



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 09:13 pm BST

PDB ID : 3PGC  
Title : Crystal Structure of HLA-DR1 with CLIP106-120, flipped peptide orientation  
Authors : Gunther, S.; Schlundt, A.; Sticht, J.; Roske, Y.; Heinemann, U.; Wiesmuller, K.-H.; Jung, G.; Falk, K.; Rotzschke, O.; Freund, C.  
Deposited on : 2010-11-01  
Resolution : 2.66 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

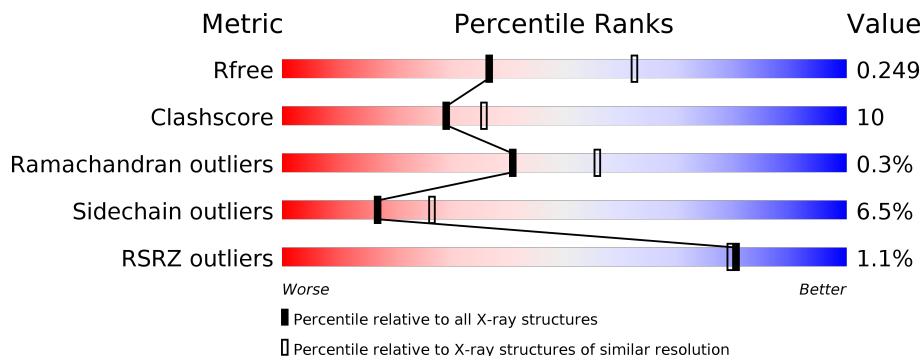
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.66 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	193	
1	D	193	
2	B	199	
2	E	199	
3	C	15	
3	F	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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
5	GOL	D	194	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6180 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 II histocompatibility antigen, DR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	177	Total	C	N	O	S	0	0	0
			1442	937	233	267	5			
1	D	178	Total	C	N	O	S	0	0	0
			1464	949	238	272	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP P01903
D	0	MET	-	EXPRESSION TAG	UNP P01903

- Molecule 2 is a protein called HLA class II histocompatibility antigen, DRB1-1 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	184	Total	C	N	O	S	0	0	0
			1471	928	257	280	6			
2	E	180	Total	C	N	O	S	0	0	0
			1443	913	253	271	6			

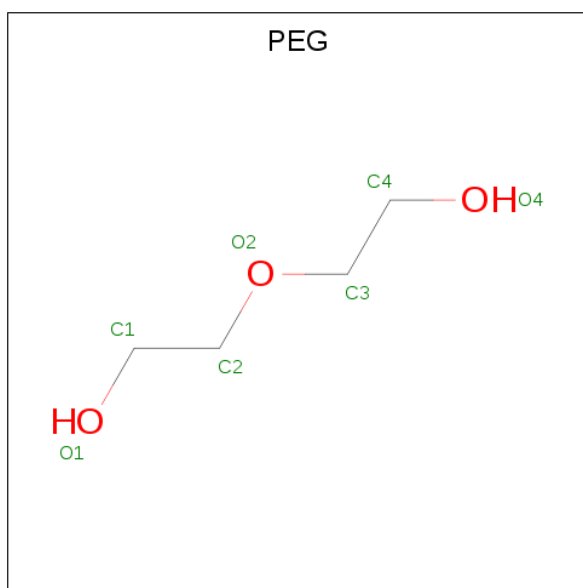
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	EXPRESSION TAG	UNP P04229
E	0	MET	-	EXPRESSION TAG	UNP P04229

- Molecule 3 is a protein called HLA class II histocompatibility antigen gamma chain.

