



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 05:29 am BST

PDB ID : 6S8V
Title : Structure of the high affinity Anticalin P3D11 in complex with the human CD98 heavy chain ectodomain
Authors : Schiefner, A.; Deuschle, F.-C.; Skerra, A.
Deposited on : 2019-07-10
Resolution : 1.80 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

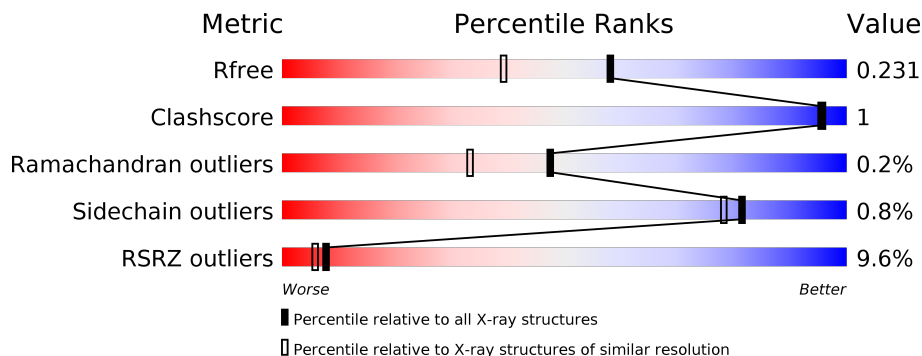
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	186	 7% 89% 5% 8%
1	C	186	 9% 86% 5% 8%
2	B	431	 9% 92% 5% 8%
2	D	431	 10% 95% 5% 8%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10265 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 Neutrophil gelatinase-associated lipocalin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	172	1391	895	237	254	5	0	2	0
1	C	172	1389	893	237	254	5	0	2	0

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	HIS	GLN	engineered mutation	UNP P80188
A	36	ARG	LEU	engineered mutation	UNP P80188
A	40	THR	ALA	engineered mutation	UNP P80188
A	41	GLY	ILE	engineered mutation	UNP P80188
A	49	GLY	GLN	engineered mutation	UNP P80188
A	52	PHE	TYR	engineered mutation	UNP P80188
A	68	TYR	SER	engineered mutation	UNP P80188
A	70	TRP	LEU	engineered mutation	UNP P80188
A	72	GLY	ARG	engineered mutation	UNP P80188
A	73	GLN	LYS	engineered mutation	UNP P80188
A	77	MET	ASP	engineered mutation	UNP P80188
A	79	SER	TRP	engineered mutation	UNP P80188
A	81	GLY	ARG	engineered mutation	UNP P80188
A	87	SER	CYS	engineered mutation	UNP P80188
A	100	ALA	TYR	engineered mutation	UNP P80188
A	103	ARG	LEU	engineered mutation	UNP P80188
A	106	TRP	TYR	engineered mutation	UNP P80188
A	125	SER	LYS	engineered mutation	UNP P80188
A	127	THR	SER	engineered mutation	UNP P80188
A	132	GLY	TYR	engineered mutation	UNP P80188
A	134	ALA	LYS	engineered mutation	UNP P80188
A	179	SER	-	expression tag	UNP P80188
A	180	ALA	-	expression tag	UNP P80188
A	181	HIS	-	expression tag	UNP P80188
A	182	HIS	-	expression tag	UNP P80188

