



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 04:59 AM GMT

PDB ID : 3S4S
Title : Crystal structure of CD4 mutant bound to HLA-DR1
Authors : Li, Y.
Deposited on : 2011-05-20
Resolution : 2.40 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

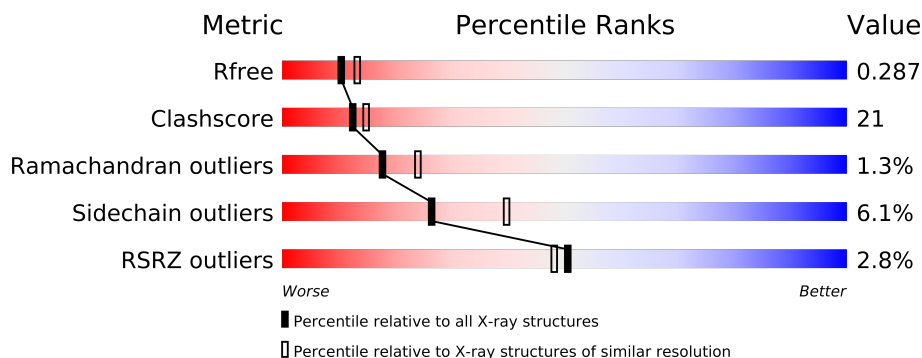
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.40 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}	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	182	
1	D	182	
2	B	193	
2	E	193	
3	C	13	
3	F	13	
4	G	191	
4	H	191	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	GOL	E	961	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8924 atoms, of which 0 are hydrogen and 0 are deuterium.

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
1	A	178	Total	C	N	O	S	0	0	0
			1464	949	237	273	5			
1	D	180	Total	C	N	O	S	0	0	0
			1472	953	239	275	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	177	GLN	HIS	CONFLICT	UNP P01903
D	177	GLN	HIS	CONFLICT	UNP P01903

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	186	Total	C	N	O	S	0	0	0
			1507	947	268	285	7			
2	E	185	Total	C	N	O	S	0	0	0
			1505	947	267	284	7			

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 Hemagglutinin peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	13	Total	C	N	O	0	0	0
			105	69	18	18			
3	F	13	Total	C	N	O	0	0	0
			103	68	18	17			

- Molecule 4 is a protein called T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	176	Total	C	N	O	S	0	0	0
			1354	852	236	262	4			
4	H	175	Total	C	N	O	S	0	0	0
			1328	833	233	258	4			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-3	ASP	-	EXPRESSION TAG	UNP P01730
G	-2	LEU	-	EXPRESSION TAG	UNP P01730
G	-1	GLY	-	EXPRESSION TAG	UNP P01730
G	0	SER	-	EXPRESSION TAG	UNP P01730
G	40	TYR	GLN	CONFLICT	UNP P01730
G	45	TRP	THR	CONFLICT	UNP P01730
G	179	ALA	-	EXPRESSION TAG	UNP P01730
G	180	ALA	-	EXPRESSION TAG	UNP P01730
G	181	ALA	-	EXPRESSION TAG	UNP P01730
G	182	HIS	-	EXPRESSION TAG	UNP P01730
G	183	HIS	-	EXPRESSION TAG	UNP P01730
G	184	HIS	-	EXPRESSION TAG	UNP P01730
G	185	HIS	-	EXPRESSION TAG	UNP P01730
G	186	HIS	-	EXPRESSION TAG	UNP P01730
G	187	HIS	-	EXPRESSION TAG	UNP P01730
H	-3	ASP	-	EXPRESSION TAG	UNP P01730
H	-2	LEU	-	EXPRESSION TAG	UNP P01730
H	-1	GLY	-	EXPRESSION TAG	UNP P01730
H	0	SER	-	EXPRESSION TAG	UNP P01730
H	40	TYR	GLN	CONFLICT	UNP P01730
H	45	TRP	THR	CONFLICT	UNP P01730
H	179	ALA	-	EXPRESSION TAG	UNP P01730
H	180	ALA	-	EXPRESSION TAG	UNP P01730
H	181	ALA	-	EXPRESSION TAG	UNP P01730
H	182	HIS	-	EXPRESSION TAG	UNP P01730
H	183	HIS	-	EXPRESSION TAG	UNP P01730
H	184	HIS	-	EXPRESSION TAG	UNP P01730
H	185	HIS	-	EXPRESSION TAG	UNP P01730
H	186	HIS	-	EXPRESSION TAG	UNP P01730
H	187	HIS	-	EXPRESSION TAG	UNP P01730

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 6 is water.