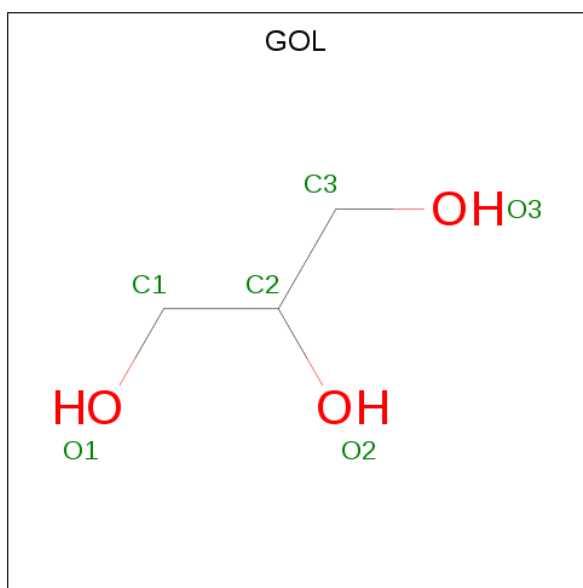
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	15	Total	C	N	O	S	0	0	0
			116	75	20	17	4			
3	F	15	Total	C	N	O	S	0	0	0
			116	75	20	17	4			

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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


- Molecule 6 is water.

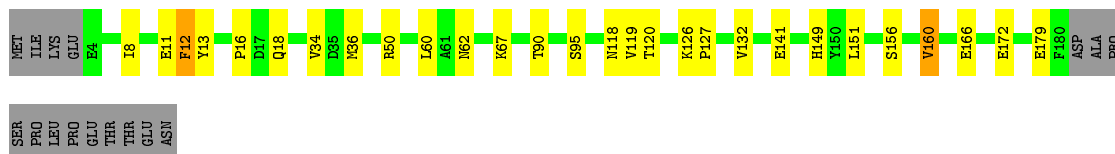
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
6	A	39	Total 39	O 39	0	0
6	B	29	Total 29	O 29	0	0
6	C	1	Total 1	O 1	0	0
6	D	19	Total 19	O 19	0	0
6	E	24	Total 24	O 24	0	0
6	F	3	Total 3	O 3	0	0

### 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.

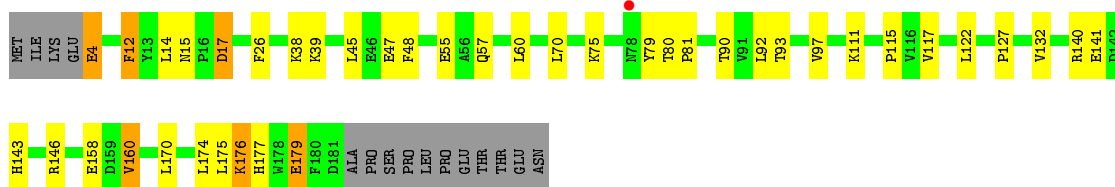
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain

Chain A: 



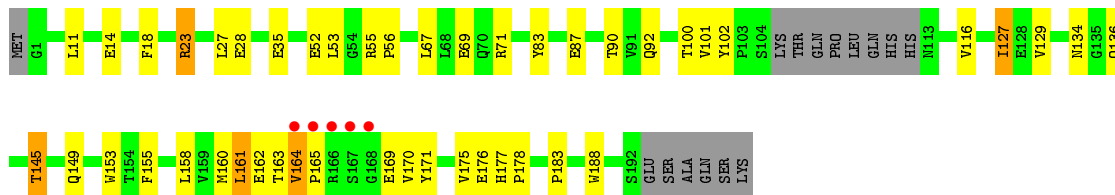
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain

Chain D: 



- Molecule 2: HLA class II histocompatibility antigen, DRB1-1 beta chain

Chain B: 



- Molecule 2: HLA class II histocompatibility antigen, DRB1-1 beta chain

Chain E: 





