wwPDB X-ray Structure Validation Summary Report (i)

Jun 24, 2024 – 04:18 PM EDT

PDB ID	:	5O14
Title	:	Co-crystal structure of a cross-reactive bactericidal human antibody targeting meningococcal vaccine antigen factor H binding protein
Authors	:	Lopez-Sagaseta, J.
Deposited on	:	2017-05-18
Resolution	:	2.19 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 (i) 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 (1)) were used in the production of this report:

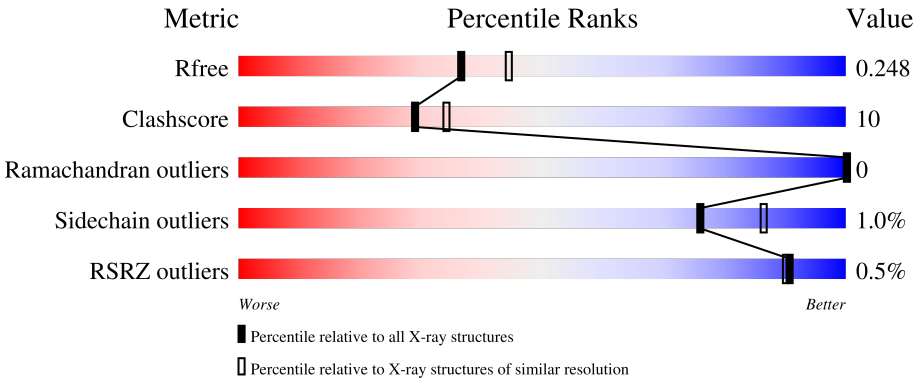
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	257	72% 16% 11%
1	B	257	% 75% 15% 10%
2	C	235	80% 14% 5%
2	H	235	% 81% 12% 6%
3	D	217	79% 20%

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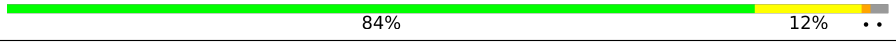
Mol	Chain	Length	Quality of chain
3	L	217	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10877 atoms, of which 24 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 Factor H binding protein variant 1.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	1	0
			1695	1056	302	336	1			
1	B	231	Total	C	N	O	S	0	0	0
			1690	1052	299	338	1			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	initiating methionine	UNP Q9JXV4
A	256	LEU	-	expression tag	UNP Q9JXV4
A	257	GLU	-	expression tag	UNP Q9JXV4
A	258	HIS	-	expression tag	UNP Q9JXV4
A	259	HIS	-	expression tag	UNP Q9JXV4
A	260	HIS	-	expression tag	UNP Q9JXV4
A	261	HIS	-	expression tag	UNP Q9JXV4
A	262	HIS	-	expression tag	UNP Q9JXV4
A	263	HIS	-	expression tag	UNP Q9JXV4
B	7	MET	-	initiating methionine	UNP Q9JXV4
B	256	LEU	-	expression tag	UNP Q9JXV4
B	257	GLU	-	expression tag	UNP Q9JXV4
B	258	HIS	-	expression tag	UNP Q9JXV4
B	259	HIS	-	expression tag	UNP Q9JXV4
B	260	HIS	-	expression tag	UNP Q9JXV4
B	261	HIS	-	expression tag	UNP Q9JXV4
B	262	HIS	-	expression tag	UNP Q9JXV4
B	263	HIS	-	expression tag	UNP Q9JXV4

- Molecule 2 is a protein called Fab 1A12 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	223	Total	C	N	O	S	0	0	0
			1666	1059	275	326	6			