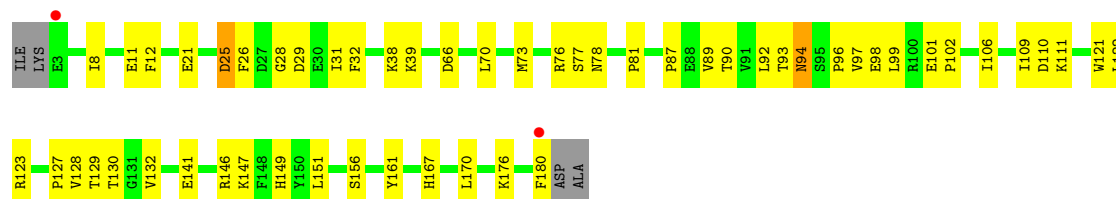
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	16	Total	O	0	0
			16	16		
6	B	15	Total	O	0	0
			15	15		
6	G	1	Total	O	0	0
			1	1		
6	D	14	Total	O	0	0
			14	14		
6	E	19	Total	O	0	0
			19	19		
6	H	3	Total	O	0	0
			3	3		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

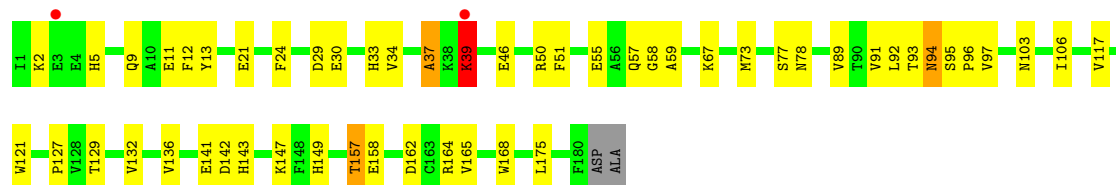
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain

Chain A: 



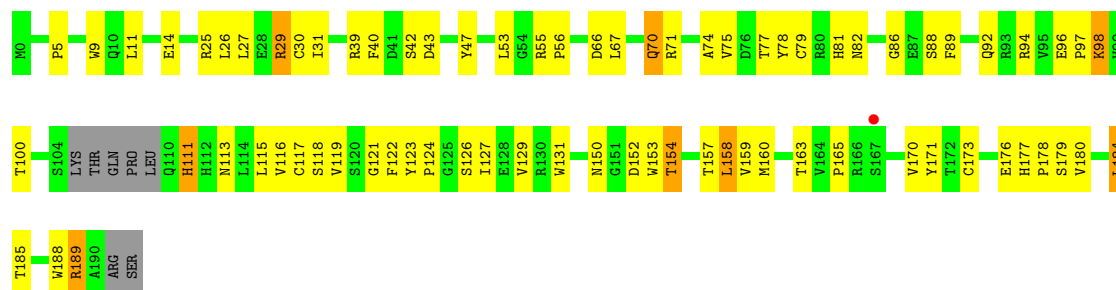
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain

Chain D: 



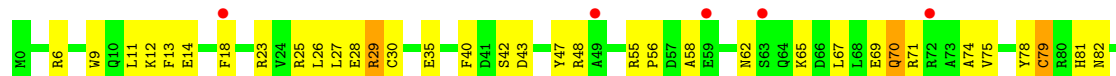
- Molecule 2: HLA class II histocompatibility antigen, DRB1-1 beta chain

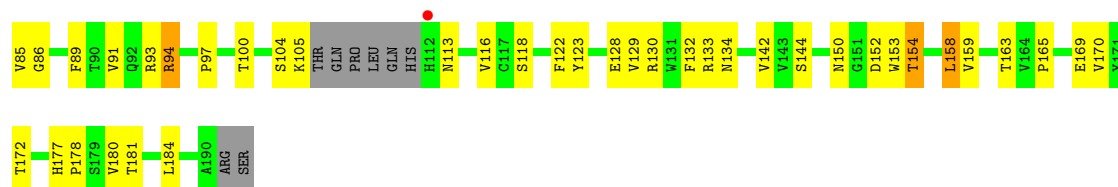
Chain B: 