- Molecule 3: HLA class II histocompatibility antigen gamma chain

Chain C: 67% 27% 7%



- Molecule 3: HLA class II histocompatibility antigen gamma chain

Chain F: 73% 27%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.15Å 138.15Å 104.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.54 – 2.66 34.54 – 2.66	Depositor EDS
% Data completeness (in resolution range)	100.0 (34.54-2.66) 100.0 (34.54-2.66)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.14 (at 2.65Å)	Xtrriage
Refinement program	PHENIX 1.5_2	Depositor
R, $R_{free}$	0.198 , 0.250 0.193 , 0.249	Depositor DCC
$R_{free}$ test set	1670 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.9	Xtrriage
Anisotropy	0.197	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 34.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6180	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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	0.46	0/1487	0.60	0/2031
1	D	0.45	0/1509	0.56	0/2058
2	B	0.46	0/1507	0.58	0/2050
2	E	0.43	0/1479	0.55	0/2013
3	C	0.46	0/117	0.65	0/155
3	F	0.41	0/117	0.65	0/155
All	All	0.45	0/6216	0.58	0/8462

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	1442	0	1371	13	1
1	D	1464	0	1401	32	0
2	B	1471	0	1379	30	0
2	E	1443	0	1353	44	0
3	C	116	0	133	3	0
3	F	116	0	133	3	0
4	D	7	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	6	0	8	5	0
6	A	39	0	0	2	0
6	B	29	0	0	3	0
6	C	1	0	0	0	0
6	D	19	0	0	1	0
6	E	24	0	0	1	0
6	F	3	0	0	0	0
All	All	6180	0	5788	114	1

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 10.