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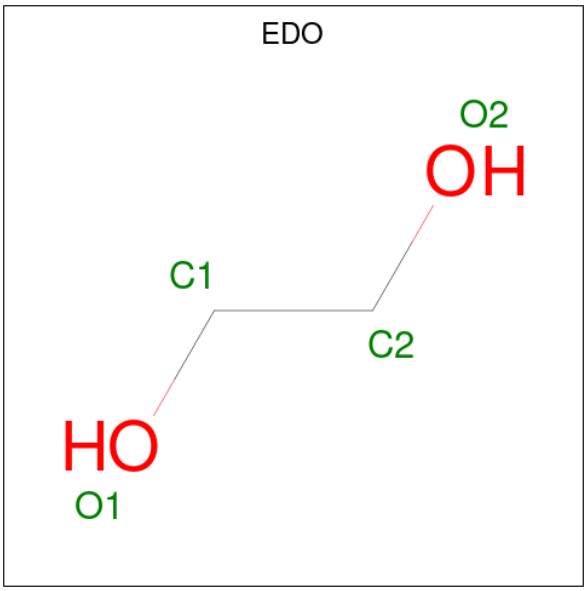
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	221	Total	C	N	O	S	0	0	0
			1644	1045	271	322	6			

- Molecule 3 is a protein called Fab 1A12 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	215	Total	C	N	O	S	0	0	0
			1622	1014	273	328	7			
3	L	212	Total	C	N	O	S	0	0	0
			1605	1004	267	328	6			

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total Cl 1 1	0	0

- Molecule 6 is water.

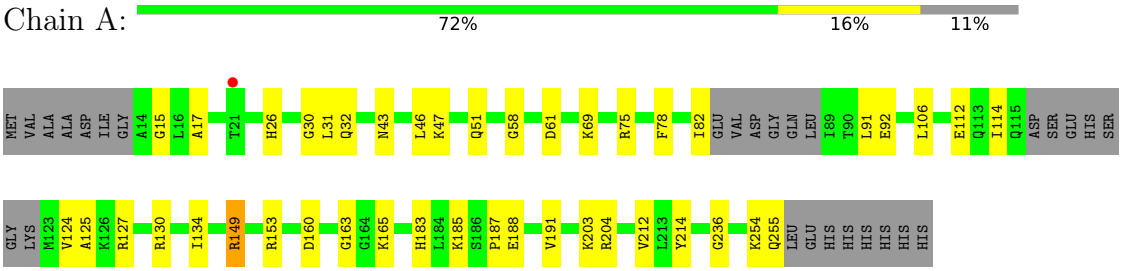
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	161	Total H O 165 4 161	0	0
6	B	126	Total O 126 126	0	0
6	C	186	Total H O 200 14 186	0	0
6	D	170	Total H O 172 2 170	0	0
6	L	131	Total H O 133 2 131	0	0
6	H	143	Total H O 145 2 143	0	0

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.

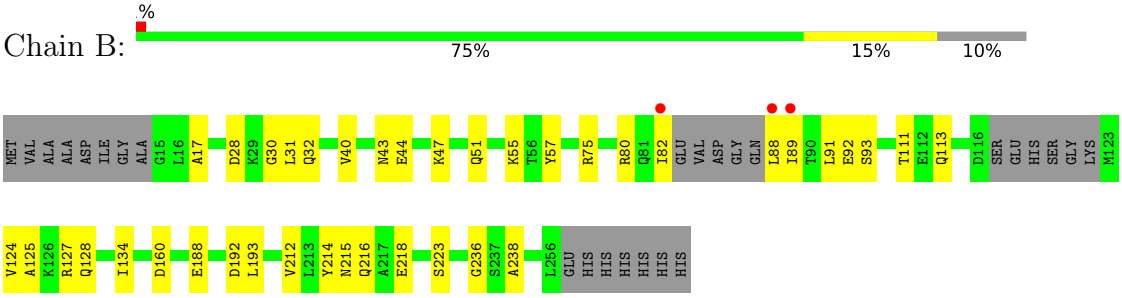
• Molecule 1: Factor H binding protein variant 1.1

Chain A:



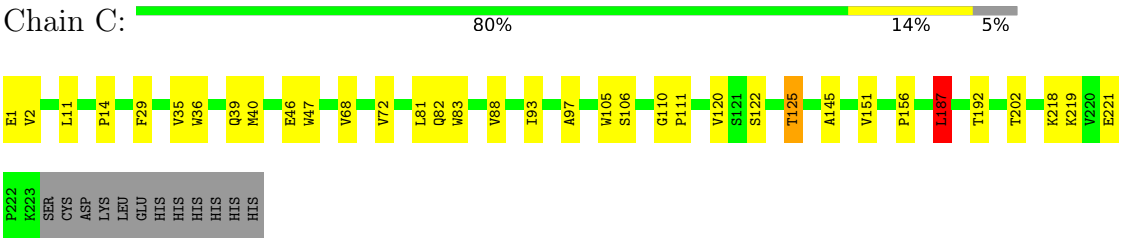
• Molecule 1: Factor H binding protein variant 1.1

Chain B:



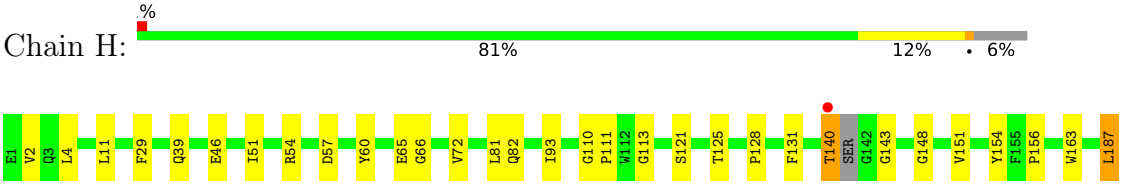
• Molecule 2: Fab 1A12 Heavy Chain

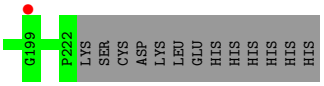
Chain C:



• Molecule 2: Fab 1A12 Heavy Chain

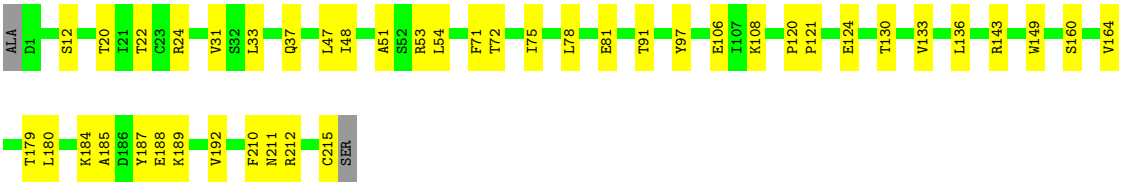
Chain H:





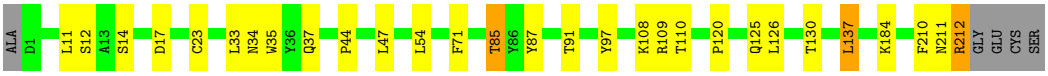
• Molecule 3: Fab 1A12 Light Chain

Chain D:



• Molecule 3: Fab 1A12 Light Chain

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	42.82Å 163.95Å 110.66Å 90.00° 97.70° 90.00°	Depositor
Resolution (Å)	48.91 – 2.19 48.91 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.3 (48.91-2.19) 96.4 (48.91-2.20)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.192 , 0.250 0.191 , 0.248	Depositor DCC
R_{free} test set	3601 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	26.6	Xtriage
Anisotropy	0.623	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 43.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10877	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.35	0/1719	0.51	0/2312
1	B	0.33	0/1711	0.52	0/2304
2	C	0.35	0/1713	0.52	1/2345 (0.0%)
2	H	0.33	0/1690	0.50	0/2315
3	D	0.35	0/1656	0.52	0/2253
3	L	0.34	0/1639	0.52	0/2231
All	All	0.34	0/10128	0.51	1/13760 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	187	LEU	CA-CB-CG	5.34	127.58	115.30

There are no chirality outliers.

