



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 07:05 am BST

PDB ID : 4WJ5  
Title : Structure of HLA-A2 in complex with an altered peptide ligands based on Mart-1 variant epitope  
Authors : Celie, P.H.N.; Rodenko, B.; Ovaa, H.  
Deposited on : 2014-09-29  
Resolution : 1.65 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

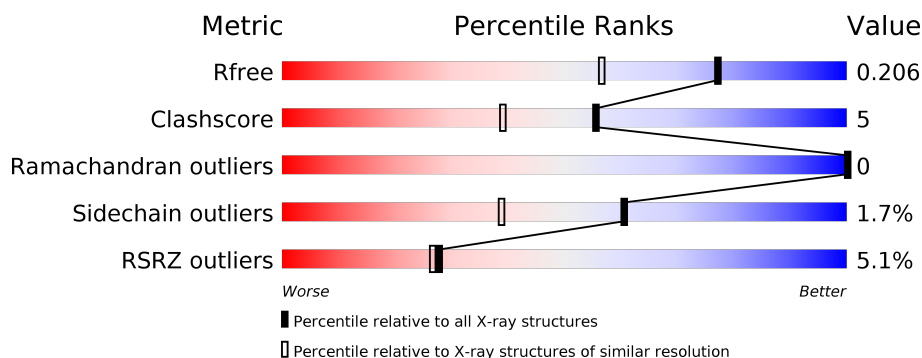
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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  $\geq 3$ , 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	275	<div> <div>5%</div> <div> <div></div> <div>90%</div> <div>10%</div> </div> </div>
1	D	275	<div> <div>6%</div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>
2	B	100	<div> <div>4%</div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>
2	E	100	<div> <div>4%</div> <div> <div></div> <div>86%</div> <div>14%</div> </div> </div>
3	C	10	<div> <div></div> <div> <div></div> <div>90%</div> <div>10%</div> </div> </div>
3	F	10	<div> <div></div> <div> <div></div> <div>80%</div> <div>20%</div> </div> </div>

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
3	NVA	C	1[A]	X	-	-	-
3	NVA	C	1[B]	X	-	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7465 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 HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	24	0
			2438	1519	450	459	10			
1	D	275	Total	C	N	O	S	0	23	0
			2444	1520	449	466	9			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	5	0
			873	554	147	168	4			
2	E	100	Total	C	N	O	S	0	12	0
			942	594	158	184	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
E	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called Melanoma antigen recognized by T-cells 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	1	0
			77	53	11	13			
3	F	10	Total	C	N	O	0	1	0
			77	52	11	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	GRN	GLU	conflict	UNP Q16655
C	1	NVA	ALA	conflict	UNP Q16655

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Chain	Residue	Modelled	Actual	Comment	Reference
C	9	LPH	VAL	conflict	UNP Q16655
F	0	GRN	GLU	conflict	UNP Q16655
F	1	NVA	ALA	conflict	UNP Q16655
F	9	LPH	VAL	conflict	UNP Q16655

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total 6	C 3	O 3	0	0
4	E	1	Total 6	C 3	O 3	0	0
4	E	1	Total 6	C 3	O 3	0	0
4	E	1	Total 6	C 3	O 3	0	0

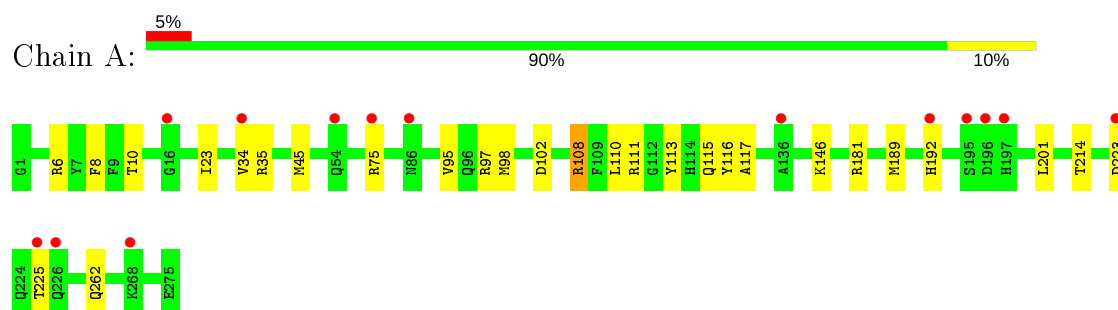
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	186	Total 186	O 186	0	0
5	B	88	Total 88	O 88	0	0
5	C	7	Total 7	O 7	0	0
5	D	167	Total 167	O 167	0	0
5	E	81	Total 81	O 81	0	0
5	F	7	Total 7	O 7	0	0

