



wwPDB X-ray Structure Validation Summary Report

Feb 26, 2024 – 03:53 PM EST

PDB ID : 8VY8
Title : Recombinant alpha bungarotoxin complexed with HAP peptide
Authors : Xu, J.; Lei, X.; Chen, L.
Deposited on : 2024-02-07
Resolution : 2.40 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (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

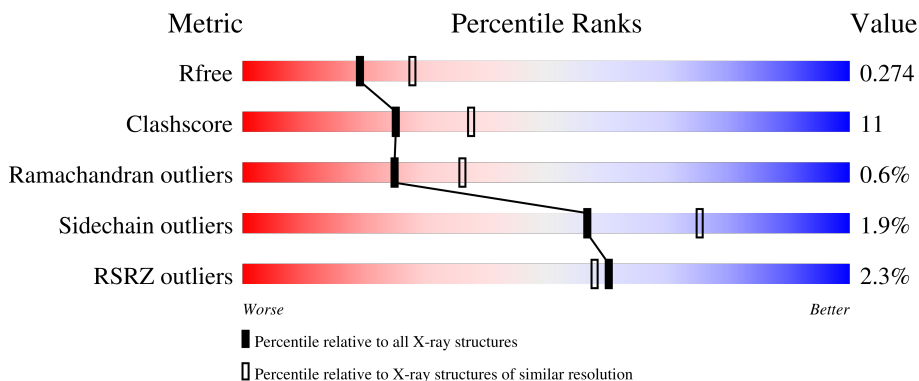
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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.



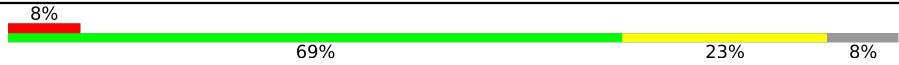

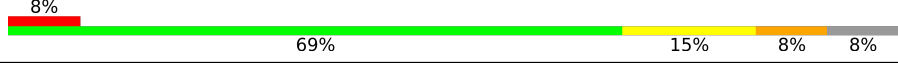
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	A	76	80% (green), 18% (yellow), 2% (grey), 0% (red)
1	B	76	3% (red), 75% (green), 22% (yellow), 0% (grey)
1	E	76	78% (green), 20% (yellow), 2% (grey), 0% (red)
1	G	76	4% (red), 82% (green), 17% (yellow), 0% (grey)
2	C	13	69% (green), 23% (yellow), 8% (grey), 0% (red)

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Mol	Chain	Length	Quality of chain
2	D	13	
2	F	13	
2	H	13	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5555 atoms, of which 2612 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 Alpha-bungarotoxin isoform V31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	B	75	1094	342	537	98	106	11	0	0	0
1	A	75	1094	342	537	98	106	11	0	0	0
1	E	74	1087	340	534	97	105	11	0	0	0
1	G	75	1093	342	537	98	105	11	0	0	0

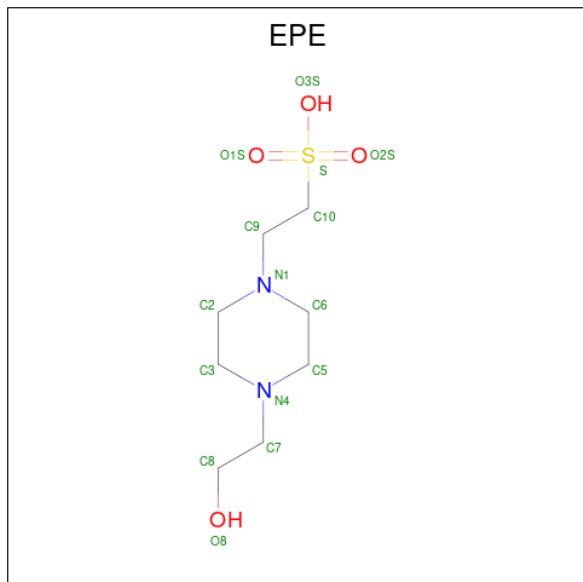
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	MET	-	expression tag	UNP P60616
B	0	GLY	-	expression tag	UNP P60616
A	-1	MET	-	expression tag	UNP P60616
A	0	GLY	-	expression tag	UNP P60616
E	-1	MET	-	expression tag	UNP P60616
E	0	GLY	-	expression tag	UNP P60616
G	-1	MET	-	expression tag	UNP P60616
G	0	GLY	-	expression tag	UNP P60616

- Molecule 2 is a protein called HAP peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	D	12	216	77	104	16	19	0	0	0
2	C	12	216	77	104	16	19	0	0	0
2	F	12	216	77	104	16	19	0	0	0
2	H	12	216	77	104	16	19	0	0	0

