



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2024 – 07:36 AM EDT

PDB ID : 3IH5  
Title : Crystal Structure of Electron Transfer Flavoprotein alpha-subunit from *Bacteroides thetaiotaomicron*  
Authors : Kim, Y.; Sather, A.; Clancy, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2009-07-29  
Resolution : 2.60 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](mailto: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>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

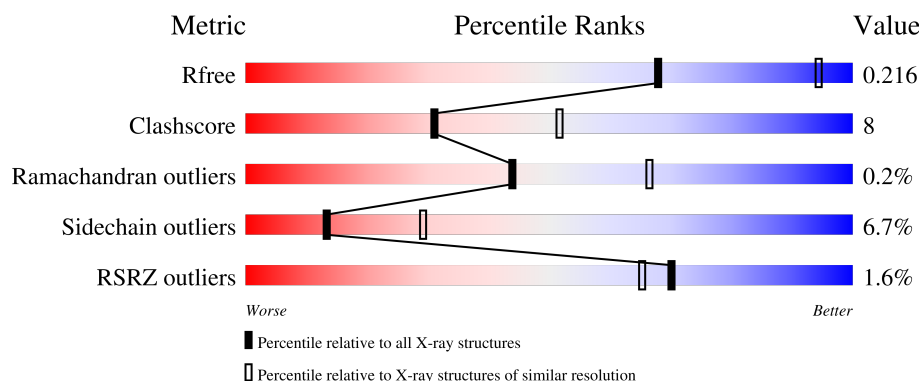
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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  $\geq 3$ , 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	217	<div> <div></div> <div>76% 16% 6%</div> </div>
1	B	217	<div> <div>2%</div> <div>82% 15% ..</div> </div>
1	C	217	<div> <div></div> <div>76% 20% ..</div> </div>
1	D	217	<div> <div></div> <div>76% 17% 6%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6851 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.

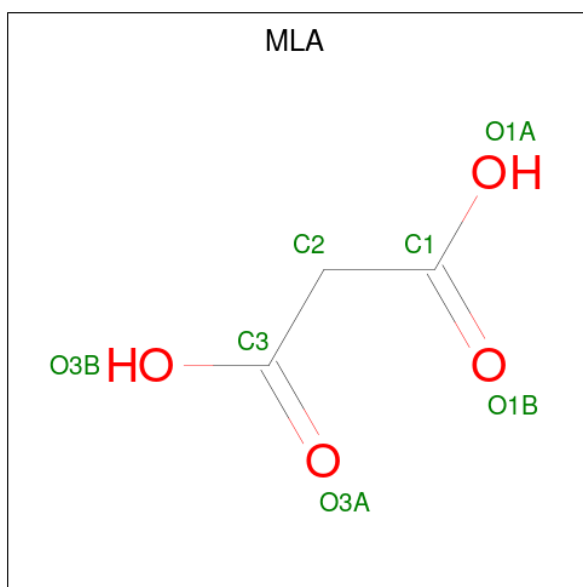
- Molecule 1 is a protein called Electron transfer flavoprotein alpha-subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	Se	0	3	0
			1606	1018	268	313	4	3			
1	B	214	Total	C	N	O	S	Se	0	0	0
			1661	1053	282	319	4	3			
1	C	212	Total	C	N	O	S	Se	0	0	0
			1644	1043	278	316	4	3			
1	D	205	Total	C	N	O	S	Se	0	2	0
			1601	1016	268	310	4	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q8A6S1
A	-1	ASN	-	expression tag	UNP Q8A6S1
A	0	ALA	-	expression tag	UNP Q8A6S1
B	-2	SER	-	expression tag	UNP Q8A6S1
B	-1	ASN	-	expression tag	UNP Q8A6S1
B	0	ALA	-	expression tag	UNP Q8A6S1
C	-2	SER	-	expression tag	UNP Q8A6S1
C	-1	ASN	-	expression tag	UNP Q8A6S1
C	0	ALA	-	expression tag	UNP Q8A6S1
D	-2	SER	-	expression tag	UNP Q8A6S1
D	-1	ASN	-	expression tag	UNP Q8A6S1
D	0	ALA	-	expression tag	UNP Q8A6S1