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

Chain E: 





- Molecule 3: Hemagglutinin peptide

Chain C:



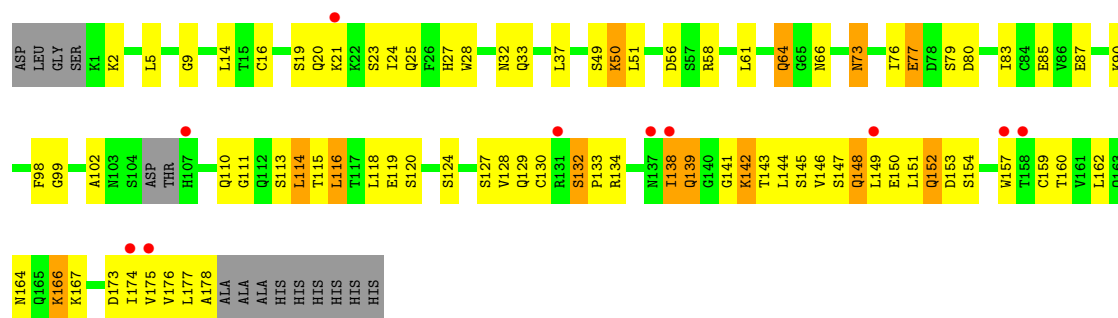
- Molecule 3: Hemagglutinin peptide

Chain F:



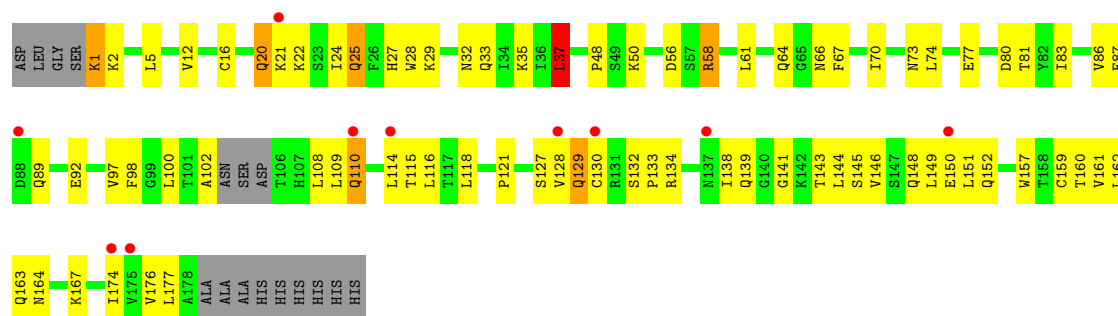
- Molecule 4: T-cell surface glycoprotein CD4

Chain G:



- Molecule 4: T-cell surface glycoprotein CD4

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.26Å 137.29Å 88.29Å 90.00° 106.64° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 46.98 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.40) 99.2 (46.98-2.39)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.251 , 0.286 0.254 , 0.287	Depositor DCC
R_{free} test set	3011 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	37.7	Xtriage
Anisotropy	0.733	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 31.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 60314 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8924	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

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	0/1508	0.69	0/2056
1	D	0.44	0/1516	0.67	0/2066
2	B	0.42	0/1543	0.66	0/2092
2	E	0.41	0/1541	0.65	0/2091
3	C	0.43	0/106	0.69	0/141
3	F	0.38	0/104	0.62	0/138
4	G	0.35	0/1374	0.63	0/1854
4	H	0.33	0/1348	0.60	1/1816 (0.1%)
All	All	0.41	0/9040	0.65	1/12254 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	37	LEU	CA-CB-CG	5.07	126.97	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1464	0	1404	37	0
1	D	1472	0	1409	39	0
2	B	1507	0	1431	65	0
2	E	1505	0	1432	66	0
3	C	105	0	119	12	0
3	F	103	0	114	14	0
4	G	1354	0	1360	84	0
4	H	1328	0	1317	83	0
5	B	6	0	8	2	0
5	D	6	0	8	1	0
5	E	6	0	8	1	0
6	A	16	0	0	1	0
6	B	15	0	0	0	0
6	D	14	0	0	0	0
6	E	19	0	0	0	0
6	G	1	0	0	0	0
6	H	3	0	0	0	0
All	All	8924	0	8610	369	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 21.