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			S
3	D	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		
3	C	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		
3	F	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	47	Total	O	0	0
			47	47		
4	D	5	Total	O	0	0
			5	5		
4	A	44	Total	O	0	0
			44	44		
4	C	6	Total	O	0	0
			6	6		
4	E	54	Total	O	0	0
			54	54		
4	F	10	Total	O	0	0
			10	10		
4	G	48	Total	O	0	0
			48	48		

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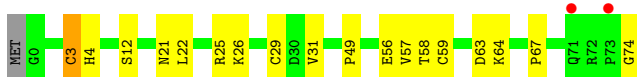
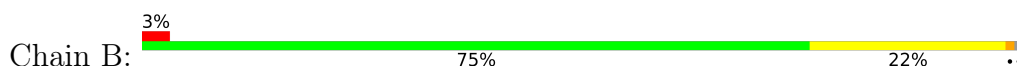
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	13	Total	O	0	0
			13	13		

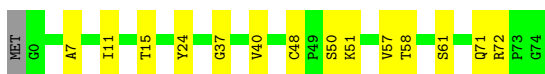
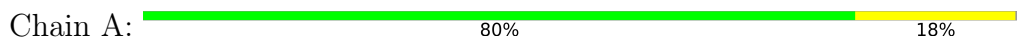
3 Residue-property plots [i](#)

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.

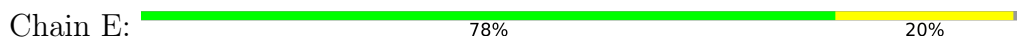
- Molecule 1: Alpha-bungarotoxin isoform V31



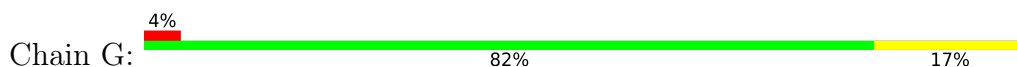
- Molecule 1: Alpha-bungarotoxin isoform V31



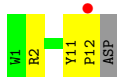
- Molecule 1: Alpha-bungarotoxin isoform V31



- Molecule 1: Alpha-bungarotoxin isoform V31

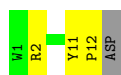


- Molecule 2: HAP peptide



- Molecule 2: HAP peptide

Chain C:  69% 23% 8%



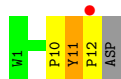
● Molecule 2: HAP peptide

Chain F:  8% 54% 23% 15% 8%



● Molecule 2: HAP peptide

Chain H:  8% 69% 15% 8% 8%



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.53Å 73.11Å 79.84Å 90.00° 103.68° 90.00°	Depositor
Resolution (Å)	53.20 – 2.40 53.21 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.3 (53.20-2.40) 88.4 (53.21-2.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.28 (at 2.39Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.237 , 0.277 0.236 , 0.274	Depositor DCC
R_{free} test set	984 reflections (5.45%)	wwPDB-VP
Wilson B-factor (Å ²)	18.0	Xtrriage
Anisotropy	0.778	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 20.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.285 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	5555	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.03% 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: EPE

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	0.28	0/571	0.55	0/775
1	B	0.39	0/571	0.62	1/775 (0.1%)
1	E	0.28	0/567	0.60	0/770
1	G	0.32	0/570	0.58	0/775
2	C	0.37	0/118	0.72	0/162
2	D	0.30	0/118	0.55	0/162
2	F	1.01	1/118 (0.8%)	1.56	3/162 (1.9%)
2	H	0.28	0/118	0.57	0/162
All	All	0.38	1/2751 (0.0%)	0.66	4/3743 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	12	PRO	N-CD	5.63	1.55	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	11	TYR	C-N-CD	11.98	153.57	128.40
2	F	12	PRO	N-CD-CG	-7.83	91.46	103.20
1	B	3	CYS	CA-CB-SG	-5.04	104.92	114.00
2	F	11	TYR	C-N-CA	-5.02	100.90	122.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	2	ARG	Sidechain

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	557	537	539	11	0
1	B	557	537	539	17	0
1	E	553	534	536	12	0
1	G	556	537	539	11	0
2	C	112	104	104	2	0
2	D	112	104	104	4	0
2	F	112	104	104	3	0
2	H	112	104	104	2	0
3	C	15	17	17	0	0
3	D	15	17	17	1	0
3	F	15	17	17	0	0
4	A	44	0	0	6	1
4	B	47	0	0	9	1
4	C	6	0	0	0	0
4	D	5	0	0	2	0
4	E	54	0	0	6	2
4	F	10	0	0	0	0
4	G	48	0	0	5	1
4	H	13	0	0	2	1
All	All	2943	2612	2620	57	3

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 11.