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Chain	Residue	Modelled	Actual	Comment	Reference
A	183	HIS	-	expression tag	UNP P80188
A	184	HIS	-	expression tag	UNP P80188
A	185	HIS	-	expression tag	UNP P80188
A	186	HIS	-	expression tag	UNP P80188
C	28	HIS	GLN	engineered mutation	UNP P80188
C	36	ARG	LEU	engineered mutation	UNP P80188
C	40	THR	ALA	engineered mutation	UNP P80188
C	41	GLY	ILE	engineered mutation	UNP P80188
C	49	GLY	GLN	engineered mutation	UNP P80188
C	52	PHE	TYR	engineered mutation	UNP P80188
C	68	TYR	SER	engineered mutation	UNP P80188
C	70	TRP	LEU	engineered mutation	UNP P80188
C	72	GLY	ARG	engineered mutation	UNP P80188
C	73	GLN	LYS	engineered mutation	UNP P80188
C	77	MET	ASP	engineered mutation	UNP P80188
C	79	SER	TRP	engineered mutation	UNP P80188
C	81	GLY	ARG	engineered mutation	UNP P80188
C	87	SER	CYS	engineered mutation	UNP P80188
C	100	ALA	TYR	engineered mutation	UNP P80188
C	103	ARG	LEU	engineered mutation	UNP P80188
C	106	TRP	TYR	engineered mutation	UNP P80188
C	125	SER	LYS	engineered mutation	UNP P80188
C	127	THR	SER	engineered mutation	UNP P80188
C	132	GLY	TYR	engineered mutation	UNP P80188
C	134	ALA	LYS	engineered mutation	UNP P80188
C	179	SER	-	expression tag	UNP P80188
C	180	ALA	-	expression tag	UNP P80188
C	181	HIS	-	expression tag	UNP P80188
C	182	HIS	-	expression tag	UNP P80188
C	183	HIS	-	expression tag	UNP P80188
C	184	HIS	-	expression tag	UNP P80188
C	185	HIS	-	expression tag	UNP P80188
C	186	HIS	-	expression tag	UNP P80188

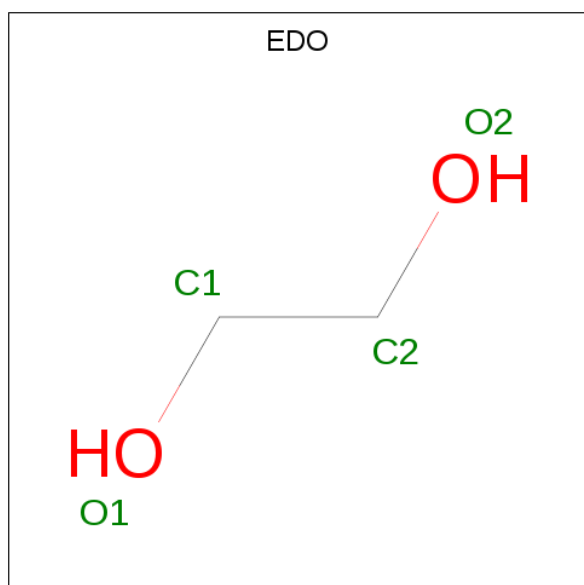
- Molecule 2 is a protein called 4F2 cell-surface antigen heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	416	3286	2082	562	637	5	0	7	0
2	D	420	3290	2092	560	633	5	0	4	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	99	ALA	-	expression tag	UNP P08195
B	100	SER	-	expression tag	UNP P08195
B	101	TRP	-	expression tag	UNP P08195
B	102	SER	-	expression tag	UNP P08195
B	103	HIS	-	expression tag	UNP P08195
B	104	PRO	-	expression tag	UNP P08195
B	105	GLN	-	expression tag	UNP P08195
B	106	PHE	-	expression tag	UNP P08195
B	107	GLU	-	expression tag	UNP P08195
B	108	LYS	-	expression tag	UNP P08195
B	109	GLY	-	expression tag	UNP P08195
B	110	ALA	-	expression tag	UNP P08195
D	99	ALA	-	expression tag	UNP P08195
D	100	SER	-	expression tag	UNP P08195
D	101	TRP	-	expression tag	UNP P08195
D	102	SER	-	expression tag	UNP P08195
D	103	HIS	-	expression tag	UNP P08195
D	104	PRO	-	expression tag	UNP P08195
D	105	GLN	-	expression tag	UNP P08195
D	106	PHE	-	expression tag	UNP P08195
D	107	GLU	-	expression tag	UNP P08195
D	108	LYS	-	expression tag	UNP P08195
D	109	GLY	-	expression tag	UNP P08195
D	110	ALA	-	expression tag	UNP P08195

