



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 06:05 AM UTC

PDB ID : 9Q1L / pdb_00009q1l
Title : Crystal structure of the walnut allergen Jug r 2 bound to the human-derived Fab 6D12
Authors : Pedersen, L.C.; Lytle, I.R.; Mueller, G.A.; Croote, D.C.
Deposited on : 2025-08-14
Resolution : 1.56 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

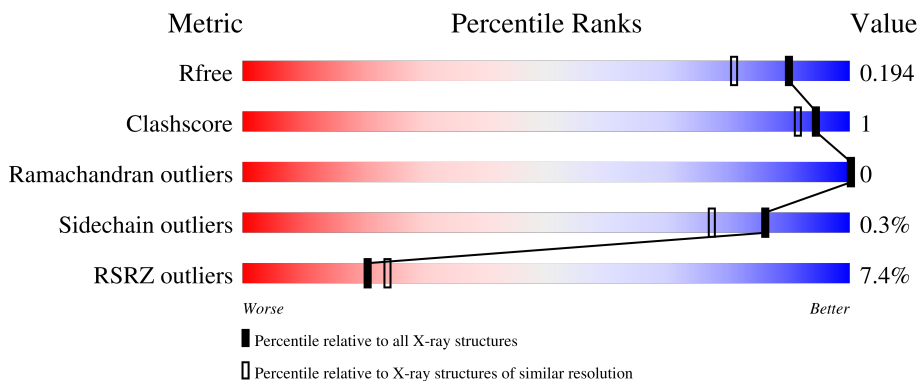
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.56 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}	180053	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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 $\leq 5\%$. 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	B	214	 2% 96%
1	E	214	 2% 99%
2	A	230	 7% 90% 7%
2	D	230	 11% 93%
3	C	47	 4% 77% 19%

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Mol	Chain	Length	Quality of chain
3	F	47	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment on the left labeled '34%', a green segment labeled '77%', a yellow segment labeled '6%', and a grey segment on the right labeled '17%'. The segments are stacked horizontally, with the red segment starting from the left and the grey segment ending at the right.</p>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 15492 atoms, of which 7074 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 6D12 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	B	213	Total	C	H	N	O	S	0	12	0
			3328	1062	1630	286	343	7			
1	E	214	Total	C	H	N	O	S	0	6	0
			3235	1038	1576	272	342	7			

- Molecule 2 is a protein called 6D12 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	A	215	Total	C	H	N	O	S	0	21	0
			3374	1077	1660	290	337	10			
2	D	221	Total	C	H	N	O	S	0	9	0
			3274	1055	1600	279	330	10			

- Molecule 3 is a protein called Vicilin Jug r 2.0102 hairpinin alpha 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
3	C	38	Total	C	H	N	O	S	0	1	0
			601	187	279	67	64	4			
3	F	39	Total	C	H	N	O	S	0	0	0
			557	176	254	63	60	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	206	GLY	-	expression tag	UNP Q9SEW4
C	207	MET	-	expression tag	UNP Q9SEW4
F	206	GLY	-	expression tag	UNP Q9SEW4
F	207	MET	-	expression tag	UNP Q9SEW4

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	1
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	E	1	Total	C	H	O	0	0
			6	2	3	1		
4	E	1	Total	C	H	O	0	0
			10	2	6	2		
4	E	1	Total	C	H	O	0	0
			10	2	6	2		
4	E	1	Total	C	H	O	0	0
			10	2	6	2		
4	D	1	Total	C	H	O	0	0
			10	2	6	2		
4	D	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

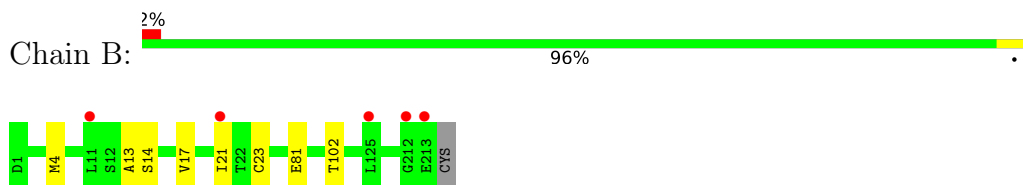
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	268	Total O 274 274	0	9
6	A	247	Total O 252 252	0	9
6	C	41	Total O 41 41	0	1
6	E	243	Total O 246 246	0	5
6	D	160	Total O 161 161	0	2
6	F	22	Total O 22 22	0	0

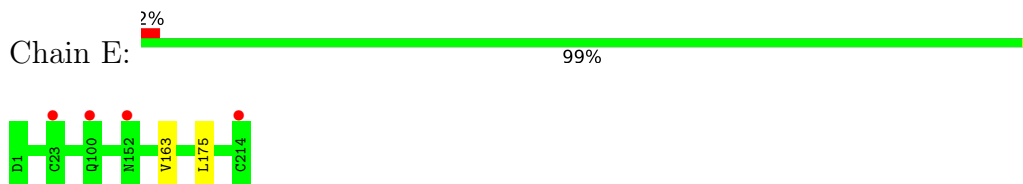
3 Residue-property plots [i](#)

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.