- Molecule 2 is MALONIC ACID (three-letter code: MLA) (formula: C<sub>3</sub>H<sub>4</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	3	4		
2	A	1	Total	C	O	0	0
			7	3	4		
2	D	1	Total	C	O	0	0
			7	3	4		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



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

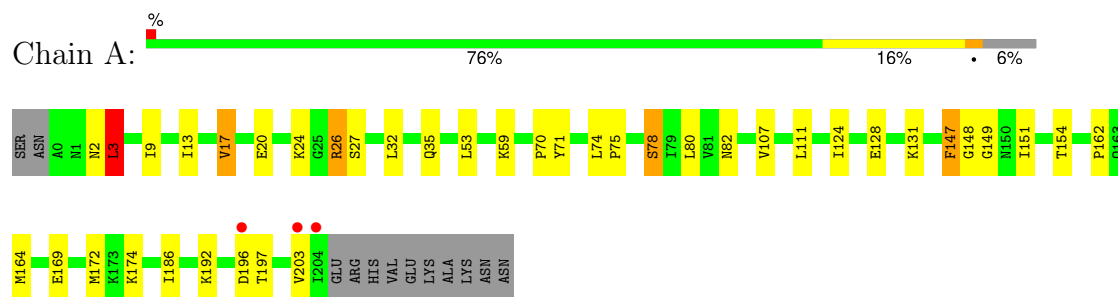
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	83	Total	O	0	0
			83	83		
5	B	71	Total	O	0	0
			71	71		
5	C	78	Total	O	0	0
			78	78		
5	D	81	Total	O	0	0
			81	81		

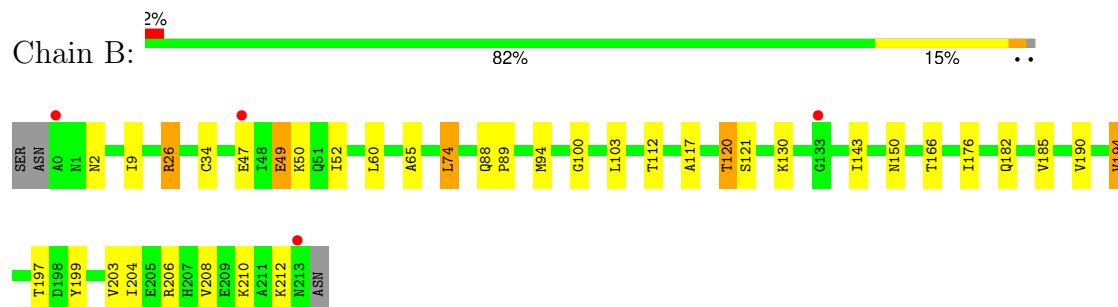
### 3 Residue-property plots [i](#)

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.

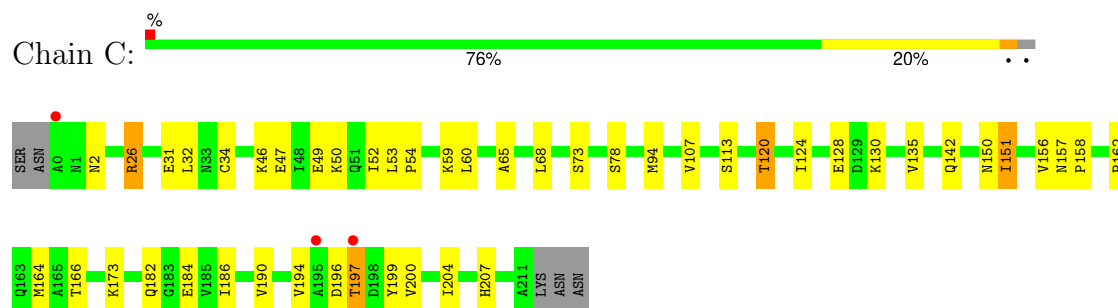
- Molecule 1: Electron transfer flavoprotein alpha-subunit



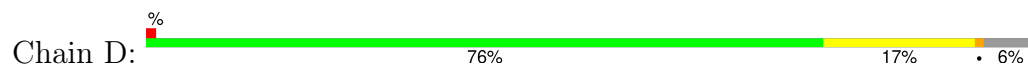
- Molecule 1: Electron transfer flavoprotein alpha-subunit