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

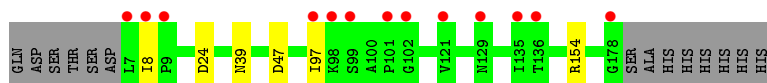
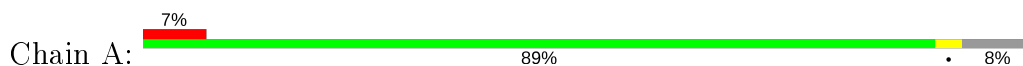
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	169	Total O 170 170	0	1
4	B	305	Total O 306 306	0	1
4	C	131	Total O 131 131	0	0
4	D	290	Total O 290 290	0	0

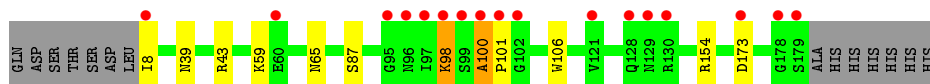
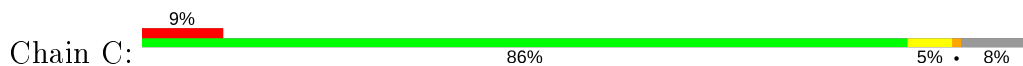
3 Residue-property plots [i](#)

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.

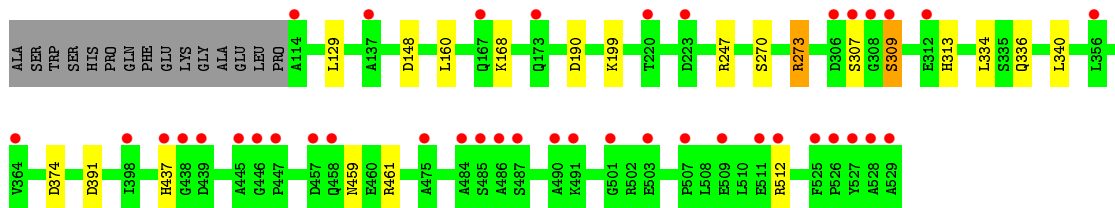
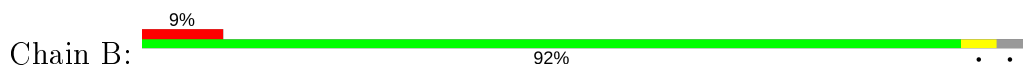
- Molecule 1: Neutrophil gelatinase-associated lipocalin



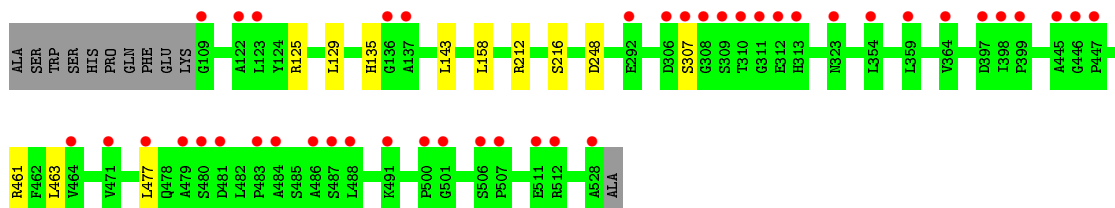
- Molecule 1: Neutrophil gelatinase-associated lipocalin



- Molecule 2: 4F2 cell-surface antigen heavy chain



- Molecule 2: 4F2 cell-surface antigen heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	202.81Å 46.05Å 137.09Å 90.00° 106.64° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80 29.70 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-1.80) 99.9 (29.70-1.80)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 1.80Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.184 , 0.226 0.197 , 0.231	Depositor DCC
R_{free} test set	2234 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtrriage
Anisotropy	0.251	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10265	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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

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	1.06	0/1429	0.93	4/1935 (0.2%)
1	C	0.95	1/1427 (0.1%)	0.87	2/1932 (0.1%)
2	B	0.94	1/3358 (0.0%)	0.90	7/4553 (0.2%)
2	D	0.91	1/3363 (0.0%)	0.88	4/4562 (0.1%)
All	All	0.95	3/9577 (0.0%)	0.90	17/12982 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	216	SER	CB-OG	-5.54	1.35	1.42
1	C	106	TRP	CB-CG	5.37	1.59	1.50
2	B	336	GLN	N-CA	5.04	1.56	1.46