All (114) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:LYS:HG2	1:D:60:LEU:HD11	1.30	1.14
2:E:170:VAL:HG21	2:E:189:ARG:HH21	1.44	0.82
2:E:103:PRO:HG3	2:E:188:TRP:CZ2	2.19	0.77
2:B:161:LEU:HD12	2:B:162:GLU:N	2.02	0.75
1:D:79:TYR:O	1:D:81:PRO:HD3	1.90	0.72
2:B:92:GLN:HG2	6:B:219:HOH:O	1.90	0.70
1:D:14:LEU:HD22	1:D:115:PRO:HD2	1.71	0.70
2:E:149:GLN:HG3	2:E:155:PHE:CE2	2.28	0.68
1:A:8:ILE:HG12	2:B:14:GLU:HG2	1.77	0.66
1:D:160:VAL:HG22	1:D:177:HIS:CE1	2.32	0.65
2:B:149:GLN:HG3	2:B:155:PHE:CE2	2.32	0.64
2:B:127:ILE:HG13	2:B:177:HIS:CD2	2.32	0.64
2:E:81:HIS:CD2	3:F:114:LEU:HD22	2.33	0.64
2:E:116:VAL:HG22	2:E:160:MET:HG3	1.80	0.63
1:A:160:VAL:HG22	1:A:179:GLU:HB3	1.80	0.63
1:D:47:GLU:HB3	5:D:194:GOL:H12	1.82	0.62
1:A:132:VAL:HG12	1:A:151:LEU:HD13	1.80	0.62
1:D:12:PHE:C	1:D:12:PHE:CD1	2.73	0.61
2:B:162:GLU:O	2:B:163:THR:HG23	2.01	0.60
1:D:39:LYS:HG2	1:D:60:LEU:CD1	2.20	0.59
2:E:34:GLN:HG2	2:E:34:GLN:O	2.04	0.57
2:E:145:THR:CG2	2:E:158:LEU:H	2.18	0.57
6:A:203:HOH:O	3:C:108:ARG:HG3	2.05	0.57
1:D:90:THR:HG22	6:D:209:HOH:O	2.04	0.57
1:D:70:LEU:HD13	2:E:9:TRP:HB2	1.86	0.56
2:E:9:TRP:CH2	2:E:30:CYS:HB3	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:127:ILE:HG13	2:B:177:HIS:HD2	1.69	0.56
2:E:57:ASP:OD1	3:F:107:MET:HG3	2.06	0.55
1:D:17:ASP:N	1:D:17:ASP:OD1	2.40	0.55
2:B:55:ARG:HB3	2:B:56:PRO:HD3	1.90	0.54
2:E:18:PHE:N	2:E:18:PHE:CD1	2.76	0.54
2:B:145:THR:CG2	2:B:158:LEU:H	2.21	0.54
2:E:189:ARG:NH1	6:E:217:HOH:O	2.42	0.52
1:D:15:ASN:O	2:E:6:ARG:HD2	2.09	0.52
2:E:60:TYR:O	2:E:63:SER:HB3	2.09	0.52
1:D:12:PHE:C	1:D:12:PHE:HD1	2.11	0.52
2:B:83:TYR:O	2:B:87:GLU:HB2	2.10	0.52
2:E:114:LEU:HD22	2:E:160:MET:HB3	1.92	0.52
2:B:90:THR:HG22	2:B:153:TRP:CH2	2.46	0.51
2:B:161:LEU:HD12	2:B:162:GLU:H	1.75	0.51
2:E:11:LEU:HD11	2:E:13:PHE:CE2	2.46	0.51
1:A:118:ASN:HB3	1:A:166:GLU:HB2	1.93	0.51
2:B:165:PRO:HB3	2:B:171:TYR:HE2	1.76	0.50
1:A:12:PHE:CD1	1:A:12:PHE:C	2.85	0.50
6:B:225:HOH:O	2:E:139:LYS:HD3	2.12	0.50
2:B:129:VAL:HG22	2:B:175:VAL:HG22	1.94	0.50
1:D:4:GLU:OE1	2:E:18:PHE:CE2	2.65	0.50
1:D:160:VAL:CG2	1:D:177:HIS:CE1	2.96	0.49
2:B:165:PRO:HB3	2:B:171:TYR:CE2	2.49	0.48
2:E:145:THR:HG21	2:E:158:LEU:H	1.79	0.48
1:A:13:TYR:CZ	1:A:67:LYS:HD2	2.49	0.48
1:D:4:GLU:HA	2:E:17:PHE:O	2.13	0.48
2:B:116:VAL:HG22	2:B:160:MET:HG3	1.95	0.47
2:B:28:GLU:OE1	2:B:71:ARG:NE	2.36	0.47
2:B:136:GLN:HA	6:B:222:HOH:O	2.15	0.47
2:B:52:GLU:OE2	2:B:55:ARG:NE	2.48	0.47
2:B:134:ASN:HD21	2:B:169:GLU:HG2	1.79	0.46
1:D:48:PHE:N	1:D:48:PHE:CD1	2.84	0.46