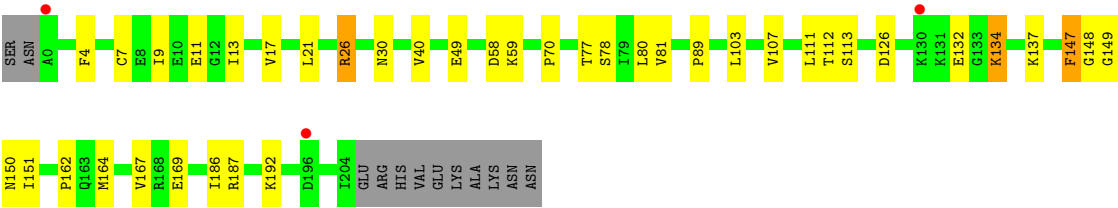


- Molecule 1: Electron transfer flavoprotein alpha-subunit



- Molecule 1: Electron transfer flavoprotein alpha-subunit





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.10Å 102.10Å 209.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.88 – 2.60 45.88 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.1 (45.88-2.60) 99.3 (45.88-2.60)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.25 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.179 , 0.215 0.181 , 0.216	Depositor DCC
$R_{free}$ test set	1972 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.6	Xtriage
Anisotropy	0.886	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 57.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6851	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>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: MLA, FMT, NA

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	0.37	0/1630	0.57	1/2205 (0.0%)
1	B	0.35	0/1685	0.50	0/2277
1	C	0.36	0/1668	0.55	0/2255
1	D	0.39	0/1624	0.56	0/2197
All	All	0.37	0/6607	0.55	1/8934 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	LEU	CA-CB-CG	5.40	127.73	115.30

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	1606	0	1624	28	0
1	B	1661	0	1690	23	0
1	C	1644	0	1671	31	0
1	D	1601	0	1622	33	0
2	A	14	0	4	2	0
2	D	7	0	2	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	A	3	0	1	0	0
5	A	83	0	0	0	0
5	B	71	0	0	1	0
5	C	78	0	0	2	0
5	D	81	0	0	2	0
All	All	6851	0	6614	106	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 8.

