Full wwPDB X-ray Structure Validation Report (i)

Sep 5, 2023 – 01:52 PM EDT

PDB ID	:	3TJE
Title	:	Crystal structure of Fas receptor extracellular domain in complex with Fab E09
Authors	:	Zuger, S.; Stirnimann, C.; Briand, C.; Grutter, M.G.
Deposited on	:	2011-08-24
Resolution	:	1.93 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 (i)) were used in the production of this report:

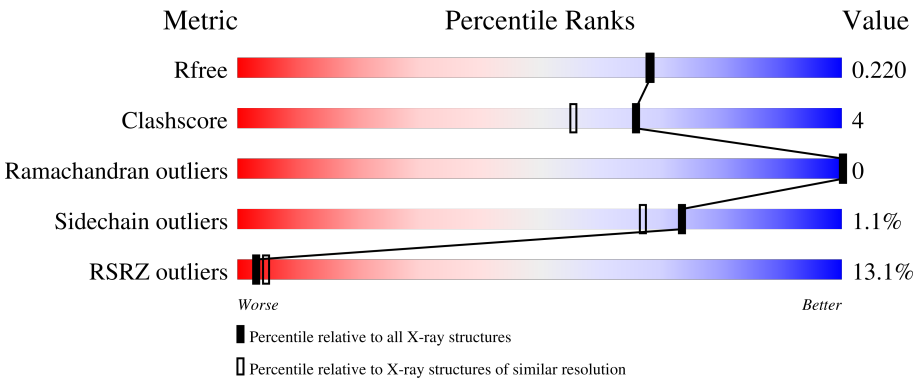
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.93 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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	L	216	7%, 92%, 6% •
2	H	245	11%, 81%, 13%, 7%
3	F	156	19%, 56%, 8% •, 36%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 8613 atoms, of which 4040 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 E09, light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	L	213	3239	1033	1599	276	327	4	0	2	0

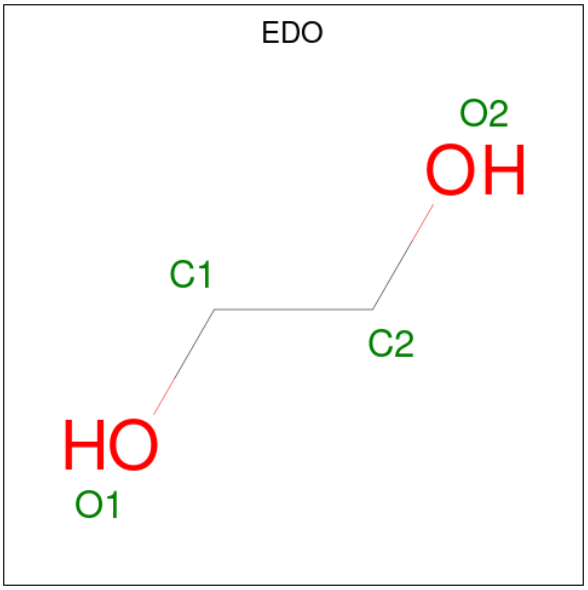
- Molecule 2 is a protein called Fab E09, heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	H	229	3429	1085	1697	292	349	6	0	5	0

- Molecule 3 is a protein called Tumor necrosis factor receptor superfamily member 6.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	F	100	1497	463	714	149	155	16	0	1	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	L	1	10	2	6	2	0	0
			Total	C	H	O		
4	L	1	10	2	6	2	0	0
			Total	C	H	O		
4	L	1	10	2	6	2	0	0
			Total	C	H	O		
4	L	1	10	2	6	2	0	0
			Total	C	H	O		
4	H	1	10	2	6	2	0	0

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

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

- Molecule 6 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cd		
6	F	2	2	2	0	0

- Molecule 7 is water.