2:E:161:LEU:HG	2:E:163:THR:HG23	1.98	0.46
2:E:170:VAL:HG21	2:E:189:ARG:NH2	2.22	0.46
2:B:177:HIS:CD2	2:B:178:PRO:HD2	2.51	0.46
2:B:176:GLU:HG2	2:B:183:PRO:HG3	1.98	0.45
1:A:16:PRO:O	1:A:18:GLN:HG3	2.17	0.45
1:A:160:VAL:CG2	1:A:179:GLU:HB3	2.45	0.45
1:D:47:GLU:CB	5:D:194:GOL:H12	2.45	0.45
1:A:11:GLU:OE1	1:A:62:ASN:HB3	2.16	0.45
2:E:55:ARG:N	2:E:56:PRO:CD	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:PHE:HB2	2:B:23:ARG:HB2	1.99	0.44
1:D:45:LEU:HD13	5:D:194:GOL:H32	1.99	0.44
1:D:170:LEU:HD13	1:D:174:LEU:HB2	1.98	0.44
2:E:174:GLN:HG3	2:E:185:THR:HG22	2.00	0.44
1:D:45:LEU:HD22	5:D:194:GOL:H32	2.00	0.44
2:B:53:LEU:HA	2:B:53:LEU:HD23	1.75	0.44
2:E:4:ARG:HA	2:E:5:PRO:HD3	1.85	0.43
2:B:69:GLU:OE1	2:E:141:GLY:N	2.51	0.43
1:D:111:LYS:HG2	1:D:140:ARG:CZ	2.49	0.43
1:D:38:LYS:HB3	1:D:38:LYS:HE2	1.87	0.43
1:D:93:THR:HG21	1:D:97:VAL:CG2	2.49	0.43
2:E:164:VAL:O	2:E:164:VAL:HG23	2.18	0.43
2:E:87:GLU:OE1	2:E:92:GLN:NE2	2.51	0.43
2:E:10:GLN:HB2	2:E:31:ILE:HB	2.01	0.43
1:D:75:LYS:HE3	1:D:75:LYS:HB2	1.74	0.42
2:E:145:THR:HG23	2:E:146:GLY:O	2.19	0.42
1:A:34:VAL:O	1:A:36:MET:HE2	2.19	0.42
1:D:176:LYS:HA	1:D:176:LYS:HD2	1.61	0.42
2:E:115:LEU:HA	2:E:115:LEU:HD12	1.91	0.42
3:F:118:LEU:HA	3:F:119:PRO:HD3	1.92	0.42
1:D:26:PHE:CE2	2:E:90:THR:HB	2.55	0.42
2:E:90:THR:OG1	2:E:91:VAL:N	2.53	0.42
1:D:55:GLU:OE2	1:D:57:GLN:HG3	2.20	0.42
2:E:145:THR:HG22	2:E:158:LEU:H	1.85	0.41
2:E:144:SER:OG	2:E:145:THR:N	2.53	0.41
1:A:126:LYS:HA	1:A:127:PRO:HD3	1.88	0.41
1:D:45:LEU:HD13	5:D:194:GOL:H11	2.02	0.41
1:A:18:GLN:NE2	6:A:216:HOH:O	2.53	0.41
1:D:143:HIS:CE1	2:E:31:ILE:HD11	2.55	0.41
1:D:177:HIS:NE2	1:D:179:GLU:HG2	2.35	0.41
2:E:40:PHE:HB2	2:E:47:TYR:CE1	2.55	0.41
2:E:74:ALA:O	2:E:78:TYR:HB3	2.21	0.41
2:B:14:GLU:HB2	2:B:27:LEU:HB3	2.03	0.41
3:C:118:LEU:HD23	3:C:118:LEU:HA	1.86	0.41
2:E:96:GLU:HA	2:E:97:PRO:HD3	1.95	0.41
2:B:101:VAL:HG12	2:B:102:TYR:N	2.35	0.41
2:B:27:LEU:HD12	2:B:27:LEU:HA	1.85	0.41
3:C:118:LEU:HA	3:C:119:PRO:HD2	1.85	0.41
2:E:177:HIS:CD2	2:E:178:PRO:HD2	2.55	0.41
1:A:119:VAL:HG11	1:A:149:HIS:CG	2.55	0.41
2:B:188:TRP:O	2:B:188:TRP:HE3	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:103:PRO:HG3	2:E:188:TRP:HZ2	1.81	0.40
2:B:164:VAL:HA	2:B:165:PRO:HD3	1.70	0.40
1:D:81:PRO:HA	2:E:7:PHE:CE2	2.56	0.40
1:D:122:LEU:HD23	1:D:127:PRO:HA	2.04	0.40
2:E:117:CYS:HB2	2:E:131:TRP:CZ2	2.57	0.40
2:E:170:VAL:CG2	2:E:189:ARG:HH21	2.24	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:GLN:OE1	1:A:18:GLN:OE1[6_555]	2.11	0.09