All (106) 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:B:94:MSE:HE2	1:B:100:GLY:HA2	1.23	1.17
1:B:94:MSE:HE1	1:B:103:LEU:HB3	1.40	1.02
1:D:59:LYS:HE2	1:D:186:ILE:HD11	1.51	0.91
1:B:94:MSE:CE	1:B:100:GLY:HA2	2.06	0.85
1:D:107:VAL:HG12	1:D:164:MSE:HE1	1.67	0.75
1:B:120:THR:HG21	1:D:70:PRO:HD3	1.72	0.72
1:B:65:ALA:HB2	1:B:190:VAL:HG21	1.71	0.71
1:D:17:VAL:HG23	5:D:295:HOH:O	1.90	0.71
1:D:59:LYS:HE2	1:D:186:ILE:CD1	2.21	0.70
1:B:49:GLU:HG2	1:B:185:VAL:HG21	1.73	0.70
1:A:162:PRO:HG2	1:A:164:MSE:HE2	1.77	0.67
1:D:17:VAL:HG22	1:D:169:GLU:HB2	1.75	0.66
1:A:74:LEU:HD12	1:C:151:ILE:HD13	1.78	0.65
1:A:59:LYS:HE3	1:A:186:ILE:HD11	1.79	0.65
1:C:197:THR:HG22	1:C:199:TYR:CE1	2.32	0.65
1:D:113:SER:HB2	5:D:276:HOH:O	1.96	0.64
1:D:150:ASN:HB2	2:D:215:MLA:HC21	1.80	0.63
1:A:24:LYS:HG2	1:A:172:MSE:HE3	1.81	0.62
1:C:199:TYR:CE2	1:D:151:ILE:HG23	2.37	0.60
1:D:111:LEU:HD12	1:D:164:MSE:CE	2.31	0.60
1:A:186:ILE:HD12	1:A:186:ILE:H	1.68	0.59
1:A:186:ILE:HD12	1:A:186:ILE:N	2.19	0.57
1:D:7:CYS:HB2	1:D:40:VAL:HG22	1.85	0.57
1:C:59:LYS:HE2	1:C:186:ILE:HD11	1.86	0.57
1:D:17:VAL:HG22	1:D:169:GLU:CB	2.35	0.57
1:A:26:ARG:O	1:A:26:ARG:HD3	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:THR:HG22	1:D:112:THR:O	2.05	0.56
1:A:111:LEU:HD12	1:A:164:MSE:HE1	1.88	0.56
1:A:70:PRO:HD3	1:C:120:THR:HG21	1.88	0.56
1:B:210:LYS:O	1:B:210:LYS:HG3	2.06	0.54
1:B:206:ARG:HD3	5:B:276:HOH:O	2.06	0.54
1:D:132:GLU:HG2	1:D:134:LYS:HD3	1.91	0.53
1:C:128:GLU:HG2	1:C:135:VAL:HG22	1.89	0.53
1:A:192:LYS:HE2	2:A:216:MLA:O3A	2.08	0.53
1:C:65:ALA:HB2	1:C:190:VAL:HG21	1.92	0.52
1:A:107:VAL:HG12	1:A:164:MSE:HE1	1.91	0.52
1:D:147:PHE:O	1:D:148:GLY:C	2.48	0.52
1:A:17:VAL:HG13	1:A:169:GLU:HA	1.92	0.51
1:C:32:LEU:HD21	1:C:124:ILE:HD12	1.93	0.51
1:C:26:ARG:O	1:C:26:ARG:HD3	2.12	0.50
1:A:78:SER:OG	1:A:197:THR:HG23	2.12	0.49
1:D:192:LYS:C	1:D:192:LYS:HD3	2.33	0.49
1:B:26:ARG:O	1:B:26:ARG:HD3	2.12	0.49
1:B:120:THR:CG2	1:D:70:PRO:HD3	2.40	0.49
1:C:156:VAL:HG23	1:C:158:PRO:HD3	1.95	0.49
1:B:52:ILE:HG21	1:B:60:LEU:HD13	1.95	0.49
1:A:3:LEU:C	1:A:3:LEU:HD12	2.34	0.48
1:D:59:LYS:CE	1:D:186:ILE:HD11	2.34	0.48
1:C:65:ALA:HB3	1:C:68:LEU:HG	1.95	0.48
1:A:71:TYR:C	1:A:71:TYR:CD1	2.87	0.48
1:D:26:ARG:NH1	1:D:30:ASN:OD1	2.46	0.48
1:A:128:GLU:O	1:A:128:GLU:HG3	2.13	0.48
1:B:94:MSE:O	1:B:166:THR:HA	2.13	0.48
1:D:21:LEU:HD21	1:D:167:VAL:HB	1.97	0.47
1:D:11:GLU:O	1:D:13:ILE:HD12	2.14	0.47
1:C:52:ILE:HG21	1:C:60:LEU:HD13	1.96	0.47