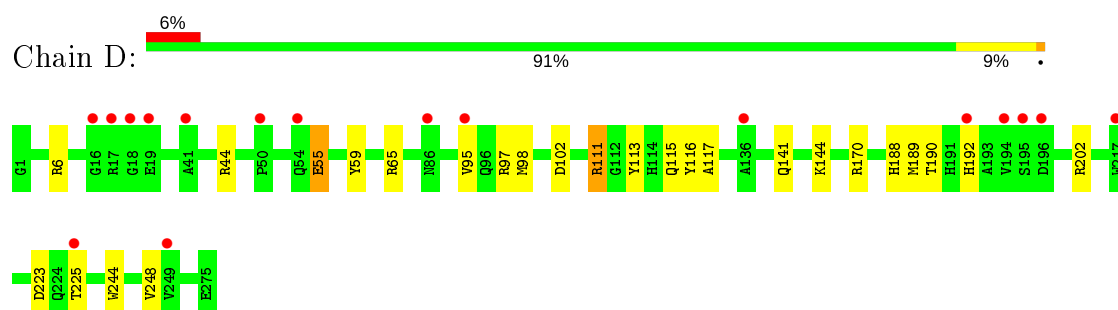
### 3 Residue-property plots [i](#)

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.

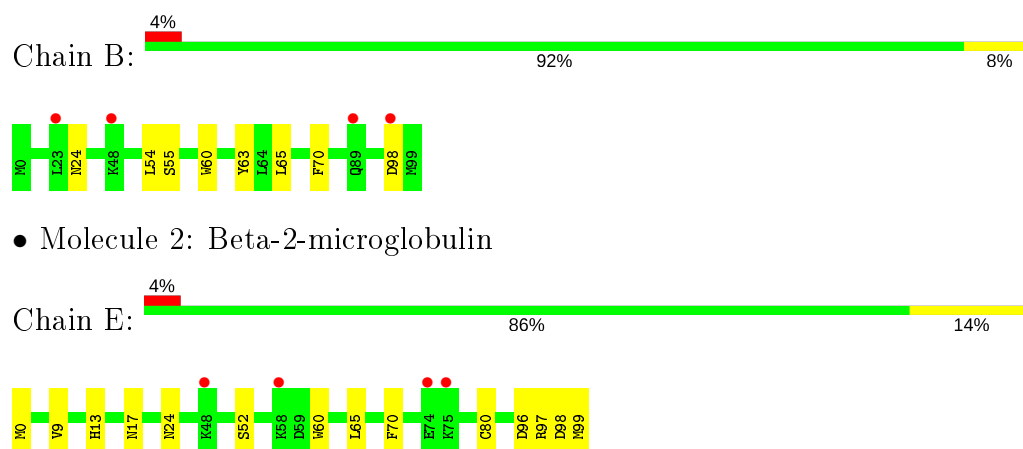
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain




- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin




- Molecule 3: Melanoma antigen recognized by T-cells 1

Chain C:  90% 10%



- Molecule 3: Melanoma antigen recognized by T-cells 1

Chain F:  80% 20%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.18Å 87.14Å 79.19Å 90.00° 90.15° 90.00°	Depositor
Resolution (Å)	19.94 – 1.65 19.94 – 1.65	Depositor EDS
% Data completeness (in resolution range)	98.8 (19.94-1.65) 99.2 (19.94-1.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.91 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.155 , 0.179 0.180 , 0.206	Depositor DCC
$R_{free}$ test set	5123 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.5	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 46.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.068 for h,-k,-l	Xtriage
Reported twinning fraction	0.747 for H, K, L 0.253 for -h,-k,l	Depositor
Outliers	0 of 103143 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7465	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% 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: GRN, GOL, NVA, LPH

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	0.62	0/2514	0.84	2/3407 (0.1%)
1	D	0.61	0/2510	0.83	4/3401 (0.1%)
2	B	0.66	0/896	0.80	0/1210
2	E	0.64	0/964	0.80	0/1295
3	C	0.54	0/43	0.80	0/57
3	F	0.40	0/49	0.95	0/64
All	All	0.63	0/6976	0.83	6/9434 (0.1%)