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	247	ARG	NE-CZ-NH1	8.14	124.37	120.30
2	D	248	ASP	CB-CG-OD1	7.38	124.94	118.30
2	D	125	ARG	NE-CZ-NH1	7.37	123.99	120.30
2	B	437	HIS	CB-CA-C	-7.26	95.89	110.40
2	B	273	ARG	NE-CZ-NH1	6.94	123.77	120.30

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	1391	0	1367	2	0
1	C	1389	0	1360	3	1
2	B	3286	0	3226	8	0
2	D	3290	0	3249	7	0
3	A	4	0	6	0	0
3	B	4	0	6	0	0
3	D	4	0	6	0	0
4	A	170	0	0	0	0
4	B	306	0	0	0	0
4	C	131	0	0	0	0
4	D	290	0	0	0	0
All	All	10265	0	9220	20	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 1.

The worst 5 of 20 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:158[B]:LEU:HD12	2:D:158[B]:LEU:O	1.57	1.05
2:D:158[B]:LEU:HD12	2:D:158[B]:LEU:C	1.93	0.88
2:D:463[A]:LEU:HD21	2:D:477:LEU:CD1	2.21	0.71
2:D:463[A]:LEU:HD21	2:D:477:LEU:HD12	1.76	0.66
2:B:129:LEU:HD11	2:B:160:LEU:HD11	1.80	0.62

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)
1:C:98:LYS:NZ	1:C:173:ASP:OD2[1_545]	2.17	0.03

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	172/186 (92%)	165 (96%)	7 (4%)	0	100	100
1	C	172/186 (92%)	165 (96%)	6 (4%)	1 (1%)	25	12
2	B	421/431 (98%)	408 (97%)	12 (3%)	1 (0%)	47	33
2	D	422/431 (98%)	410 (97%)	12 (3%)	0	100	100
All	All	1187/1234 (96%)	1148 (97%)	37 (3%)	2 (0%)	47	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	100	ALA
2	B	309	SER

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	153/164 (93%)	152 (99%)	1 (1%)	84	81
1	C	152/164 (93%)	150 (99%)	2 (1%)	69	62
2	B	357/362 (99%)	354 (99%)	3 (1%)	81	78
2	D	357/362 (99%)	355 (99%)	2 (1%)	86	84
All	All	1019/1052 (97%)	1011 (99%)	8 (1%)	81	78

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	512	ARG
2	D	307	SER
1	C	98	LYS
2	B	309	SER
1	C	87	SER

Some 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 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	$\# Z > 2$
3	EDO	A	201	-	3,3,3	0.71	0	2,2,2	0.38	0
3	EDO	D	601	-	3,3,3	0.59	0	2,2,2	0.10	0
3	EDO	B	601	-	3,3,3	0.56	0	2,2,2	0.48	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
3	EDO	A	201	-	-	0/1/1/1	-
3	EDO	D	601	-	-	0/1/1/1	-
3	EDO	B	601	-	-	0/1/1/1	-

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.

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 [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	172/186 (92%)	0.18	13 (7%) 13 10	17, 27, 54, 74	0
1	C	172/186 (92%)	0.40	17 (9%) 7 5	21, 31, 65, 101	0
2	B	416/431 (96%)	0.30	40 (9%) 8 6	17, 31, 69, 93	0
2	D	420/431 (97%)	0.36	43 (10%) 6 5	19, 33, 63, 89	0
All	All	1180/1234 (95%)	0.32	113 (9%) 8 6	17, 31, 66, 101	0

The worst 5 of 113 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	97	ILE	11.1
1	C	101	PRO	8.0
1	C	100	ALA	7.2
2	B	527	TYR	7.1
2	D	307	SER	7.0

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 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(\AA^2)	Q<0.9
3	EDO	A	201	4/4	0.84	0.13	37,38,40,41	0
3	EDO	B	601	4/4	0.94	0.10	25,26,27,27	0
3	EDO	D	601	4/4	0.96	0.08	29,29,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.