Full wwPDB X-ray Structure Validation Report (i)

Oct 15, 2023 – 12:30 AM EDT

PDB ID	:	7ST5
Title	:	Structure of Fab CC-95251 in complex with SIRP-alpha
Authors	:	Fenalti, G.
Deposited on	:	2021-11-12
Resolution	:	2.20 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*
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:

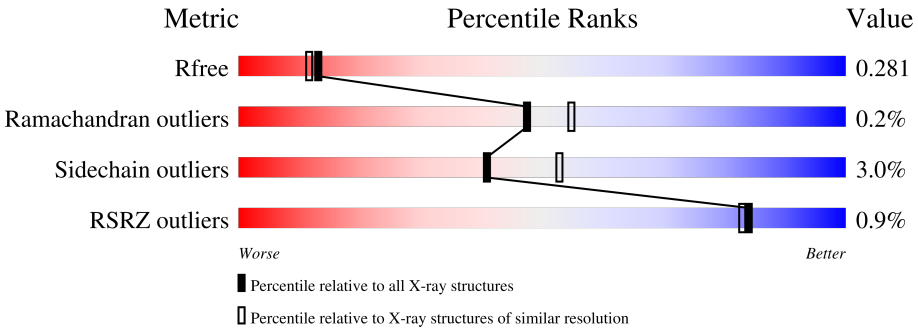
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.20 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)
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	H	227	87% · 9%
1	h	227	% 88% · 9%
2	L	214	94% 5% ·
2	l	214	95% · ·
3	A	125	3% 82% · 17%
3	F	125	2% 80% · 18%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7644 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 Fab CC-95251 anti-SIRP-alpha heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	206	Total	C	N	O	S	0	0	0
			1487	943	249	288	7			
1	h	206	Total	C	N	O	S	0	0	0
			1465	929	247	282	7			

- Molecule 2 is a protein called Fab CC-95251 anti-SIRP-alpha light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	211	Total	C	N	O	S	0	0	0
			1510	955	254	296	5			
2	l	211	Total	C	N	O	S	0	0	0
			1473	938	247	284	4			

- Molecule 3 is a protein called Tyrosine-protein phosphatase non-receptor type substrate 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	102	Total	C	N	O	S	0	0	0
			750	476	133	138	3			
3	A	104	Total	C	N	O	S	0	0	0
			761	482	137	139	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	120	SER	-	expression tag	UNP P78324
F	121	GLY	-	expression tag	UNP P78324
F	122	LEU	-	expression tag	UNP P78324
F	123	VAL	-	expression tag	UNP P78324
F	124	PRO	-	expression tag	UNP P78324
F	125	ARG	-	expression tag	UNP P78324
A	120	SER	-	expression tag	UNP P78324
A	121	GLY	-	expression tag	UNP P78324

