



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 12:35 PM GMT

PDB ID : 3BE5  
Title : Crystal structure of FitE (crystal form 1), a group III periplasmic siderophore binding protein  
Authors : Shi, R.; Matte, A.; Cygler, M.; Montreal-Kingston Bacterial Structural Genomics Initiative (BSGI)  
Deposited on : 2007-11-16  
Resolution : 2.20 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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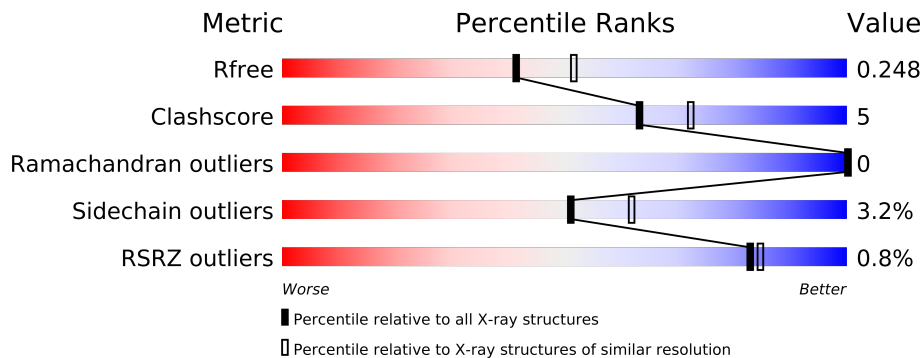
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	297	
1	B	297	
1	C	297	
1	D	297	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9668 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Putative iron compound-binding protein of ABC transporter family.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	Se	0	2	0
			2264	1431	399	427	2	5			
1	B	294	Total	C	N	O	S	Se	0	2	0
			2265	1432	400	425	2	6			
1	C	294	Total	C	N	O	S	Se	0	3	0
			2272	1437	400	427	2	6			
1	D	294	Total	C	N	O	S	Se	0	0	0
			2256	1424	400	425	2	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	259	THR	ALA	SEE REMARK 999	UNP Q8XBR1
B	259	THR	ALA	SEE REMARK 999	UNP Q8XBR1
C	259	THR	ALA	SEE REMARK 999	UNP Q8XBR1
D	259	THR	ALA	SEE REMARK 999	UNP Q8XBR1

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	2	Total	Cl	0	0
			2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	145	Total	O	0	0
			145	145		
3	B	121	Total	O	0	0
			121	121		

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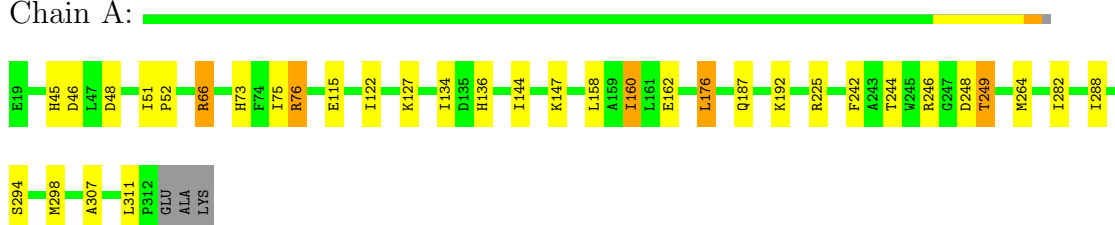
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	160	Total 160	O 160	0	0
3	D	183	Total 183	O 183	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

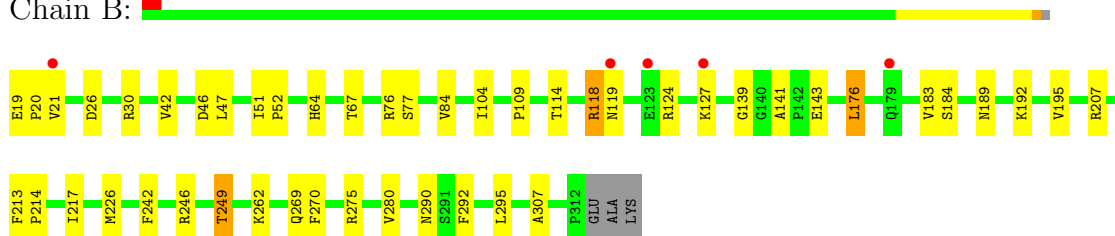
- Molecule 1: Putative iron compound-binding protein of ABC transporter family