## 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	175/193 (91%)	167 (95%)	8 (5%)	0	100	100
1	D	176/193 (91%)	165 (94%)	10 (6%)	1 (1%)	25	37
2	B	180/199 (90%)	170 (94%)	10 (6%)	0	100	100
2	E	176/199 (88%)	169 (96%)	7 (4%)	0	100	100
3	C	13/15 (87%)	12 (92%)	0	1 (8%)	1	0
3	F	13/15 (87%)	13 (100%)	0	0	100	100
All	All	733/814 (90%)	696 (95%)	35 (5%)	2 (0%)	41	56

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	80	THR
3	C	119	PRO

### 5.3.2 Protein sidechains [i](#)

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	159/177 (90%)	149 (94%)	10 (6%)	18	28
1	D	163/177 (92%)	150 (92%)	13 (8%)	12	18
2	B	158/179 (88%)	148 (94%)	10 (6%)	18	28
2	E	155/179 (87%)	147 (95%)	8 (5%)	23	36
3	C	13/13 (100%)	11 (85%)	2 (15%)	2	3
3	F	13/13 (100%)	13 (100%)	0	100	100
All	All	661/738 (90%)	618 (94%)	43 (6%)	17	26

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	PHE
1	A	50	ARG
1	A	60	LEU
1	A	90	THR
1	A	95	SER
1	A	120	THR
1	A	141	GLU
1	A	156	SER
1	A	160	VAL
1	A	172	GLU
2	B	11	LEU
2	B	23	ARG
2	B	35	GLU
2	B	67	LEU
2	B	100	THR
2	B	127	ILE
2	B	145	THR
2	B	161	LEU
2	B	164	VAL
2	B	170	VAL
3	C	106	LYS
3	C	107	MET

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Mol	Chain	Res	Type
1	D	4	GLU
1	D	12	PHE
1	D	17	ASP
1	D	92	LEU
1	D	117	VAL
1	D	132	VAL
1	D	141	GLU
1	D	146	ARG
1	D	158	GLU
1	D	160	VAL
1	D	175	LEU
1	D	176	LYS
1	D	179	GLU
2	E	18	PHE
2	E	23	ARG
2	E	63	SER
2	E	66	ASP
2	E	88	SER
2	E	100	THR
2	E	138	GLU
2	E	189	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	HIS
2	B	81	HIS
2	B	156	GLN
1	D	149	HIS
2	E	92	GLN
2	E	156	GLN

### 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](#)

2 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
5	GOL	D	194	-	5,5,5	0.56	0	5,5,5	0.33	0
4	PEG	D	193	-	6,6,6	0.53	0	5,5,5	1.59	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
5	GOL	D	194	-	-	2/4/4/4	-
4	PEG	D	193	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	194	GOL	O1-C1-C2-O2
5	D	194	GOL	O1-C1-C2-C3
4	D	193	PEG	O1-C1-C2-O2
4	D	193	PEG	C1-C2-O2-C3
4	D	193	PEG	C4-C3-O2-C2

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	194	GOL	5	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, 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	177/193 (91%)	-0.66	0 <b>100</b>   <b>100</b>	31, 44, 61, 74	0
1	D	178/193 (92%)	-0.52	1 (0%) <b>89</b>   <b>89</b>	32, 54, 77, 96	0
2	B	184/199 (92%)	-0.36	5 (2%) 54   50	33, 51, 85, 112	0
2	E	180/199 (90%)	-0.43	2 (1%) <b>80</b>   <b>79</b>	32, 56, 89, 104	0
3	C	15/15 (100%)	-0.48	0 <b>100</b>   <b>100</b>	40, 44, 87, 100	0
3	F	15/15 (100%)	-0.44	0 <b>100</b>   <b>100</b>	32, 41, 70, 87	0
All	All	749/814 (92%)	-0.49	8 (1%) <b>80</b>   <b>79</b>	31, 50, 83, 112	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	167	SER	3.4
2	B	165	PRO	3.3
2	B	168	GLY	2.8
2	B	166	ARG	2.6
1	D	78	ASN	2.4
2	B	164	VAL	2.3
2	E	113	ASN	2.1
2	E	134	ASN	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. 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
5	GOL	D	194	6/6	0.86	0.36	47,53,57,57	0
4	PEG	D	193	7/7	0.86	0.17	62,74,81,83	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.