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
3	C	2	0

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	D	189	MET	CG-SD-CE	-6.66	89.54	100.20
1	A	97	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	A	181	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	D	97	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	D	102	ASP	CB-CG-OD1	5.38	123.14	118.30
1	D	111	ARG	CG-CD-NE	5.02	122.34	111.80

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	1[A]	NVA	CA
3	C	1[B]	NVA	CA

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	2438	0	2287	28	0
1	D	2444	0	2277	24	0
2	B	873	0	834	7	0
2	E	942	0	894	18	0
3	C	77	0	80	1	0
3	F	77	0	80	1	0
4	A	12	0	16	2	0
4	B	12	0	16	0	0
4	D	36	0	48	5	0
4	E	18	0	24	3	0
5	A	186	0	0	3	0
5	B	88	0	0	0	0
5	C	7	0	0	0	0
5	D	167	0	0	5	0
5	E	81	0	0	3	0
5	F	7	0	0	0	0
All	All	7465	0	6556	69	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 5.

All (69) 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:A:108[B]:ARG:HG2	1:A:108[B]:ARG:HH11	1.07	1.11
1:A:192[A]:HIS:HE1	2:B:98[A]:ASP:OD2	1.47	0.97
2:E:52:SER:HA	4:E:102:GOL:H32	1.50	0.93
1:A:108[B]:ARG:HH11	1:A:108[B]:ARG:CG	1.82	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108[B]:ARG:HG2	1:A:108[B]:ARG:NH1	1.89	0.86
1:A:10[B]:THR:HG21	2:B:54:LEU:HD23	1.56	0.86
1:D:248[B]:VAL:HG23	1:D:248[B]:VAL:O	1.75	0.83
1:A:192[A]:HIS:CE1	2:B:98[A]:ASP:OD2	2.35	0.77
2:E:9[B]:VAL:HG11	2:E:80:CYS:HB2	1.67	0.77
1:A:34[B]:VAL:CG1	1:A:45:MET:SD	2.72	0.77
2:E:9[B]:VAL:CG1	2:E:80:CYS:HB2	2.17	0.74
1:D:111:ARG:HD2	1:D:113:TYR:OH	1.88	0.73
1:D:188:HIS:HD2	5:D:508:HOH:O	1.73	0.72
1:A:8:PHE:CZ	4:A:302:GOL:H12	2.27	0.70
2:E:9[B]:VAL:HG11	2:E:80:CYS:CB	2.24	0.68
1:A:75:ARG:HG3	5:A:493:HOH:O	1.96	0.65
1:D:248[B]:VAL:CG2	1:D:248[B]:VAL:O	2.42	0.65
1:D:44[A]:ARG:HH11	1:D:44[A]:ARG:HG3	1.61	0.65
2:E:52:SER:HA	4:E:102:GOL:C3	2.22	0.65
2:E:17:ASN:OD1	2:E:97[B]:ARG:NH2	2.30	0.63
1:A:111:ARG:NH2	5:A:509:HOH:O	2.32	0.62
1:A:34[B]:VAL:HG11	1:A:45:MET:SD	2.40	0.60
1:A:95[A]:VAL:HG11	1:A:116:TYR:OH	2.02	0.59
2:E:9[B]:VAL:CG1	2:E:80:CYS:CB	2.81	0.57
1:A:8:PHE:HZ	4:A:302:GOL:H12	1.67	0.56
1:A:214[B]:THR:OG1	1:A:262:GLN:HB2	2.06	0.55
1:D:95[A]:VAL:HG11	1:D:116:TYR:OH	2.06	0.55
1:D:190:THR:HG21	2:E:98[A]:ASP:OD1	2.07	0.55
1:A:34[B]:VAL:HG13	1:A:45:MET:SD	2.46	0.54
1:A:111:ARG:HD2	1:A:113:TYR:OH	2.07	0.54
1:D:192:HIS:CE1	2:E:98[B]:ASP:O	2.61	0.53
1:D:192:HIS:NE2	2:E:98[B]:ASP:O	2.42	0.53
2:E:13:HIS:HD2	5:E:221:HOH:O	1.93	0.52