Chain A:



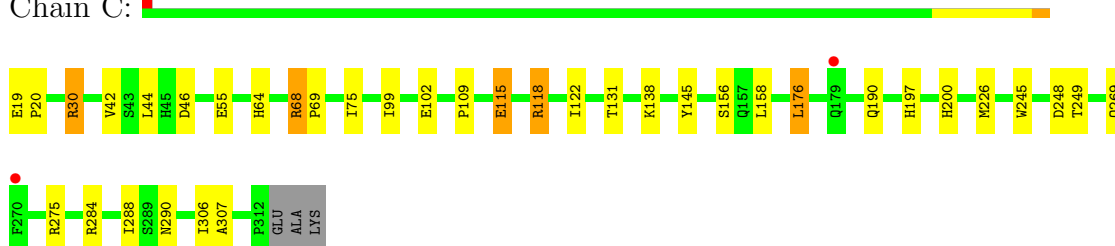
- Molecule 1: Putative iron compound-binding protein of ABC transporter family

Chain B:



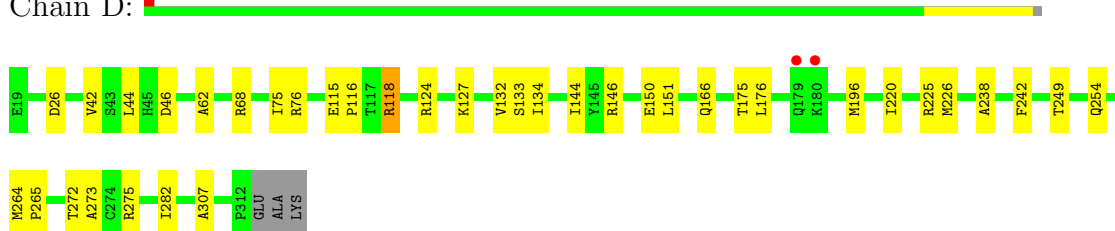
- Molecule 1: Putative iron compound-binding protein of ABC transporter family

Chain C:



- Molecule 1: Putative iron compound-binding protein of ABC transporter family

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.66Å 113.63Å 224.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.04 – 2.20 47.03 – 2.20	Depositor EDS
% Data completeness (in resolution range)	87.7 (47.04-2.20) 87.7 (47.03-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.79 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.187 , 0.245 0.188 , 0.248	Depositor DCC
$R_{free}$ test set	3042 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.2	Xtriage
Anisotropy	1.107	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 36.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 60059 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9668	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:  
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	A	0.50	0/2309	0.59	0/3129
1	B	0.51	0/2310	0.62	0/3130
1	C	0.55	0/2320	0.67	2/3144 (0.1%)
1	D	0.55	0/2295	0.61	0/3109
All	All	0.53	0/9234	0.62	2/12512 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	30	ARG	NE-CZ-NH2	-8.21	116.19	120.30
1	C	30	ARG	NE-CZ-NH1	6.91	123.75	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2264	0	2295	24	0
1	B	2265	0	2305	32	0
1	C	2272	0	2313	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2256	0	2287	24	0
2	C	2	0	0	0	0
3	A	145	0	0	4	0
3	B	121	0	0	4	0
3	C	160	0	0	1	0
3	D	183	0	0	1	0
All	All	9668	0	9200	100	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (100) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:220:ILE:HG12	1:D:226:MSE:HE3	1.44	0.99
1:C:30:ARG:NH2	1:C:131:THR:O	2.07	0.85
1:B:114:THR:OG1	1:B:118:ARG:HD3	1.79	0.82
1:B:242:PHE:CD1	1:B:280[A]:VAL:CG2	2.64	0.80
1:C:46:ASP:H	1:C:64:HIS:HD2	1.29	0.80
1:B:242:PHE:CE1	1:B:280[A]:VAL:HG21	2.16	0.80
1:B:46:ASP:H	1:B:64:HIS:HD2	1.32	0.78
1:B:242:PHE:CD1	1:B:280[A]:VAL:HG21	2.21	0.74
1:A:45:HIS:HD2	1:A:48:ASP:H	1.34	0.74
1:C:245:TRP:CH2	1:D:175:THR:HG21	2.23	0.73
1:B:19:GLU:N	1:B:20:PRO:HD3	2.04	0.72
3:B:403:HOH:O	1:C:226:MSE:CE	2.38	0.71
1:A:176:LEU:HD23	1:A:307:ALA:HB2	1.75	0.68
1:A:76:ARG:HH12	1:A:288:ILE:HD11	1.58	0.68
1:A:311:LEU:HD23	3:B:535:HOH:O	1.94	0.66
1:B:19:GLU:N	1:B:20:PRO:CD	2.58	0.66
1:D:132:VAL:HG21	1:D:151:LEU:HD11	1.78	0.66
1:C:68:ARG:HB2	1:C:69:PRO:HD2	1.79	0.65
1:D:166:GLN:HG3	3:D:592:HOH:O	1.97	0.65
1:A:136:HIS:HB3	1:A:144:ILE:HD11	1.79	0.64
1:C:176[B]:LEU:HD13	1:C:307:ALA:HB2	1.78	0.64
1:B:42:VAL:HG23	1:B:109:PRO:HB3	1.80	0.64
1:D:115:GLU:OE2	1:D:118:ARG:HG2	1.98	0.63
1:D:176:LEU:HD21	1:D:307:ALA:HB2	1.80	0.62
1:B:195:VAL:HG11	1:B:217:ILE:HG12	1.81	0.61
3:B:403:HOH:O	1:C:226:MSE:HE3	2.00	0.60
1:B:46:ASP:H	1:B:64:HIS:CD2	2.17	0.59
1:A:187:GLN:CD	3:A:928:HOH:O	2.40	0.59
1:B:139:GLY:HA3	1:B:143:GLU:HG3	1.85	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:264:MSE:HE3	1:D:265:PRO:HD2	1.84	0.58
1:B:246:ARG:HH12	1:B:249:THR:CG2	2.17	0.57
1:C:68:ARG:HB2	1:C:69:PRO:CD	2.36	0.56