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	1695	0	1659	41	0
1	B	1690	0	1624	40	0
2	C	1666	0	1599	31	0
2	H	1644	0	1568	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1622	0	1553	36	0
3	L	1605	0	1537	19	0
4	A	12	0	18	3	0
5	C	1	0	0	0	0
5	H	1	0	0	0	0
6	A	161	4	0	11	0
6	B	126	0	0	14	0
6	C	186	14	0	10	0
6	D	170	2	0	15	0
6	H	143	2	0	3	1
6	L	131	2	0	4	1
All	All	10853	24	9558	187	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.

The worst 5 of 187 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)
2:H:11:LEU:HD23	2:H:125:THR:HG22	1.46	0.97
1:B:80:ARG:NH1	1:B:92:GLU:OE1	2.08	0.86
3:L:109:ARG:NH1	3:L:110:THR:O	2.09	0.85
3:D:75:ILE:HG21	6:D:309:HOH:O	1.77	0.85
3:D:31:VAL:HG13	3:D:51:ALA:HB3	1.60	0.82

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)
6:L:382:HOH:O	6:H:403:HOH:O[1_655]	2.04	0.16

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	224/257 (87%)	218 (97%)	6 (3%)	0	100	100
1	B	225/257 (88%)	219 (97%)	6 (3%)	0	100	100
2	C	221/235 (94%)	215 (97%)	6 (3%)	0	100	100
2	H	217/235 (92%)	211 (97%)	6 (3%)	0	100	100
3	D	213/217 (98%)	205 (96%)	8 (4%)	0	100	100
3	L	210/217 (97%)	203 (97%)	7 (3%)	0	100	100
All	All	1310/1418 (92%)	1271 (97%)	39 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	169/200 (84%)	168 (99%)	1 (1%)	86	93
1	B	165/200 (82%)	165 (100%)	0	100	100
2	C	185/204 (91%)	182 (98%)	3 (2%)	62	76
2	H	182/204 (89%)	180 (99%)	2 (1%)	73	85
3	D	182/191 (95%)	181 (100%)	1 (0%)	88	94
3	L	182/191 (95%)	178 (98%)	4 (2%)	52	65
All	All	1065/1190 (90%)	1054 (99%)	11 (1%)	76	86

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	137	LEU
3	L	212	ARG
2	H	187	LEU
2	H	140	THR
3	D	215	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

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	EDO	A	303	-	3,3,3	0.47	0	2,2,2	0.27	0
4	EDO	A	301	-	3,3,3	0.51	0	2,2,2	0.17	0
4	EDO	A	302	-	3,3,3	0.52	0	2,2,2	0.41	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	EDO	A	303	-	-	0/1/1/1	-
4	EDO	A	301	-	-	0/1/1/1	-
4	EDO	A	302	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	302	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	303	EDO	2	0
4	A	301	EDO	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

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^{th} 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	229/257 (89%)	-0.24	1 (0%) 92 91	14, 25, 45, 62	0
1	B	231/257 (89%)	-0.05	3 (1%) 77 75	16, 32, 63, 81	0
2	C	223/235 (94%)	-0.23	0 100 100	15, 25, 39, 54	0
2	H	221/235 (94%)	-0.19	2 (0%) 84 83	15, 29, 53, 81	0
3	D	215/217 (99%)	-0.12	0 100 100	14, 25, 51, 62	0
3	L	212/217 (97%)	-0.22	0 100 100	16, 27, 46, 53	0
All	All	1331/1418 (93%)	-0.17	6 (0%) 91 90	14, 27, 50, 81	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	88	LEU	3.6
1	B	82	ILE	3.4
2	H	199	GLY	2.6
2	H	140	THR	2.3
1	B	89	ILE	2.3

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 monosaccharides 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^{th} 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
4	EDO	A	301	4/4	0.90	0.16	45,47,48,48	0
4	EDO	A	302	4/4	0.94	0.11	22,26,30,32	0
4	EDO	A	303	4/4	0.96	0.12	33,35,35,36	0
5	CL	C	301	1/1	0.99	0.09	30,30,30,30	0
5	CL	H	301	1/1	0.99	0.05	34,34,34,34	0

6.5 Other polymers (i)

There are no such residues in this entry.