



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 12:49 am BST

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 X-ray Structure Validation Summary 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 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

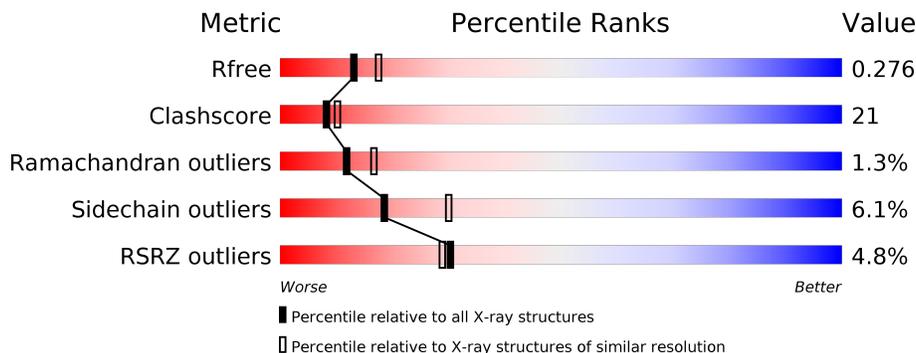
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 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	182	
1	D	182	
2	B	193	
2	E	193	
3	C	13	
3	F	13	

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Mol	Chain	Length	Quality of chain
4	G	191	
4	H	191	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8924 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	178	1464	949	237	273	5	0	0	0
1	D	180	1472	953	239	275	5	0	0	0

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
			Total	C	N	O	S			
2	B	186	1507	947	268	285	7	0	0	0
2	E	185	1505	947	267	284	7	0	0	0

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
			Total	C	N	O			
3	C	13	105	69	18	18	0	0	0
3	F	13	103	68	18	17	0	0	0

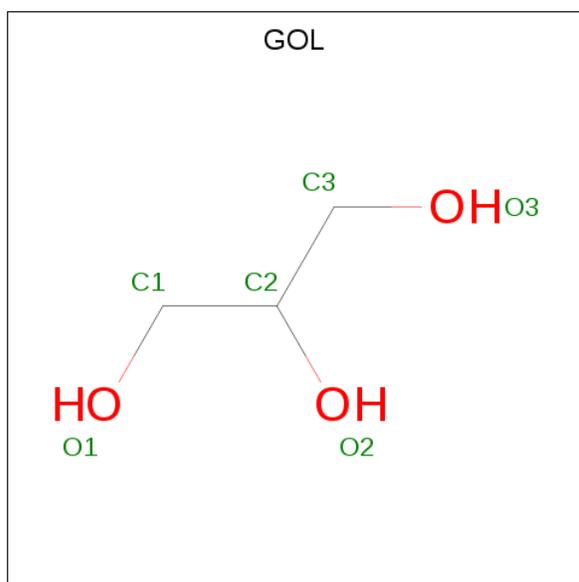
- Molecule 4 is a protein called T-cell surface glycoprotein CD4.

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

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 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0

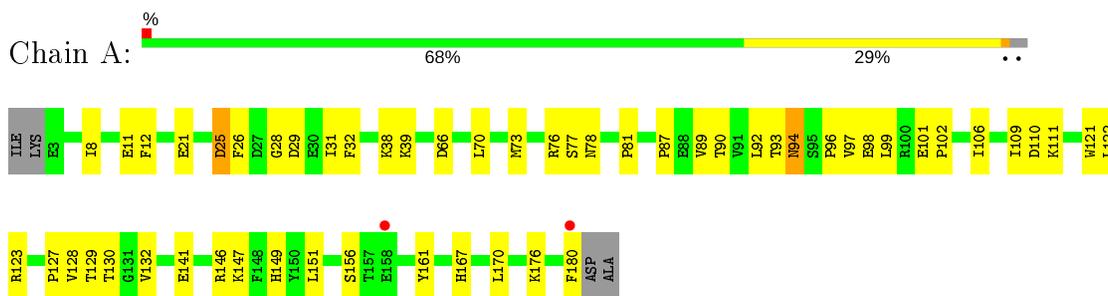
- Molecule 6 is water.