1:A:6[B]:ARG:HG3	5:A:470:HOH:O	2.09	0.52
4:D:304:GOL:H31	5:D:538:HOH:O	2.12	0.50
1:A:108[B]:ARG:CG	1:A:108[B]:ARG:NH1	2.52	0.50
1:D:111:ARG:HD3	5:D:550:HOH:O	2.12	0.50
1:D:111:ARG:NH2	4:D:303:GOL:H31	2.27	0.50
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.48	0.48
2:E:96:ASP:CG	2:E:99[B]:MET:HG3	2.34	0.48
1:D:111:ARG:NE	4:D:302:GOL:H31	2.30	0.47
1:D:55[A]:GLU:HG3	1:D:59:TYR:CG	2.49	0.47
2:E:98[A]:ASP:OD1	5:E:257:HOH:O	2.20	0.47
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.49	0.47
1:D:202:ARG:HD2	2:E:99[B]:MET:OXT	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6[B]:ARG:NH1	1:A:102:ASP:OD1	2.46	0.46
1:D:170:ARG:HD2	4:D:305:GOL:O1	2.15	0.46
1:D:244:TRP:CZ2	2:E:99[B]:MET:HE1	2.52	0.45
1:A:34[B]:VAL:CG1	1:A:35:ARG:N	2.79	0.45
1:A:95[A]:VAL:CG1	1:A:116:TYR:OH	2.64	0.44
1:A:6[A]:ARG:HD2	1:A:98:MET:SD	2.58	0.44
2:B:55[B]:SER:HB2	2:B:63:TYR:CZ	2.53	0.43
1:A:10[B]:THR:HG21	2:B:54:LEU:CD2	2.39	0.43
1:D:116:TYR:CZ	3:F:9:LPH:H1	2.53	0.43
4:D:304:GOL:C3	5:D:538:HOH:O	2.67	0.43
1:D:141:GLN:OE1	1:D:144[A]:LYS:HE3	2.19	0.43
1:A:10[B]:THR:HG22	1:A:23[B]:ILE:HB	2.01	0.42
1:D:95[A]:VAL:CG1	1:D:116:TYR:OH	2.66	0.42
1:A:189[B]:MET:CE	1:A:201:LEU:HD22	2.49	0.42
1:D:65[B]:ARG:NH2	5:D:403:HOH:O	2.36	0.41
4:E:102:GOL:C1	5:E:256:HOH:O	2.68	0.41
2:E:97[B]:ARG:HG3	2:E:98[B]:ASP:N	2.34	0.41
1:D:95[A]:VAL:HG13	1:D:116:TYR:CZ	2.55	0.41
2:E:24:ASN:HB3	2:E:65:LEU:HD11	2.02	0.41
1:A:110[A]:LEU:HG	1:A:111:ARG:NH1	2.36	0.41
1:D:98:MET:CE	1:D:115:GLN:HG2	2.51	0.41
1:A:146:LYS:NZ	3:C:8:THR:OG1	2.54	0.41
2:B:24:ASN:HB3	2:B:65:LEU:HD11	2.03	0.41
1:D:6:ARG:HD2	1:D:98:MET:SD	2.61	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	297/275 (108%)	293 (99%)	4 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	296/275 (108%)	292 (99%)	4 (1%)	0	100	100
2	B	103/100 (103%)	102 (99%)	1 (1%)	0	100	100
2	E	108/100 (108%)	107 (99%)	1 (1%)	0	100	100
3	C	7/10 (70%)	7 (100%)	0	0	100	100
3	F	8/10 (80%)	8 (100%)	0	0	100	100
All	All	819/770 (106%)	809 (99%)	10 (1%)	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	255/231 (110%)	250 (98%)	5 (2%)	55	32
1	D	254/231 (110%)	250 (98%)	4 (2%)	62	41
2	B	100/95 (105%)	99 (99%)	1 (1%)	76	62
2	E	107/95 (113%)	104 (97%)	3 (3%)	43	18
3	C	4/4 (100%)	4 (100%)	0	100	100
3	F	5/4 (125%)	4 (80%)	1 (20%)	1	0
All	All	725/660 (110%)	711 (98%)	14 (2%)	60	34

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108[A]	ARG
1	A	108[B]	ARG
1	A	115	GLN
1	A	223	ASP
1	A	225	THR
2	B	70	PHE
1	D	55[A]	GLU
1	D	55[B]	GLU