1:C:176[B]:LEU:HD21	1:C:306:ILE:CG2	2.36	0.55
1:B:246:ARG:HH12	1:B:249:THR:HG22	1.71	0.55
1:A:249:THR:HG23	1:A:249:THR:O	2.07	0.54
1:A:136:HIS:CB	1:A:144:ILE:HD11	2.38	0.54
1:B:249:THR:HG23	1:B:249:THR:O	2.07	0.54
1:D:272:THR:HG22	1:D:275:ARG:HH21	1.72	0.53
1:B:242:PHE:CD1	1:B:280[A]:VAL:HG23	2.42	0.53
1:C:176[B]:LEU:HD21	1:C:306:ILE:HG21	1.91	0.53
1:B:183:VAL:O	1:B:214:PRO:HD3	2.10	0.52
1:D:146:ARG:O	1:D:150:GLU:HG2	2.10	0.52
1:A:76:ARG:NH1	1:A:288:ILE:HD11	2.25	0.51
1:C:145:TYR:HB3	1:C:158:LEU:HD13	1.92	0.51
1:D:124:ARG:HA	1:D:127:LYS:HE3	1.92	0.51
1:B:51:ILE:HB	1:B:52:PRO:HD3	1.94	0.50
1:B:67:THR:HG21	1:C:102:GLU:HG3	1.93	0.50
1:A:249:THR:O	1:A:249:THR:CG2	2.60	0.50
1:D:42:VAL:HG22	1:D:62:ALA:HB3	1.94	0.49
1:C:46:ASP:HB2	1:C:75:ILE:HG23	1.94	0.49
1:B:207:ARG:HG2	1:B:213:PHE:CE2	2.47	0.49
1:B:141:ALA:HB2	1:B:290:ASN:HB3	1.94	0.49
1:A:242:PHE:HD1	1:A:282:ILE:CD1	2.27	0.48
1:A:158:LEU:O	1:A:162:GLU:HG3	2.14	0.47
1:C:248:ASP:HB3	1:C:249:THR:HG23	1.96	0.47
1:C:200:HIS:HA	1:C:290:ASN:HD21	1.79	0.47
1:A:294:SER:O	1:A:298:MSE:HG2	2.14	0.47
1:D:134:ILE:HG22	1:D:144:ILE:HD12	1.97	0.47
1:D:196:MSE:HG2	1:D:225:ARG:HB3	1.97	0.47
1:B:189:ASN:O	1:B:192:LYS:HG2	2.15	0.47
1:A:136:HIS:CE1	3:A:999:HOH:O	2.68	0.47
1:C:245:TRP:CH2	1:D:175:THR:CG2	2.96	0.46
1:C:44:LEU:HD22	1:C:99:ILE:HG12	1.98	0.46
1:A:134:ILE:HD12	1:A:147:LYS:HD3	1.97	0.46
1:D:242:PHE:HD1	1:D:282:ILE:HD12	1.80	0.46
1:A:160[A]:ILE:HD12	1:B:84:VAL:HG23	1.98	0.45
1:D:134:ILE:CG2	1:D:144:ILE:HD12	2.46	0.45
1:C:19:GLU:N	1:C:20:PRO:CD	2.80	0.45
1:C:42:VAL:HG23	1:C:109:PRO:HB3	1.99	0.45
1:D:44:LEU:O	1:D:118:ARG:HD2	2.16	0.45
1:B:26:ASP:OD2	1:B:30:ARG:NH2	2.50	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:262:LYS:HB2	1:B:262:LYS:HE2	1.89	0.44
1:D:26:ASP:HB2	1:D:133:SER:O	2.18	0.44
1:B:104:ILE:O	1:B:109:PRO:HD3	2.18	0.44
1:A:51:ILE:HB	1:A:52:PRO:HD3	2.00	0.44
1:A:46:ASP:HB2	1:A:75:ILE:HG23	2.00	0.43
1:B:118:ARG:HG2	1:B:119:ASN:N	2.33	0.43
1:A:244:THR:HA	1:A:282:ILE:O	2.19	0.43
1:C:55:GLU:OE1	1:C:145:TYR:OH	2.25	0.43
1:C:115[B]:GLU:HG3	1:C:118:ARG:HD3	2.00	0.43
1:D:115:GLU:HB2	1:D:116:PRO:HD2	2.01	0.43
1:D:118:ARG:HA	1:D:118:ARG:HH11	1.85	0.42
1:B:76:ARG:O	1:B:77:SER:HB2	2.20	0.42
1:C:269:GLN:HA	1:C:275:ARG:HD3	2.02	0.42
1:D:46:ASP:HB2	1:D:75:ILE:HG23	2.02	0.41
1:B:47:LEU:HD21	1:B:76:ARG:HG2	2.02	0.41
1:A:66:ARG:O	1:A:73:HIS:HA	2.20	0.41
1:C:284:ARG:HG2	1:C:288:ILE:HD13	2.03	0.41
1:D:238:ALA:O	1:D:273:ALA:HB2	2.21	0.41
1:A:246:ARG:HB3	1:A:246:ARG:HE	1.74	0.41
1:B:226:MSE:HE1	3:B:554:HOH:O	2.21	0.41
1:D:254:GLN:CD	1:D:254:GLN:H	2.24	0.41
1:B:292:PHE:HA	1:B:295:LEU:HD12	2.01	0.41
1:A:136:HIS:HE1	3:A:999:HOH:O	2.03	0.40
1:A:242:PHE:HD1	1:A:282:ILE:HD13	1.85	0.40
1:A:225:ARG:HD2	3:A:624:HOH:O	2.20	0.40
1:C:197:HIS:HD2	3:C:536:HOH:O	2.03	0.40
1:D:242:PHE:HD1	1:D:282:ILE:CD1	2.34	0.40
1:B:176:LEU:HD23	1:B:307:ALA:HB2	2.02	0.40
1:B:269:GLN:OE1	1:B:275:ARG:HD3	2.21	0.40