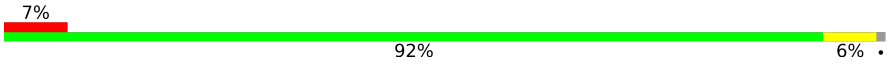
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	L	213	213	213	0	0
			Total	O		
7	H	129	129	129	0	0
			Total	O		
7	F	53	53	53	0	0

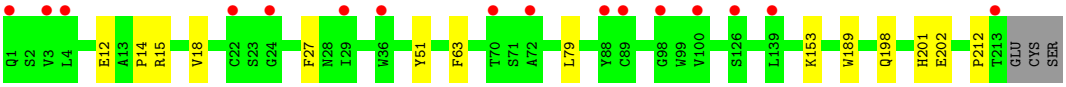
3 Residue-property plots (i)

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 E09, light chain

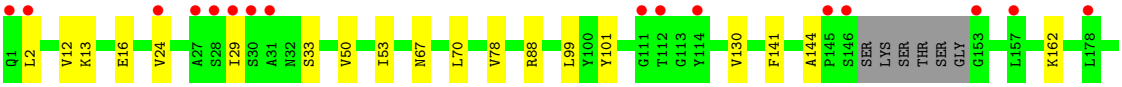
Chain L:

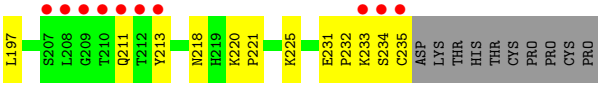




- Molecule 2: Fab E09, heavy chain

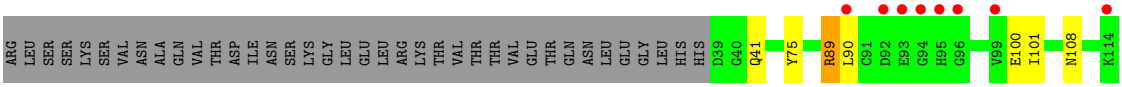
Chain H:

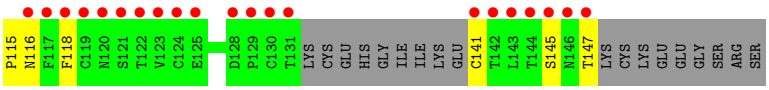




- Molecule 3: Tumor necrosis factor receptor superfamily member 6

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	89.49Å 166.40Å 110.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.09 – 1.93 46.09 – 1.93	Depositor EDS
% Data completeness (in resolution range)	98.2 (46.09-1.93) 98.3 (46.09-1.93)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.50 (at 1.94Å)	Xtriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.204 , 0.232 0.192 , 0.220	Depositor DCC
R_{free} test set	3064 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	34.9	Xtriage
Anisotropy	0.812	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 47.3	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	0.96	EDS
Total number of atoms	8613	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CD, CL, 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	L	0.51	0/1682	0.54	0/2296
2	H	0.43	0/1781	0.56	0/2431
3	F	0.34	0/797	0.49	0/1072
All	All	0.45	0/4260	0.54	0/5799

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	L	1640	1599	1597	7	0
2	H	1732	1697	1689	19	0
3	F	783	714	712	8	0
4	H	4	6	6	0	0
4	L	16	24	24	2	0
5	L	1	0	0	0	0
6	F	2	0	0	0	0
7	F	53	0	0	0	0
7	H	129	0	0	0	0
7	L	213	0	0	0	0
All	All	4573	4040	4028	33	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 4.