The worst 5 of 369 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:H:102:ALA:HB2	4:H:116:LEU:HD23	1.43	1.00
4:H:1:LYS:HG3	4:H:2:LYS:H	1.24	0.99
3:F:4:LYS:HE2	3:F:4:LYS:H	1.27	0.99
1:A:96:PRO:HG3	2:B:100:THR:HG21	1.43	0.98
4:G:50:LYS:H	4:G:50:LYS:HD2	1.28	0.97

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	176/182 (97%)	166 (94%)	10 (6%)	0	100	100
1	D	178/182 (98%)	166 (93%)	7 (4%)	5 (3%)	8	6
2	B	182/193 (94%)	168 (92%)	12 (7%)	2 (1%)	21	29
2	E	181/193 (94%)	164 (91%)	16 (9%)	1 (1%)	33	47
3	C	11/13 (85%)	11 (100%)	0	0	100	100
3	F	11/13 (85%)	11 (100%)	0	0	100	100
4	G	172/191 (90%)	153 (89%)	17 (10%)	2 (1%)	19	26
4	H	171/191 (90%)	148 (86%)	19 (11%)	4 (2%)	10	10
All	All	1082/1158 (93%)	987 (91%)	81 (8%)	14 (1%)	18	24

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	2	LYS
4	H	148	GLN
4	H	149	LEU
4	G	148	GLN
2	B	79	CYS

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	163/166 (98%)	155 (95%)	8 (5%)	35	53
1	D	163/166 (98%)	157 (96%)	6 (4%)	45	66
2	B	164/174 (94%)	154 (94%)	10 (6%)	26	40
2	E	164/174 (94%)	155 (94%)	9 (6%)	30	46
3	C	12/12 (100%)	11 (92%)	1 (8%)	16	24
3	F	11/12 (92%)	9 (82%)	2 (18%)	2	3
4	G	152/170 (89%)	135 (89%)	17 (11%)	9	12
4	H	147/170 (86%)	140 (95%)	7 (5%)	35	53
All	All	976/1044 (94%)	916 (94%)	60 (6%)	26	40

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	G	73	ASN
4	G	142	LYS
4	H	25	GLN
4	G	116	LEU
4	G	166	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
4	G	129	GLN
1	D	5	HIS
4	H	73	ASN
4	G	148	GLN
1	D	33	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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
5	GOL	B	960	-	5,5,5	0.16	0	5,5,5	0.21	0
5	GOL	D	962	-	5,5,5	0.22	0	5,5,5	0.32	0
5	GOL	E	961	-	5,5,5	0.40	0	5,5,5	0.29	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	B	960	-	-	0/4/4/4	0/0/0/0
5	GOL	D	962	-	-	0/4/4/4	0/0/0/0
5	GOL	E	961	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

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, 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	178/182 (97%)	0.11	2 (1%) 77 77	19, 32, 54, 62	0
1	D	180/182 (98%)	0.20	2 (1%) 77 77	24, 37, 63, 74	0
2	B	186/193 (96%)	0.08	1 (0%) 88 88	21, 38, 59, 70	0
2	E	185/193 (95%)	0.28	6 (3%) 45 43	24, 42, 71, 79	0
3	C	13/13 (100%)	0.12	0 100 100	37, 42, 48, 50	0
3	F	13/13 (100%)	0.36	0 100 100	48, 55, 62, 63	0
4	G	176/191 (92%)	0.54	10 (5%) 23 21	30, 57, 81, 88	0
4	H	175/191 (91%)	0.59	10 (5%) 23 21	30, 61, 81, 85	0
All	All	1106/1158 (95%)	0.30	31 (2%) 50 48	19, 43, 75, 88	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	150	GLU	5.0
4	G	138	ILE	4.0
4	H	137	ASN	3.9
4	H	130	CYS	3.6
4	G	137	ASN	3.2

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	GOL	E	961	6/6	0.24	4.70	51,52,55,56	0
5	GOL	D	962	6/6	0.20	2.00	41,44,46,47	0
5	GOL	B	960	6/6	0.19	-0.00	63,63,64,66	0

6.5 Other polymers

There are no such residues in this entry.