The worst 5 of 57 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)
1:G:48:CYS:O	4:G:102:HOH:O	1.82	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:51:LYS:NZ	4:G:103:HOH:O	1.99	0.92
1:B:56:GLU:OE2	4:B:101:HOH:O	1.86	0.91
1:B:63:ASP:O	4:B:102:HOH:O	1.90	0.90
1:E:15:THR:O	4:E:101:HOH:O	1.93	0.87

All (3) 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)
4:B:143:HOH:O	4:H:112:HOH:O[2_645]	1.89	0.31
4:A:118:HOH:O	4:E:118:HOH:O[2_655]	2.02	0.18
4:E:123:HOH:O	4:G:101:HOH:O[1_655]	2.18	0.02

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	73/76 (96%)	69 (94%)	4 (6%)	0	100	100
1	B	73/76 (96%)	69 (94%)	4 (6%)	0	100	100
1	E	72/76 (95%)	69 (96%)	3 (4%)	0	100	100
1	G	73/76 (96%)	70 (96%)	3 (4%)	0	100	100
2	C	10/13 (77%)	9 (90%)	1 (10%)	0	100	100
2	D	10/13 (77%)	9 (90%)	1 (10%)	0	100	100
2	F	10/13 (77%)	9 (90%)	0	1 (10%)	0	0
2	H	10/13 (77%)	9 (90%)	0	1 (10%)	0	0
All	All	331/356 (93%)	313 (95%)	16 (5%)	2 (1%)	25	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	11	TYR
2	H	11	TYR

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	66/67 (98%)	65 (98%)	1 (2%)	65 80
1	B	66/67 (98%)	64 (97%)	2 (3%)	41 61
1	E	66/67 (98%)	65 (98%)	1 (2%)	65 80
1	G	66/67 (98%)	66 (100%)	0	100 100
2	C	12/13 (92%)	12 (100%)	0	100 100
2	D	12/13 (92%)	11 (92%)	1 (8%)	11 17
2	F	12/13 (92%)	11 (92%)	1 (8%)	11 17
2	H	12/13 (92%)	12 (100%)	0	100 100
All	All	312/320 (98%)	306 (98%)	6 (2%)	57 75

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	SER
1	E	50	SER
2	F	12	PRO
1	B	31	VAL
1	B	3	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](#)

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	EPE	F	101	-	15,15,15	0.89	1 (6%)	18,20,20	1.95	6 (33%)
3	EPE	D	101	-	15,15,15	0.97	1 (6%)	18,20,20	1.67	5 (27%)
3	EPE	C	101	-	15,15,15	0.84	1 (6%)	18,20,20	1.69	5 (27%)

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	EPE	F	101	-	-	5/9/19/19	0/1/1/1
3	EPE	D	101	-	-	6/9/19/19	0/1/1/1
3	EPE	C	101	-	-	5/9/19/19	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	101	EPE	C10-S	3.32	1.82	1.77
3	F	101	EPE	C10-S	3.02	1.81	1.77
3	C	101	EPE	C10-S	2.78	1.81	1.77

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	101	EPE	C5-N4-C3	3.95	117.71	108.83
3	F	101	EPE	C7-N4-C3	3.64	120.54	111.23
3	F	101	EPE	C7-N4-C5	3.36	119.82	111.23
3	C	101	EPE	C5-N4-C3	3.23	116.11	108.83
3	C	101	EPE	C7-N4-C3	3.15	119.30	111.23

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	101	EPE	S-C10-C9-N1
3	F	101	EPE	S-C10-C9-N1
3	F	101	EPE	C9-C10-S-O2S
3	D	101	EPE	C9-C10-S-O3S
3	C	101	EPE	C9-C10-S-O3S

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	101	EPE	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	A	75/76 (98%)	0.08	0 100 100	11, 21, 44, 55	0
1	B	75/76 (98%)	0.18	2 (2%) 54 52	10, 22, 44, 55	0
1	E	74/76 (97%)	-0.14	0 100 100	8, 16, 36, 49	0
1	G	75/76 (98%)	0.07	3 (4%) 38 37	9, 16, 43, 49	0
2	C	12/13 (92%)	0.21	0 100 100	20, 32, 50, 53	0
2	D	12/13 (92%)	0.42	1 (8%) 11 10	15, 32, 46, 53	0
2	F	12/13 (92%)	0.29	1 (8%) 11 10	15, 21, 31, 45	0
2	H	12/13 (92%)	0.25	1 (8%) 11 10	15, 21, 27, 43	0
All	All	347/356 (97%)	0.08	8 (2%) 60 58	8, 20, 44, 55	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	73	PRO	6.5
2	D	12	PRO	2.8
2	F	12	PRO	2.7
1	G	0	GLY	2.5
1	G	74	GLY	2.3

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
3	EPE	C	101	15/15	0.59	0.33	41,59,94,105	0
3	EPE	D	101	15/15	0.74	0.31	45,64,94,116	0
3	EPE	F	101	15/15	0.81	0.40	23,53,90,93	0

6.5 Other polymers [i](#)

There are no such residues in this entry.