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

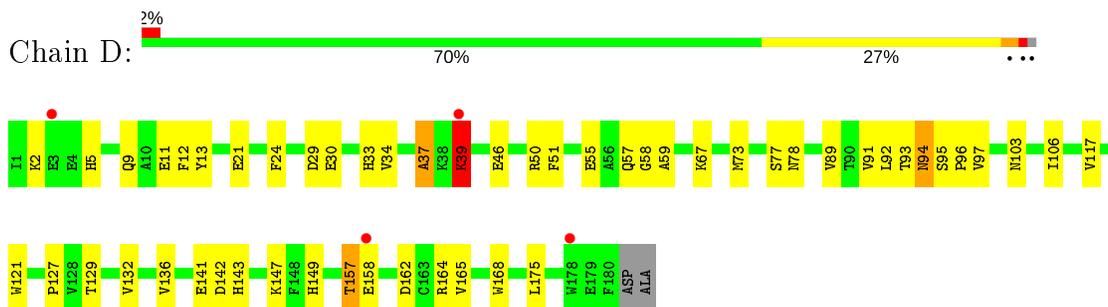
3 Residue-property plots [i](#)

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.

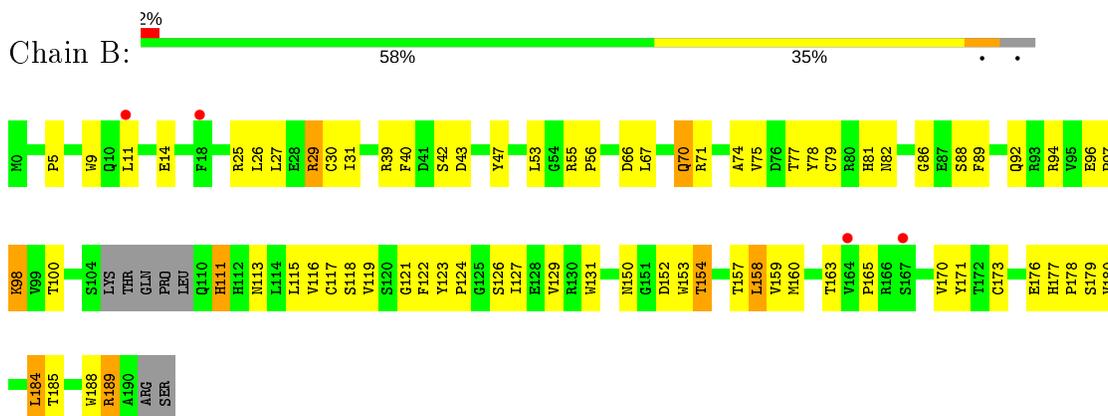
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain



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

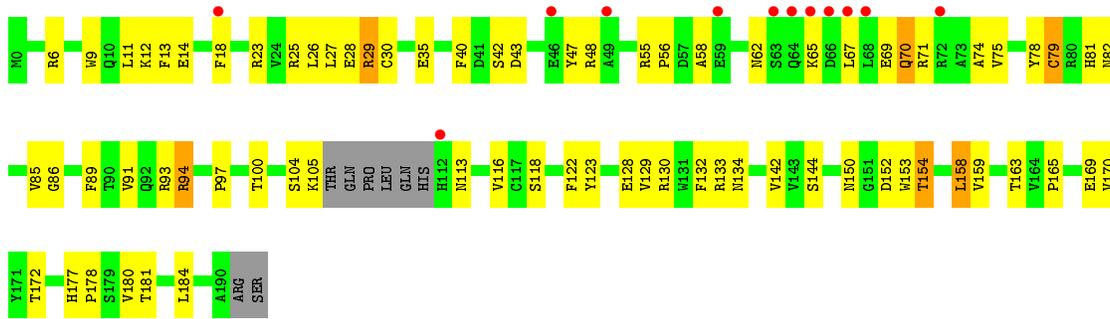


- Molecule 2: HLA class II histocompatibility antigen, DRB1-1 beta chain



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





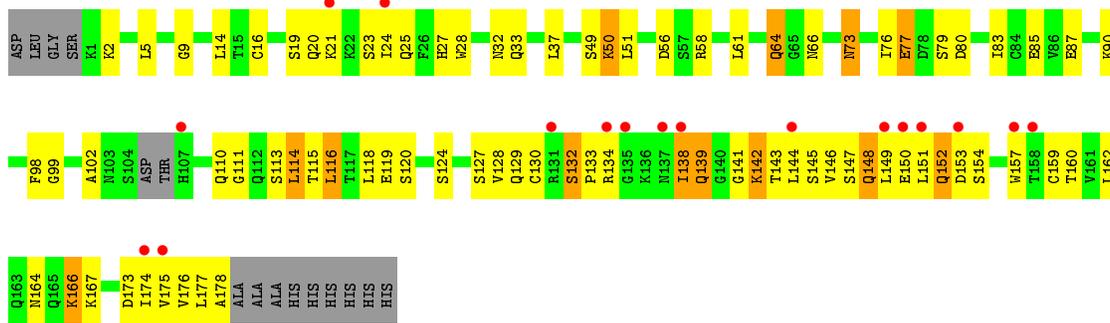
• Molecule 3: Hemagglutinin peptide



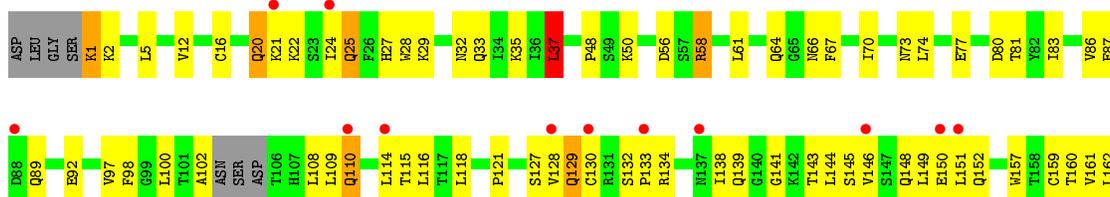
• Molecule 3: Hemagglutinin peptide



• Molecule 4: T-cell surface glycoprotein CD4



• Molecule 4: T-cell surface glycoprotein CD4



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)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.251 , 0.286 0.243 , 0.276	Depositor DCC
R_{free} test set	3011 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	37.7	Xtrriage
Anisotropy	0.733	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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.

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

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($^{\circ}$)	Ideal($^{\circ}$)
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 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	1464	0	1404	37	0
1	D	1472	0	1409	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 21.

The worst 5 of 369 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)
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 [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	176/182 (97%)	166 (94%)	10 (6%)	0	100	100
1	D	178/182 (98%)	166 (93%)	7 (4%)	5 (3%)	5	4
2	B	182/193 (94%)	168 (92%)	12 (7%)	2 (1%)	14	20
2	E	181/193 (94%)	164 (91%)	16 (9%)	1 (1%)	25	36
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%)	13	19
4	H	171/191 (90%)	148 (86%)	19 (11%)	4 (2%)	6	7
All	All	1082/1158 (93%)	987 (91%)	81 (8%)	14 (1%)	12	17

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 [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	163/166 (98%)	155 (95%)	8 (5%)	25	40
1	D	163/166 (98%)	157 (96%)	6 (4%)	34	53
2	B	164/174 (94%)	154 (94%)	10 (6%)	18	30
2	E	164/174 (94%)	155 (94%)	9 (6%)	21	35
3	C	12/12 (100%)	11 (92%)	1 (8%)	11	17
3	F	11/12 (92%)	9 (82%)	2 (18%)	1	2
4	G	152/170 (89%)	135 (89%)	17 (11%)	6	8
4	H	147/170 (86%)	140 (95%)	7 (5%)	25	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	976/1044 (94%)	916 (94%)	60 (6%)	18 30

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 [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](#)

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	0.21	0	5,5,5	0.22	0
5	GOL	E	961	-	5,5,5	0.49	0	5,5,5	0.27	0
5	GOL	D	962	-	5,5,5	0.31	0	5,5,5	0.31	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	-
5	GOL	E	961	-	-	0/4/4/4	-
5	GOL	D	962	-	-	0/4/4/4	-

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.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	960	GOL	2	0
5	E	961	GOL	1	0
5	D	962	GOL	1	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, 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%)	0.27	2 (1%) 80 79	19, 32, 54, 62	0
1	D	180/182 (98%)	0.34	4 (2%) 62 60	24, 37, 63, 74	0
2	B	186/193 (96%)	0.22	4 (2%) 62 60	21, 38, 59, 70	0
2	E	185/193 (95%)	0.47	12 (6%) 18 17	24, 42, 71, 79	0
3	C	13/13 (100%)	0.23	0 100 100	37, 42, 48, 50	0
3	F	13/13 (100%)	0.35	0 100 100	48, 55, 62, 63	0
4	G	176/191 (92%)	0.68	17 (9%) 7 7	30, 57, 81, 88	0
4	H	175/191 (91%)	0.71	14 (8%) 12 11	30, 61, 81, 85	0
All	All	1106/1158 (95%)	0.44	53 (4%) 30 29	19, 43, 75, 88	0

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	150	GLU	7.1
4	G	150	GLU	3.9
2	E	18	PHE	3.6
4	G	138	ILE	3.6
4	G	137	ASN	3.6

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, 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	GOL	E	961	6/6	0.80	0.25	51,52,55,56	0
5	GOL	B	960	6/6	0.87	0.20	63,63,64,66	0
5	GOL	D	962	6/6	0.90	0.22	41,44,46,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.