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Mol	Chain	Res	Type
1	D	223	ASP
1	D	225	THR
2	E	0[A]	MET
2	E	0[B]	MET
2	E	70	PHE
3	F	7	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	HIS
1	D	188	HIS
2	E	13	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 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	$\# Z  > 2$
3	NVA	C	1[A]	3	5,6,7	0.77	0	2,6,8	0.67	0
3	NVA	F	1	3	5,6,7	2.79	1 (20%)	2,6,8	1.90	1 (50%)
3	NVA	C	1[B]	3	5,6,7	1.50	1 (20%)	2,6,8	0.74	0
3	LPH	F	9	3	3,7,7	1.96	1 (33%)	2,8,8	0.67	0
3	LPH	C	9	3	3,7,7	2.34	2 (66%)	2,8,8	1.13	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
3	NVA	C	1[A]	3	1/1/1/2	3/4/5/7	-
3	NVA	F	1	3	-	1/4/5/7	-
3	NVA	C	1[B]	3	1/1/1/2	2/4/5/7	-
3	LPH	F	9	3	-	0/2/7/7	-
3	LPH	C	9	3	-	0/2/7/7	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	NVA	CB-CA	-5.94	1.45	1.53
3	C	9	LPH	CG-CD	3.28	1.27	1.18
3	F	9	LPH	CG-CD	3.20	1.27	1.18
3	C	1[B]	NVA	CB-CA	-3.07	1.49	1.53
3	C	9	LPH	CA-N	-2.37	1.41	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	NVA	CD-CG-CB	-2.50	101.23	113.29

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	1[A]	NVA	CA
3	C	1[B]	NVA	CA

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1[A]	NVA	O-C-CA-CB
3	C	1[B]	NVA	C-CA-CB-CG
3	C	1[A]	NVA	CA-CB-CG-CD
3	C	1[A]	NVA	C-CA-CB-CG
3	C	1[B]	NVA	CA-CB-CG-CD
3	F	1	NVA	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	9	LPH	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

13 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	B	101	-	5,5,5	0.37	0	5,5,5	0.34	0
4	GOL	E	101	-	5,5,5	0.28	0	5,5,5	0.46	0
4	GOL	D	301	-	5,5,5	0.36	0	5,5,5	0.23	0
4	GOL	D	305	-	5,5,5	0.26	0	5,5,5	0.32	0
4	GOL	B	102	-	5,5,5	0.45	0	5,5,5	0.28	0
4	GOL	D	302	-	5,5,5	0.43	0	5,5,5	0.69	0
4	GOL	D	306	-	5,5,5	0.28	0	5,5,5	0.33	0
4	GOL	E	103	-	5,5,5	0.38	0	5,5,5	0.53	0
4	GOL	D	304	-	5,5,5	0.25	0	5,5,5	0.31	0
4	GOL	D	303	-	5,5,5	0.34	0	5,5,5	0.48	0
4	GOL	A	302	-	5,5,5	0.29	0	5,5,5	0.98	0
4	GOL	E	102	-	5,5,5	0.30	0	5,5,5	0.69	0
4	GOL	A	301	-	5,5,5	0.44	0	5,5,5	0.56	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	B	101	-	-	2/4/4/4	-
4	GOL	E	101	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	D	301	-	-	0/4/4/4	-
4	GOL	D	305	-	-	0/4/4/4	-
4	GOL	B	102	-	-	2/4/4/4	-
4	GOL	D	302	-	-	4/4/4/4	-
4	GOL	D	306	-	-	2/4/4/4	-
4	GOL	E	103	-	-	2/4/4/4	-
4	GOL	D	304	-	-	0/4/4/4	-
4	GOL	D	303	-	-	4/4/4/4	-
4	GOL	A	302	-	-	2/4/4/4	-
4	GOL	E	102	-	-	4/4/4/4	-
4	GOL	A	301	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	101	GOL	C1-C2-C3-O3
4	E	101	GOL	O1-C1-C2-C3
4	B	102	GOL	C1-C2-C3-O3
4	D	302	GOL	O1-C1-C2-O2
4	D	302	GOL	O1-C1-C2-C3
4	E	103	GOL	C1-C2-C3-O3
4	D	303	GOL	O1-C1-C2-C3
4	D	302	GOL	C1-C2-C3-O3
4	D	306	GOL	C1-C2-C3-O3
4	E	102	GOL	O1-C1-C2-C3
4	E	102	GOL	C1-C2-C3-O3
4	B	101	GOL	O2-C2-C3-O3
4	E	101	GOL	O1-C1-C2-O2
4	D	306	GOL	O2-C2-C3-O3
4	E	103	GOL	O2-C2-C3-O3
4	D	303	GOL	O1-C1-C2-O2
4	B	102	GOL	O2-C2-C3-O3
4	D	302	GOL	O2-C2-C3-O3
4	E	102	GOL	O2-C2-C3-O3
4	D	303	GOL	C1-C2-C3-O3
4	D	303	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	A	302	GOL	O2-C2-C3-O3
4	A	302	GOL	C1-C2-C3-O3
4	E	102	GOL	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	305	GOL	1	0
4	D	302	GOL	1	0
4	D	304	GOL	2	0
4	D	303	GOL	1	0
4	A	302	GOL	2	0
4	E	102	GOL	3	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 ⓘ