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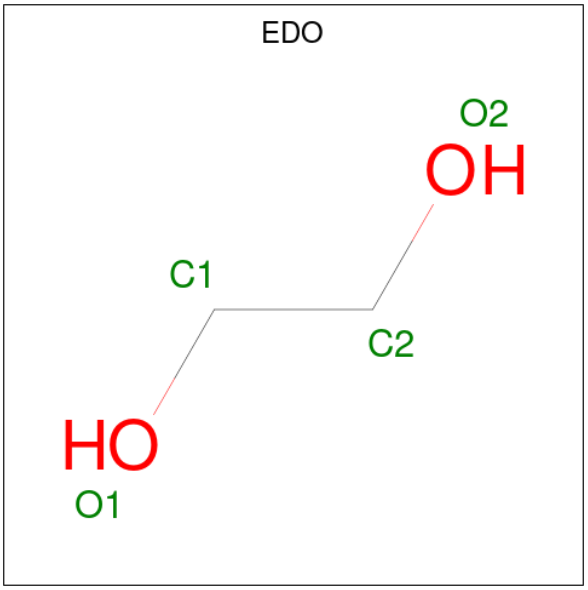
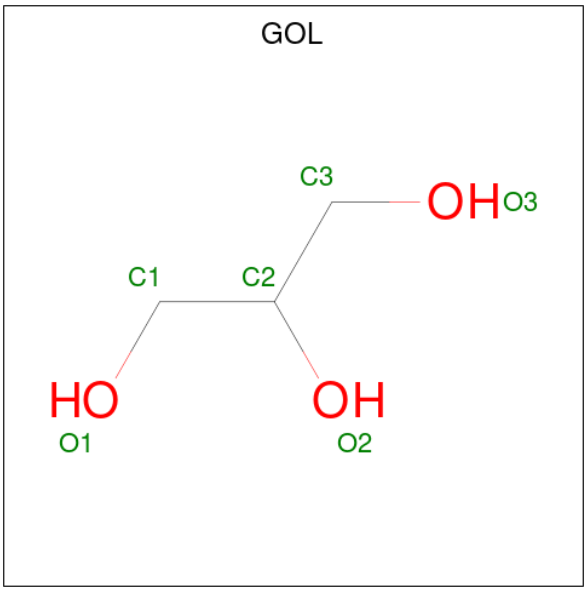
Chain	Residue	Modelled	Actual	Comment	Reference
A	122	LEU	-	expression tag	UNP P78324
A	123	VAL	-	expression tag	UNP P78324
A	124	PRO	-	expression tag	UNP P78324
A	125	ARG	-	expression tag	UNP P78324

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



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

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



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

- Molecule 6 is water.

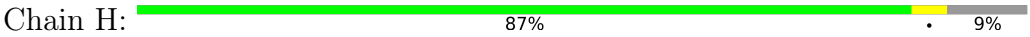
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	44	Total O 44 44	0	0
6	L	29	Total O 29 29	0	0
6	F	18	Total O 18 18	0	0
6	h	34	Total O 34 34	0	0
6	l	26	Total O 26 26	0	0
6	A	17	Total O 17 17	0	0

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.

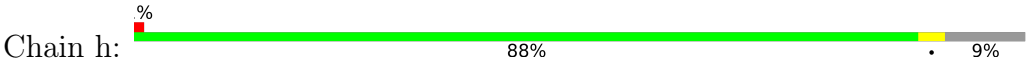
• Molecule 1: Fab CC-95251 anti-SIRP-alpha heavy chain

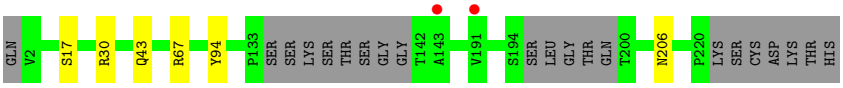
Chain H:



• Molecule 1: Fab CC-95251 anti-SIRP-alpha heavy chain

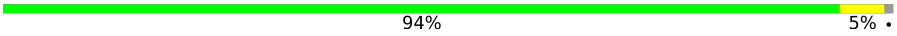
Chain h:





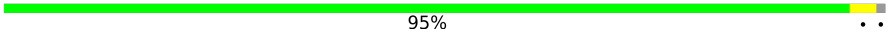
• Molecule 2: Fab CC-95251 anti-SIRP-alpha light chain

Chain L:



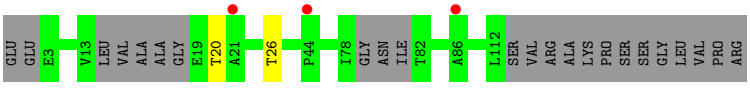
• Molecule 2: Fab CC-95251 anti-SIRP-alpha light chain

Chain l:



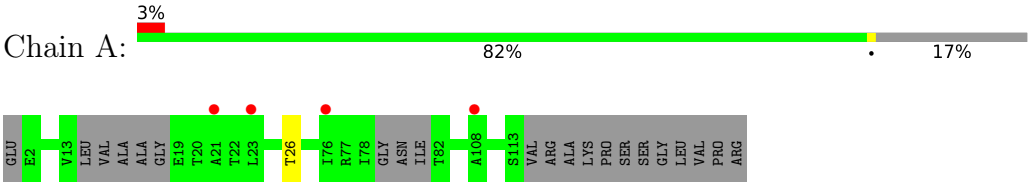
• Molecule 3: Tyrosine-protein phosphatase non-receptor type substrate 1