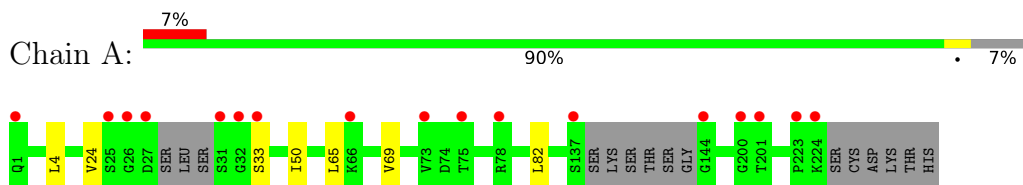
- Molecule 1: 6D12 Fab light chain



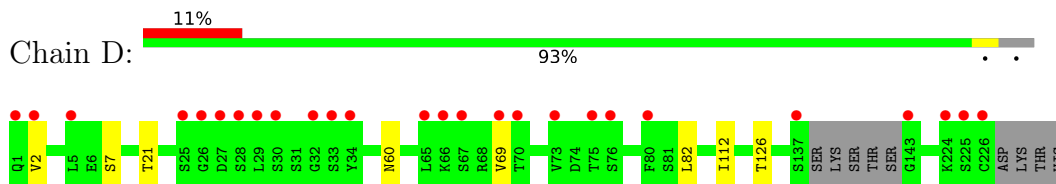
- Molecule 1: 6D12 Fab light chain



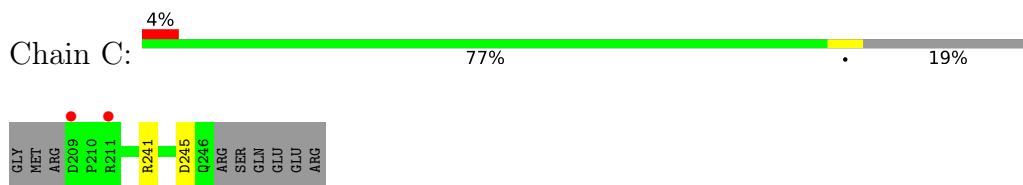
- Molecule 2: 6D12 Fab Heavy Chain




- Molecule 2: 6D12 Fab Heavy Chain

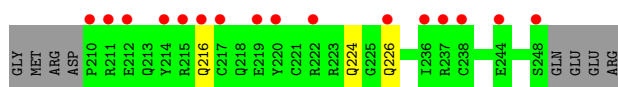


- Molecule 3: Vicilin Jug r 2.0102 hairpinin alpha 4



- Molecule 3: Vicilin Jug r 2.0102 hairpinin alpha 4

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	98.54Å 49.51Å 111.09Å 90.00° 104.73° 90.00°	Depositor
Resolution (Å)	42.41 – 1.56 42.41 – 1.56	Depositor EDS
% Data completeness (in resolution range)	97.3 (42.41-1.56) 97.4 (42.41-1.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 1.56Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.168 , 0.195 0.168 , 0.194	Depositor DCC
R_{free} test set	1980 reflections (1.34%)	wwPDB-VP
Wilson B-factor (Å ²)	17.5	Xtrriage
Anisotropy	0.372	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 45.4	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	0.96	EDS
Total number of atoms	15492	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.17% 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: 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	B	0.23	0/1740	0.48	0/2370
1	E	0.24	0/1694	0.48	0/2310
2	A	0.23	0/1750	0.49	0/2383
2	D	0.21	0/1714	0.46	0/2344
3	C	0.21	0/324	0.41	0/431
3	F	0.19	0/305	0.41	0/407
All	All	0.23	0/7527	0.47	0/10245

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	B	1698	1630	1610	4	0
1	E	1659	1576	1572	1	0
2	A	1714	1660	1653	4	0
2	D	1674	1600	1592	7	0
3	C	322	279	278	1	0
3	F	303	254	254	3	0
4	A	16	24	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	12	18	18	0	0
4	D	8	12	12	0	0
4	E	15	21	21	0	0
5	E	1	0	0	0	0
6	A	252	0	0	0	0
6	B	274	0	0	0	0
6	C	41	0	0	0	0
6	D	161	0	0	1	0
6	E	246	0	0	0	0
6	F	22	0	0	1	0
All	All	8418	7074	7034	19	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 1.