All (33) 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)
3:F:141:CYS:N	3:F:147:THR:HG1	1.61	0.99
2:H:2:LEU:HD11	2:H:24:VAL:HG13	1.77	0.66
1:L:63:PHE:CE2	4:L:217:EDO:H21	2.39	0.58
2:H:13:LYS:O	2:H:16[A]:GLU:HB3	2.03	0.57
2:H:24:VAL:HG21	2:H:29:ILE:HG21	1.91	0.53
2:H:231:GLU:HB2	2:H:232:PRO:HD2	1.90	0.53
3:F:141:CYS:N	3:F:147:THR:OG1	2.36	0.53
1:L:189:TRP:O	1:L:212:PRO:HG3	2.11	0.50
2:H:53:ILE:HD13	2:H:78:VAL:HG23	1.95	0.49
3:F:75:TYR:CZ	3:F:108:ASN:HB2	2.48	0.49
2:H:211:GLN:HG2	2:H:213:TYR:CZ	2.48	0.49
2:H:2:LEU:CD1	2:H:24:VAL:HG13	2.44	0.48
2:H:33:SER:OG	3:F:41:GLN:HG2	2.14	0.48
1:L:18:VAL:HG13	1:L:79:LEU:HD11	1.96	0.47
2:H:99:LEU:HD23	2:H:101:TYR:OH	2.14	0.47
3:F:115:PRO:O	3:F:116:ASN:HB2	2.14	0.47
2:H:234:SER:O	2:H:235:CYS:HB2	2.15	0.46
2:H:197:LEU:C	2:H:197:LEU:HD12	2.36	0.46
1:L:201:HIS:CE1	1:L:202:GLU:HG2	2.50	0.46
2:H:50:VAL:HG13	2:H:70:LEU:HD13	1.97	0.45
2:H:141:PHE:CE2	2:H:162[A]:LYS:HD3	2.51	0.45
2:H:67:ASN:HB3	2:H:70:LEU:HD12	1.99	0.45
2:H:220:LYS:N	2:H:221:PRO:CD	2.81	0.44
2:H:141:PHE:HE2	2:H:162[A]:LYS:HD3	1.83	0.43
3:F:89[B]:ARG:HG2	3:F:90:LEU:N	2.33	0.43
3:F:118:PHE:CD2	3:F:118:PHE:C	2.91	0.43
1:L:14:PRO:O	1:L:15:ARG:HB2	2.19	0.43
1:L:27:PHE:CE1	4:L:218:EDO:H21	2.54	0.42
1:L:153:LYS:HE3	1:L:198:GLN:OE1	2.20	0.42
2:H:144:ALA:HB3	2:H:233:LYS:HG3	2.02	0.41
2:H:218[B]:ASN:OD1	2:H:225:LYS:HG3	2.21	0.41
3:F:100:GLU:HG2	3:F:101:ILE:HG13	2.03	0.40
2:H:12:VAL:O	2:H:130:VAL:HA	2.21	0.40

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	L	213/216 (99%)	207 (97%)	6 (3%)	0	100	100
2	H	230/245 (94%)	221 (96%)	9 (4%)	0	100	100
3	F	97/156 (62%)	95 (98%)	2 (2%)	0	100	100
All	All	540/617 (88%)	523 (97%)	17 (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	L	185/186 (100%)	183 (99%)	2 (1%)	73	67
2	H	198/208 (95%)	197 (100%)	1 (0%)	88	88
3	F	93/143 (65%)	90 (97%)	3 (3%)	39	25
All	All	476/537 (89%)	470 (99%)	6 (1%)	73	62

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	12	GLU
1	L	51	TYR
2	H	88	ARG
3	F	89[A]	ARG
3	F	89[B]	ARG

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Mol	Chain	Res	Type
3	F	145	SER