Chain F:



• Molecule 3: Tyrosine-protein phosphatase non-receptor type substrate 1

Chain A:


3%
82%
17%
GLU
E2
V13
LEU
VAL
ALA
ALA
GLY
E19
T20
A21
T22
L23
T26
I76
R77
I78
GLY
ASN
ILE
T82
A108
S113
VAL
ARG
ALA
LYS
PRO
SER
SER
GLY
LEU
VAL
PRO
ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	42.96Å 97.70Å 103.39Å 77.18° 85.92° 85.74°	Depositor
Resolution (Å)	50.01 – 2.20 49.12 – 2.20	Depositor EDS
% Data completeness (in resolution range)	88.2 (50.01-2.20) 88.2 (49.12-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.245 , 0.280 0.249 , 0.281	Depositor DCC
R_{free} test set	3601 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	37.3	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 34.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7644	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% 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: GOL, EDO

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	H	0.88	1/1522 (0.1%)	0.90	4/2081 (0.2%)
1	h	0.89	1/1500 (0.1%)	0.87	3/2050 (0.1%)
2	L	0.85	0/1545	0.89	4/2117 (0.2%)
2	l	0.82	0/1508	0.86	2/2070 (0.1%)
3	A	0.74	0/775	0.88	0/1049
3	F	0.73	0/765	0.88	0/1039
All	All	0.84	2/7615 (0.0%)	0.88	13/10406 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	h	94	TYR	CE1-CZ	-7.45	1.28	1.38
1	H	52	SER	CB-OG	5.04	1.48	1.42

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	67	ARG	NE-CZ-NH1	-8.59	116.00	120.30
1	h	67	ARG	NE-CZ-NH1	-7.65	116.47	120.30
1	H	67	ARG	NE-CZ-NH2	7.51	124.06	120.30
2	L	108	ARG	NE-CZ-NH2	7.33	123.97	120.30
2	L	185	ASP	CB-CG-OD1	7.20	124.78	118.30
1	h	67	ARG	NE-CZ-NH2	7.00	123.80	120.30
2	l	108	ARG	NE-CZ-NH2	6.96	123.78	120.30
2	L	108	ARG	NE-CZ-NH1	-6.13	117.23	120.30
1	h	30	ARG	NE-CZ-NH2	6.05	123.33	120.30
2	l	108	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	H	38	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	H	108	ASP	CB-CG-OD1	5.26	123.04	118.30
2	L	61	ARG	NE-CZ-NH1	5.14	122.87	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	H	200/227 (88%)	192 (96%)	8 (4%)	0	100	100
1	h	200/227 (88%)	191 (96%)	9 (4%)	0	100	100
2	L	209/214 (98%)	195 (93%)	13 (6%)	1 (0%)	29	31
2	l	209/214 (98%)	195 (93%)	13 (6%)	1 (0%)	29	31
3	A	98/125 (78%)	91 (93%)	7 (7%)	0	100	100
3	F	96/125 (77%)	90 (94%)	6 (6%)	0	100	100
All	All	1012/1132 (89%)	954 (94%)	56 (6%)	2 (0%)	47	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	l	204	PRO
2	L	204	PRO

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	H	144/189 (76%)	140 (97%)	4 (3%)	43	56
1	h	133/189 (70%)	130 (98%)	3 (2%)	50	63
2	L	146/184 (79%)	140 (96%)	6 (4%)	30	39
2	l	128/184 (70%)	123 (96%)	5 (4%)	32	41
3	A	72/104 (69%)	71 (99%)	1 (1%)	67	80
3	F	73/104 (70%)	71 (97%)	2 (3%)	44	57
All	All	696/954 (73%)	675 (97%)	21 (3%)	41	53