The worst 5 of 19 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:D:2:VAL:HG13	2:D:112:ILE:HD13	1.63	0.81
1:B:13:ALA:HB1	1:B:17:VAL:HG21	1.68	0.73
1:B:14:SER:O	1:B:17:VAL:HG22	1.99	0.63
2:A:50:ILE:HG23	2:A:65[A]:LEU:HD13	1.83	0.61
2:D:2:VAL:CG1	2:D:112:ILE:HD13	2.34	0.58

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	B	222/214 (104%)	216 (97%)	6 (3%)	0	100	100
1	E	217/214 (101%)	211 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	227/230 (99%)	221 (97%)	6 (3%)	0	100	100
2	D	226/230 (98%)	223 (99%)	3 (1%)	0	100	100
3	C	37/47 (79%)	37 (100%)	0	0	100	100
3	F	37/47 (79%)	37 (100%)	0	0	100	100
All	All	966/982 (98%)	945 (98%)	21 (2%)	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	B	191/189 (101%)	190 (100%)	1 (0%)	81	68
1	E	187/189 (99%)	187 (100%)	0	100	100
2	A	196/201 (98%)	194 (99%)	2 (1%)	68	47
2	D	186/201 (92%)	186 (100%)	0	100	100
3	C	32/44 (73%)	32 (100%)	0	100	100
3	F	29/44 (66%)	29 (100%)	0	100	100
All	All	821/868 (95%)	818 (100%)	3 (0%)	86	73

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	81	GLU
2	A	33[A]	SER
2	A	33[B]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	226	GLN

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Mol	Chain	Res	Type
3	F	213	GLN
2	A	60	ASN
2	A	41	GLN
2	A	214	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 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	E	301	-	2,2,3	0.47	0	1,1,2	0.31	0
4	EDO	A	304	-	3,3,3	0.38	0	2,2,2	0.29	0
4	EDO	B	303	-	3,3,3	0.40	0	2,2,2	0.43	0
4	EDO	E	303	-	3,3,3	0.57	0	2,2,2	0.16	0
4	EDO	E	304	-	3,3,3	0.41	0	2,2,2	0.28	0
4	EDO	D	302	-	3,3,3	0.44	0	2,2,2	0.33	0
4	EDO	B	302	-	3,3,3	0.42	0	2,2,2	0.28	0
4	EDO	D	301	-	3,3,3	0.60	0	2,2,2	0.05	0
4	EDO	B	301	-	3,3,3	0.53	0	2,2,2	0.26	0
4	EDO	A	301	-	3,3,3	0.40	0	2,2,2	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	A	302[B]	-	3,3,3	0.41	0	2,2,2	0.35	0
4	EDO	A	303	-	3,3,3	0.52	0	2,2,2	0.21	0
4	EDO	E	302	-	3,3,3	0.41	0	2,2,2	0.28	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	304	-	-	0/1/1/1	-
4	EDO	B	303	-	-	0/1/1/1	-
4	EDO	E	303	-	-	0/1/1/1	-
4	EDO	E	304	-	-	1/1/1/1	-
4	EDO	D	302	-	-	0/1/1/1	-
4	EDO	B	302	-	-	0/1/1/1	-
4	EDO	D	301	-	-	0/1/1/1	-
4	EDO	B	301	-	-	0/1/1/1	-
4	EDO	A	301	-	-	0/1/1/1	-
4	EDO	A	302[B]	-	-	0/1/1/1	-
4	EDO	A	303	-	-	0/1/1/1	-
4	EDO	E	302	-	-	0/1/1/1	-

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	E	304	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

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	B	213/214 (99%)	-0.11	5 (2%) 61 69	10, 22, 37, 67	11 (5%)
1	E	214/214 (100%)	-0.04	4 (1%) 66 75	7, 25, 41, 78	6 (2%)
2	A	215/230 (93%)	0.18	17 (7%) 18 22	9, 21, 50, 72	21 (9%)
2	D	221/230 (96%)	0.62	26 (11%) 9 11	7, 30, 67, 83	9 (4%)
3	C	38/47 (80%)	0.61	2 (5%) 32 39	11, 34, 58, 66	1 (2%)
3	F	39/47 (82%)	1.93	16 (41%) 0 0	45, 56, 79, 84	0
All	All	940/982 (95%)	0.26	70 (7%) 20 24	7, 25, 60, 84	48 (5%)

The worst 5 of 70 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	26[A]	GLY	11.5
2	D	226	CYS	7.1
2	A	31[B]	SER	6.2
2	D	25	SER	6.1
1	E	214	CYS	5.5

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 oligosaccharides 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	E	304	4/4	0.74	0.16	42,51,62,62	0
4	EDO	D	302	4/4	0.74	0.16	40,48,55,61	0
4	EDO	A	304	4/4	0.78	0.18	32,39,46,56	0
4	EDO	B	302	4/4	0.81	0.18	28,33,38,46	0
4	EDO	E	303	4/4	0.87	0.15	23,32,39,39	0
4	EDO	E	302	4/4	0.88	0.12	28,38,51,61	0
5	CL	E	305	1/1	0.89	0.14	49,49,49,49	0
4	EDO	B	303	4/4	0.91	0.13	22,36,41,43	0
4	EDO	E	301	3/4	0.92	0.17	26,36,46,46	0
4	EDO	A	302[B]	4/4	0.92	0.12	18,24,39,39	10
4	EDO	B	301	4/4	0.92	0.11	19,32,39,39	0
4	EDO	A	303	4/4	0.93	0.10	20,26,32,32	0
4	EDO	A	301	4/4	0.94	0.09	23,28,35,35	0
4	EDO	D	301	4/4	0.96	0.08	17,23,23,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.