0	100	100
3	C	238/257 (93%)	231 (97%)	7 (3%)	0	100	100
3	F	237/257 (92%)	231 (98%)	6 (2%)	0	100	100
All	All	1318/1400 (94%)	1290 (98%)	28 (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	182/192 (95%)	181 (100%)	1 (0%)	81	70
1	D	182/192 (95%)	182 (100%)	0	100	100
2	B	193/196 (98%)	193 (100%)	0	100	100
2	E	193/196 (98%)	193 (100%)	0	100	100
3	C	187/200 (94%)	187 (100%)	0	100	100
3	F	186/200 (93%)	185 (100%)	1 (0%)	81	70
All	All	1123/1176 (96%)	1121 (100%)	2 (0%)	87	81

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	PRO
3	F	41	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
2	B	165	GLN
3	C	128	GLN
3	C	215	ASN
3	C	216	GLN
1	D	197	GLN
2	E	152	GLN
2	E	165	GLN
3	F	215	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	C	301	-	5,5,5	0.63	0	5,5,5	1.03	1 (20%)
4	GOL	F	301	-	5,5,5	0.74	0	5,5,5	0.65	0
5	ACT	D	301	-	3,3,3	2.02	2 (66%)	3,3,3	1.43	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	C	301	-	-	0/4/4/4	-
4	GOL	F	301	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	301	ACT	CH3-C	2.85	1.60	1.49
5	D	301	ACT	O-C	2.03	1.31	1.22

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	301	GOL	C3-C2-C1	-2.04	104.30	111.80

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	301	GOL	O1-C1-C2-C3
4	F	301	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [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	209/223 (93%)	-1.17	0 100 100	12, 22, 46, 65	1 (0%)
1	D	209/223 (93%)	-1.13	0 100 100	13, 22, 47, 67	1 (0%)
2	B	217/220 (98%)	-1.06	0 100 100	16, 28, 45, 60	0
2	E	216/220 (98%)	-0.96	0 100 100	16, 28, 47, 65	0
3	C	241/257 (93%)	-1.08	0 100 100	12, 27, 48, 68	1 (0%)
3	F	241/257 (93%)	-1.07	0 100 100	16, 27, 47, 74	0
All	All	1333/1400 (95%)	-1.08	0 100 100	12, 26, 47, 74	3 (0%)

There are no RSRZ outliers to report.

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 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, 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	B-factors(Å ²)	Q<0.9
5	ACT	D	301	4/4	0.97	0.07	33,35,43,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	C	301	6/6	0.98	0.05	21,27,32,33	0
4	GOL	F	301	6/6	0.99	0.05	22,31,36,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.