1:B:121:SER:HB2	1:B:143:ILE:HB	1.97	0.47
1:D:162:PRO:HG2	1:D:164:MSE:HE2	1.97	0.47
1:B:26:ARG:HD3	1:B:26:ARG:C	2.32	0.47
1:A:82:ASN:HD21	1:A:196[B]:ASP:CG	2.18	0.47
1:B:88:GLN:N	1:B:89:PRO:HD3	2.30	0.47
1:C:26:ARG:HD3	1:C:26:ARG:C	2.33	0.46
1:D:26:ARG:O	1:D:26:ARG:HD3	2.15	0.46
1:D:111:LEU:HD12	1:D:164:MSE:HE1	1.96	0.46
1:A:20:GLU:HG2	1:A:174:LYS:HB3	1.97	0.46
1:D:4:PHE:CD1	1:D:89:PRO:HB3	2.51	0.46
1:D:26:ARG:NH2	1:D:58:ASP:OD2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:VAL:HG12	1:B:194:VAL:HB	1.98	0.46
1:A:13:ILE:N	1:A:13:ILE:HD12	2.32	0.45
1:A:82:ASN:ND2	1:A:196[B]:ASP:OD2	2.49	0.45
1:C:142:GLN:HE22	1:C:157:ASN:HD22	1.64	0.45
1:D:162:PRO:CG	1:D:164:MSE:HE2	2.47	0.45
1:A:74:LEU:HB2	1:A:75:PRO:HD3	1.98	0.45
1:C:94:MSE:O	1:C:166:THR:HA	2.16	0.45
1:D:17:VAL:CG2	1:D:169:GLU:HB2	2.46	0.44
1:A:151:ILE:HG23	1:B:199:TYR:CE1	2.52	0.44
1:C:113:SER:HB2	1:C:162:PRO:O	2.18	0.44
1:C:47:GLU:HB3	1:C:50:LYS:HD2	1.99	0.44
1:C:107:VAL:HG12	1:C:164:MSE:HE1	1.98	0.44
1:D:77:THR:O	1:D:81:VAL:HG23	2.17	0.44
1:C:31:GLU:O	1:C:31:GLU:HG3	2.19	0.43
1:C:53:LEU:HD23	1:C:53:LEU:HA	1.75	0.43
1:A:70:PRO:HD3	1:C:120:THR:CG2	2.48	0.43
1:B:120:THR:HG21	1:D:70:PRO:CD	2.46	0.43
1:C:162:PRO:HG2	1:C:164:MSE:HE2	2.00	0.43
1:A:192:LYS:CE	2:A:216:MLA:O3A	2.67	0.43
1:B:47:GLU:OE1	1:B:50:LYS:HE2	2.18	0.43
1:C:197:THR:HG22	1:C:199:TYR:CD1	2.53	0.43
1:A:32:LEU:HD21	1:A:124:ILE:HD12	2.01	0.42
1:D:134:LYS:HB2	1:D:134:LYS:NZ	2.35	0.42
1:C:157:ASN:ND2	5:C:265:HOH:O	2.51	0.42
1:B:2:ASN:HD22	1:B:34:CYS:HB2	1.84	0.42
1:C:53:LEU:N	1:C:54:PRO:CD	2.82	0.42
1:C:73:SER:CB	1:D:150:ASN:HD21	2.32	0.42
1:C:204:ILE:HB	1:C:207:HIS:ND1	2.35	0.42
1:C:59:LYS:HG3	1:C:184:GLU:HB3	2.01	0.42
1:A:147:PHE:O	1:A:148:GLY:C	2.58	0.41
1:D:126:ASP:OD1	1:D:137:LYS:HA	2.21	0.41
1:B:94:MSE:HE2	1:B:100:GLY:CA	2.16	0.41
1:B:117:ALA:HA	1:B:166:THR:OG1	2.21	0.41
1:A:53:LEU:HD23	1:A:53:LEU:HA	1.83	0.41
1:C:2:ASN:HD22	1:C:34:CYS:HB2	1.84	0.41
1:A:2:ASN:HB3	1:A:35:GLN:O	2.21	0.40
1:C:173:LYS:HG2	5:C:252:HOH:O	2.21	0.40
1:B:74:LEU:HD22	1:B:74:LEU:HA	1.77	0.40
1:C:150:ASN:O	1:C:151:ILE:HD12	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	206/217 (95%)	202 (98%)	3 (2%)	1 (0%)	25	47
1	B	212/217 (98%)	206 (97%)	6 (3%)	0	100	100
1	C	210/217 (97%)	206 (98%)	4 (2%)	0	100	100
1	D	205/217 (94%)	197 (96%)	7 (3%)	1 (0%)	25	47
All	All	833/868 (96%)	811 (97%)	20 (2%)	2 (0%)	44	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	149	GLY
1	A	149	GLY