There are no symmetry-related clashes.

## 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	A	294/297 (99%)	286 (97%)	8 (3%)	0	100	100
1	B	294/297 (99%)	288 (98%)	6 (2%)	0	100	100
1	C	295/297 (99%)	288 (98%)	7 (2%)	0	100	100
1	D	292/297 (98%)	288 (99%)	4 (1%)	0	100	100
All	All	1175/1188 (99%)	1150 (98%)	25 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	A	246/242 (102%)	234 (95%)	12 (5%)	35	40
1	B	247/242 (102%)	239 (97%)	8 (3%)	51	62
1	C	248/242 (102%)	238 (96%)	10 (4%)	42	51
1	D	245/242 (101%)	241 (98%)	4 (2%)	75	85
All	All	986/968 (102%)	952 (97%)	34 (3%)	51	59

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ARG
1	A	76	ARG
1	A	115	GLU
1	A	122	ILE
1	A	127	LYS
1	A	160[A]	ILE
1	A	160[B]	ILE
1	A	176	LEU
1	A	192	LYS
1	A	248	ASP
1	A	249	THR
1	A	264	MSE
1	B	21	VAL
1	B	118	ARG

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Mol	Chain	Res	Type
1	B	124	ARG
1	B	127	LYS
1	B	176	LEU
1	B	184	SER
1	B	249	THR
1	B	270	PHE
1	C	68	ARG
1	C	115[A]	GLU
1	C	115[B]	GLU
1	C	118	ARG
1	C	122	ILE
1	C	138	LYS
1	C	156	SER
1	C	176[A]	LEU
1	C	176[B]	LEU
1	C	190	GLN
1	D	68	ARG
1	D	76	ARG
1	D	118	ARG
1	D	249	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	HIS
1	A	136	HIS
1	A	168	GLN
1	A	170	ASN
1	A	190	GLN
1	B	22	GLN
1	B	64	HIS
1	B	73	HIS
1	B	168	GLN
1	B	170	ASN
1	B	197	HIS
1	C	64	HIS
1	C	170	ASN
1	C	197	HIS
1	C	290	ASN
1	D	22	GLN
1	D	73	HIS
1	D	303	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

## 5.7 Other polymers ⓘ

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 ⓘ

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	294/297 (98%)	-0.40	0 100 100	23, 32, 45, 52	0
1	B	294/297 (98%)	-0.26	5 (1%) 67 68	21, 30, 45, 55	0
1	C	294/297 (98%)	-0.42	2 (0%) 84 86	18, 26, 36, 51	0
1	D	294/297 (98%)	-0.46	2 (0%) 84 86	20, 29, 38, 45	0
All	All	1176/1188 (98%)	-0.39	9 (0%) 83 85	18, 29, 42, 55	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	179	GLN	3.4
1	C	270	PHE	3.3
1	B	179	GLN	2.6
1	B	127	LYS	2.4
1	B	21	VAL	2.2
1	B	119	ASN	2.2
1	D	180	LYS	2.2
1	B	123	GLU	2.1
1	C	179	GLN	2.0

### 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 carbohydrates in this entry.

## 6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CL	C	402	1/1	0.07	-10.62	41,41,41,41	0
2	CL	C	401	1/1	0.07	-12.08	30,30,30,30	0

## 6.5 Other polymers

There are no such residues in this entry.