### 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	275/275 (100%)	0.43	14 (5%) 28 27	13, 24, 44, 56	0
1	D	275/275 (100%)	0.49	17 (6%) 20 19	15, 26, 48, 65	0
2	B	100/100 (100%)	0.34	4 (4%) 38 38	14, 24, 43, 50	0
2	E	100/100 (100%)	0.32	4 (4%) 38 38	16, 24, 41, 47	0
3	C	7/10 (70%)	0.36	0 100 100	20, 26, 29, 34	0
3	F	7/10 (70%)	0.23	0 100 100	22, 26, 31, 32	0
All	All	764/770 (99%)	0.42	39 (5%) 28 27	13, 25, 44, 65	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	196	ASP	6.6
1	D	195	SER	5.9
1	A	196	ASP	5.9
1	A	136	ALA	5.6
1	D	194	VAL	5.3
1	D	86	ASN	4.0
1	A	226	GLN	3.6
1	D	17	ARG	3.5
1	D	136	ALA	3.5
1	D	192	HIS	3.5
1	A	54	GLN	3.4
1	D	54	GLN	3.3
1	D	16	GLY	3.2
1	D	18	GLY	3.1
1	D	95[A]	VAL	3.0
2	E	48	LYS	2.9
1	A	197[A]	HIS	2.9
1	A	195	SER	2.9
1	D	225	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	217	TRP	2.6
1	A	192[A]	HIS	2.6
2	B	89	GLN	2.6
1	A	34[A]	VAL	2.5
1	D	50[A]	PRO	2.5
1	D	41	ALA	2.5
1	A	268	LYS	2.5
2	E	75	LYS	2.5
2	B	48	LYS	2.4
2	B	23	LEU	2.4
2	E	74	GLU	2.4
1	A	225	THR	2.3
2	B	98[A]	ASP	2.3
1	A	75	ARG	2.2
1	A	223	ASP	2.2
1	D	19	GLU	2.2
2	E	58	LYS	2.2
1	A	86	ASN	2.2
1	A	16	GLY	2.2
1	D	249	VAL	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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(Å <sup>2</sup> )	Q<0.9
3	LPH	F	9	8/8	0.86	0.13	22,25,28,29	0
3	LPH	C	9	8/8	0.91	0.10	21,24,29,30	0
3	NVA	C	1[A]	7/8	0.93	0.12	10,11,13,13	7
3	NVA	C	1[B]	7/8	0.93	0.12	7,7,9,9	7
3	NVA	F	1	7/8	0.94	0.14	9,10,11,11	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. 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(Å <sup>2</sup> )	Q<0.9
4	GOL	D	301	6/6	0.73	0.16	52,57,57,62	0
4	GOL	D	304	6/6	0.77	0.16	37,48,50,54	0
4	GOL	D	305	6/6	0.78	0.21	41,55,62,67	0
4	GOL	A	302	6/6	0.79	0.18	27,34,45,45	0
4	GOL	B	102	6/6	0.81	0.23	39,45,46,50	0
4	GOL	B	101	6/6	0.81	0.18	28,35,39,52	0
4	GOL	E	101	6/6	0.81	0.31	34,46,54,68	0
4	GOL	E	103	6/6	0.83	0.20	20,40,51,51	0
4	GOL	A	301	6/6	0.83	0.18	28,36,40,41	0
4	GOL	D	302	6/6	0.85	0.24	38,47,49,51	0
4	GOL	D	303	6/6	0.85	0.16	31,42,46,66	0
4	GOL	D	306	6/6	0.86	0.12	45,58,59,61	0
4	GOL	E	102	6/6	0.91	0.35	31,36,41,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.