### 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	178/183 (97%)	167 (94%)	11 (6%)	15	33
1	B	183/183 (100%)	167 (91%)	16 (9%)	8	17
1	C	181/183 (99%)	169 (93%)	12 (7%)	14	30
1	D	177/183 (97%)	168 (95%)	9 (5%)	20	42
All	All	719/732 (98%)	671 (93%)	48 (7%)	13	29

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	9	ILE
1	A	17	VAL
1	A	26	ARG
1	A	27	SER
1	A	78	SER
1	A	80	LEU
1	A	131	LYS
1	A	147	PHE
1	A	154	THR
1	A	203	VAL
1	B	9	ILE
1	B	26	ARG
1	B	49	GLU
1	B	74	LEU
1	B	112	THR
1	B	120	THR
1	B	130	LYS
1	B	150	ASN
1	B	176	ILE
1	B	182	GLN
1	B	194	VAL
1	B	197	THR
1	B	203	VAL
1	B	204	ILE
1	B	208	VAL
1	B	212	LYS
1	C	26	ARG
1	C	46	LYS
1	C	49	GLU
1	C	78	SER
1	C	120	THR
1	C	130	LYS
1	C	151	ILE
1	C	182	GLN
1	C	194	VAL
1	C	196	ASP
1	C	197	THR
1	C	200	VAL
1	D	9	ILE
1	D	26	ARG
1	D	49	GLU
1	D	78	SER

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Mol	Chain	Res	Type
1	D	80	LEU
1	D	103	LEU
1	D	134	LYS
1	D	147	PHE
1	D	187	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	ASN
1	A	150	ASN
1	A	157	ASN
1	B	1	ASN
1	B	2	ASN
1	B	35	GLN
1	B	150	ASN
1	C	2	ASN
1	C	90	GLN
1	C	157	ASN
1	D	142	GLN
1	D	157	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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	FMT	A	218	-	2,2,2	0.78	0	1,1,1	0.30	0
2	MLA	D	215	-	6,6,6	1.82	2 (33%)	7,7,7	1.59	1 (14%)
2	MLA	A	215	-	6,6,6	1.84	2 (33%)	7,7,7	1.50	1 (14%)
2	MLA	A	216	-	6,6,6	1.79	2 (33%)	7,7,7	1.45	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
2	MLA	D	215	-	-	2/4/4/4	-
2	MLA	A	215	-	-	2/4/4/4	-
2	MLA	A	216	-	-	0/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	215	MLA	O3A-C3	3.78	1.34	1.22
2	D	215	MLA	O3A-C3	3.64	1.34	1.22
2	A	216	MLA	O3A-C3	3.48	1.33	1.22
2	A	216	MLA	O3B-C3	-2.54	1.22	1.30
2	D	215	MLA	O3B-C3	-2.29	1.23	1.30
2	A	215	MLA	O3B-C3	-2.20	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	215	MLA	O1A-C1-C2	2.23	121.42	114.51
2	D	215	MLA	O3B-C3-C2	2.11	121.05	114.51

There are no chirality outliers.

All (4) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
2	A	215	MLA	C1-C2-C3-O3A
2	A	215	MLA	C1-C2-C3-O3B
2	D	215	MLA	C1-C2-C3-O3B
2	D	215	MLA	C1-C2-C3-O3A

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	215	MLA	1	0
2	A	216	MLA	2	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, 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	202/217 (93%)	-0.54	3 (1%) 71 67	22, 44, 69, 104	3 (1%)
1	B	211/217 (97%)	-0.51	4 (1%) 66 61	35, 50, 88, 111	0
1	C	209/217 (96%)	-0.58	3 (1%) 73 68	36, 48, 80, 109	0
1	D	202/217 (93%)	-0.57	3 (1%) 71 67	29, 45, 73, 97	2 (0%)
All	All	824/868 (94%)	-0.55	13 (1%) 70 65	22, 47, 81, 111	5 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	196[A]	ASP	3.9
1	C	0	ALA	3.3
1	A	203	VAL	3.2
1	B	213	ASN	2.6
1	B	0	ALA	2.6
1	C	195	ALA	2.6
1	C	197	THR	2.6
1	B	133	GLY	2.5
1	B	47	GLU	2.4
1	D	196	ASP	2.3
1	D	0	ALA	2.2
1	D	130	LYS	2.0
1	A	204	ILE	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, 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	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NA	A	217	1/1	0.45	0.25	68,68,68,68	0
3	NA	D	216	1/1	0.47	0.20	60,60,60,60	0
2	MLA	A	216	7/7	0.57	0.23	63,75,91,91	0
2	MLA	D	215	7/7	0.64	0.15	57,72,80,98	0
2	MLA	A	215	7/7	0.83	0.17	70,78,85,89	0
4	FMT	A	218	3/3	0.93	0.25	20,20,20,20	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.