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 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 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	H	246	-	3,3,3	0.55	0	2,2,2	0.65	0
4	EDO	L	217	-	3,3,3	0.49	0	2,2,2	0.22	0
4	EDO	L	219	-	3,3,3	0.49	0	2,2,2	0.31	0
4	EDO	L	220	-	3,3,3	0.49	0	2,2,2	0.25	0
4	EDO	L	218	-	3,3,3	0.47	0	2,2,2	0.27	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	246	-	-	1/1/1/1	-
4	EDO	L	217	-	-	1/1/1/1	-
4	EDO	L	219	-	-	1/1/1/1	-
4	EDO	L	220	-	-	1/1/1/1	-
4	EDO	L	218	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	220	EDO	O1-C1-C2-O2
4	L	217	EDO	O1-C1-C2-O2
4	H	246	EDO	O1-C1-C2-O2
4	L	219	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	217	EDO	1	0
4	L	218	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 (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	L	213/216 (98%)	0.85	16 (7%)	14	20	24, 34, 56, 86	0
2	H	229/245 (93%)	1.00	26 (11%)	5	7	27, 44, 84, 105	0
3	F	100/156 (64%)	1.58	29 (29%)	0	0	31, 60, 112, 136	0
All	All	542/617 (87%)	1.05	71 (13%)	3	5	24, 41, 86, 136	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	143	LEU	8.4
3	F	123	VAL	7.6
3	F	130	CYS	6.9
3	F	147	THR	6.6
2	H	234	SER	5.9
3	F	131	THR	5.8
2	H	233	LYS	5.5
3	F	129	PRO	5.4
2	H	114	TYR	5.2
2	H	208	LEU	5.2
3	F	144	THR	5.1
3	F	122	THR	5.0
1	L	1	GLN	4.9
2	H	1	GLN	4.7
2	H	235	CYS	4.4
3	F	141	CYS	4.3
2	H	29	ILE	4.1
3	F	119	CYS	4.1
3	F	118	PHE	3.7
3	F	116	ASN	3.6
3	F	117	PHE	3.6
3	F	142	THR	3.5
2	H	153	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
2	H	146	SER	3.5
3	F	145	SER	3.5
2	H	145	PRO	3.5
2	H	209	GLY	3.4
3	F	146	ASN	3.4
2	H	27	ALA	3.3
2	H	28	SER	3.2
2	H	210	THR	3.1
2	H	212	THR	3.0
2	H	211	GLN	3.0
3	F	120	ASN	2.9
1	L	89	CYS	2.9
3	F	121	SER	2.9
3	F	125	GLU	2.8
3	F	95	HIS	2.7
1	L	72	ALA	2.7
3	F	124	CYS	2.7
2	H	31	ALA	2.6
2	H	24	VAL	2.6
2	H	30	SER	2.5
3	F	99	VAL	2.5
3	F	93	GLU	2.5
3	F	94	GLY	2.5
2	H	157	LEU	2.5
2	H	207	SER	2.5
1	L	3	VAL	2.4
3	F	92	ASP	2.4
3	F	114	LYS	2.4
1	L	24	GLY	2.4
2	H	213	TYR	2.4
2	H	2	LEU	2.3
3	F	90	LEU	2.3
3	F	96	GLY	2.3
1	L	139	LEU	2.3
1	L	29	ILE	2.3
2	H	112	THR	2.3
2	H	111	GLY	2.2
1	L	213	THR	2.2
3	F	128	ASP	2.2
1	L	70	THR	2.2
1	L	126	SER	2.2
1	L	4	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	22	CYS	2.1
1	L	98	GLY	2.1
2	H	178	LEU	2.1
1	L	100	VAL	2.0
1	L	88	TYR	2.0
1	L	36	TRP	2.0

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 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, 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
4	EDO	L	220	4/4	0.78	0.29	48,66,78,79	0
4	EDO	L	218	4/4	0.83	0.18	61,73,79,84	0
4	EDO	L	217	4/4	0.86	0.18	44,61,66,73	0
4	EDO	H	246	4/4	0.87	0.18	32,43,55,55	0
6	CD	F	157	1/1	0.93	0.05	70,70,70,70	1
4	EDO	L	219	4/4	0.94	0.29	45,63,70,78	0
6	CD	F	158	1/1	0.95	0.10	64,64,64,64	0
5	CL	L	221	1/1	0.99	0.14	31,31,31,31	0

6.5 Other polymers (i)

There are no such residues in this entry.