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	17	SER
1	H	43	GLN
1	H	88	SER
1	H	190	THR
2	L	30	SER
2	L	55	GLN
2	L	89	GLN
2	L	90	GLN
2	L	105	GLU
2	L	158	ASN
3	F	20	THR
3	F	26	THR
1	h	17	SER
1	h	43	GLN
1	h	206	ASN
2	l	30	SER
2	l	89	GLN
2	l	90	GLN
2	l	105	GLU
2	l	158	ASN
3	A	26	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	39	GLN
1	H	178	GLN
2	L	38	GLN
2	L	55	GLN

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Mol	Chain	Res	Type
2	L	89	GLN
2	L	90	GLN
2	L	155	GLN
2	L	158	ASN
2	L	166	GLN
1	h	39	GLN
1	h	178	GLN
2	l	38	GLN
2	l	55	GLN
2	l	89	GLN
2	l	90	GLN
2	l	158	ASN
2	l	166	GLN

5.3.3 RNA

There are no RNA molecules 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 monosaccharides in this entry.

5.6 Ligand geometry

7 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	EDO	H	301	-	3,3,3	0.88	0	2,2,2	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	EDO	F	201	-	3,3,3	0.80	0	2,2,2	0.54	0
4	EDO	A	201	-	3,3,3	0.56	0	2,2,2	0.13	0
4	EDO	l	303	-	3,3,3	0.51	0	2,2,2	0.17	0
4	EDO	l	301	-	3,3,3	0.75	0	2,2,2	0.24	0
5	GOL	L	301	-	5,5,5	0.47	0	5,5,5	0.79	0
4	EDO	l	302	-	3,3,3	0.89	0	2,2,2	0.60	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	H	301	-	-	1/1/1/1	-
4	EDO	F	201	-	-	1/1/1/1	-
4	EDO	A	201	-	-	1/1/1/1	-
4	EDO	l	303	-	-	1/1/1/1	-
4	EDO	l	301	-	-	0/1/1/1	-
5	GOL	L	301	-	-	2/4/4/4	-
4	EDO	l	302	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	301	EDO	O1-C1-C2-O2
5	L	301	GOL	O1-C1-C2-C3
4	l	303	EDO	O1-C1-C2-O2
5	L	301	GOL	O1-C1-C2-O2
4	A	201	EDO	O1-C1-C2-O2
4	l	302	EDO	O1-C1-C2-O2
4	F	201	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	H	206/227 (90%)	-0.38	0 100 100	16, 37, 74, 82	0
1	h	206/227 (90%)	-0.24	2 (0%) 82 81	17, 41, 84, 96	0
2	L	211/214 (98%)	-0.40	0 100 100	18, 42, 64, 77	0
2	l	211/214 (98%)	-0.39	0 100 100	18, 44, 65, 77	0
3	A	104/125 (83%)	0.04	4 (3%) 40 38	26, 52, 66, 77	0
3	F	102/125 (81%)	0.10	3 (2%) 51 49	24, 54, 74, 77	0
All	All	1040/1132 (91%)	-0.27	9 (0%) 84 83	16, 44, 74, 96	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	108	ALA	3.9
3	A	21	ALA	3.0
1	h	191	VAL	2.7
1	h	143	ALA	2.5
3	F	21	ALA	2.3
3	A	23	LEU	2.3
3	F	44	PRO	2.2
3	A	76	ILE	2.2
3	F	86	ALA	2.1

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	H	301	4/4	0.89	0.11	50,52,53,53	0
4	EDO	l	303	4/4	0.90	0.11	53,59,60,61	0
4	EDO	l	302	4/4	0.92	0.14	33,41,42,43	0
4	EDO	l	301	4/4	0.92	0.10	39,47,52,52	0
4	EDO	A	201	4/4	0.92	0.15	58,61,61,62	0
5	GOL	L	301	6/6	0.92	0.13	44,47,50,51	0
4	EDO	F	201	4/4	0.95	0.09	39,40,42,43	0

6.5 Other polymers (i)

There are no such residues in this entry.