



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 28, 2017 – 06:06 PM EST

PDB ID : 5NUR  
Title : Structural basis for maintenance of bacterial outer membrane lipid asymmetry  
Authors : Abellon-Ruiz, J.; Kaptan, S.S.; Basle, A.; Claudi, B.; Bumann, D.;  
Kleinekathofer, U.; van den Berg, B.  
Deposited on : unknown  
Resolution : 3.29 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

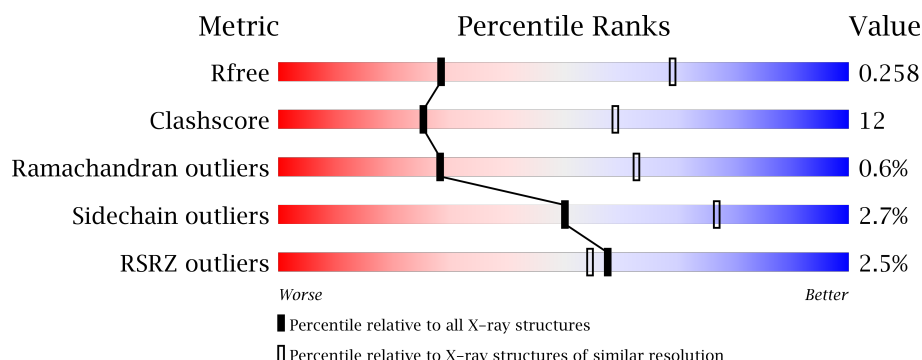
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.29 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))
$R_{free}$	100719	1034 (3.36-3.24)
Clashscore	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)
RSRZ outliers	101464	1039 (3.36-3.24)

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. 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	340	<div> <div style="width: 71%; background-color: green;"></div> <div style="width: 28%; background-color: yellow;"></div> <div style="width: 1%; background-color: orange;"></div> <div style="width: 1%; background-color: red;"></div> <div style="width: 1%; background-color: grey;"></div> </div> <div>71% 28% .</div>
1	C	340	<div> <div style="width: 75%; background-color: green;"></div> <div style="width: 23%; background-color: yellow;"></div> <div style="width: 1%; background-color: orange;"></div> <div style="width: 1%; background-color: red;"></div> <div style="width: 1%; background-color: grey;"></div> </div> <div>75% 23% .</div>
1	E	340	<div> <div style="width: 79%; background-color: green;"></div> <div style="width: 20%; background-color: yellow;"></div> <div style="width: 1%; background-color: orange;"></div> <div style="width: 1%; background-color: red;"></div> <div style="width: 1%; background-color: grey;"></div> </div> <div>79% 20% .</div>
2	B	236	<div> <div style="width: 58%; background-color: green;"></div> <div style="width: 25%; background-color: yellow;"></div> <div style="width: 16%; background-color: grey;"></div> </div> <div>58% 25% . 16%</div>
2	D	236	<div> <div style="width: 59%; background-color: green;"></div> <div style="width: 23%; background-color: yellow;"></div> <div style="width: 16%; background-color: grey;"></div> </div> <div>59% 23% . 16%</div>

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Mol	Chain	Length	Quality of chain
2	F	236	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	KDO	C	404	-	-	-	X
6	L1L	A	407	X	-	-	-
6	L1L	C	405	X	-	-	-
6	L1L	E	404	X	-	-	-
8	C8E	A	402	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12920 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 Outer membrane protein F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			
1	A	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			
1	E	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			

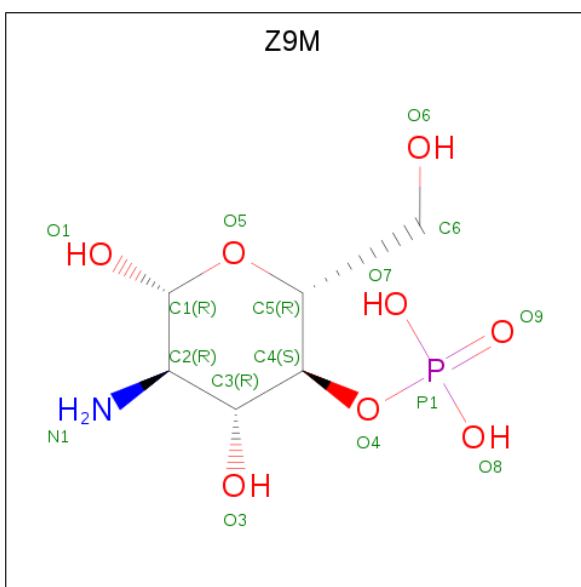
- Molecule 2 is a protein called ABC transporter permease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	199	Total	C	N	O	S	0	0	0
			1597	1031	271	287	8			
2	B	198	Total	C	N	O	S	0	0	0
			1586	1025	267	286	8			
2	F	198	Total	C	N	O	S	0	0	0
			1586	1025	267	286	8			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

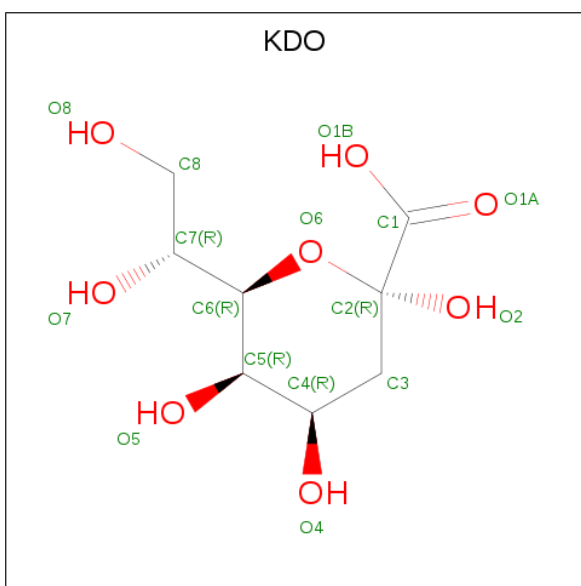
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	E	1	Total	Ca	0	0
			1	1		

- Molecule 4 is 2-amino-2-deoxy-4-O-phosphono-beta-D-glucopyranose (three-letter code: Z9M) (formula: C<sub>6</sub>H<sub>14</sub>NO<sub>8</sub>P).



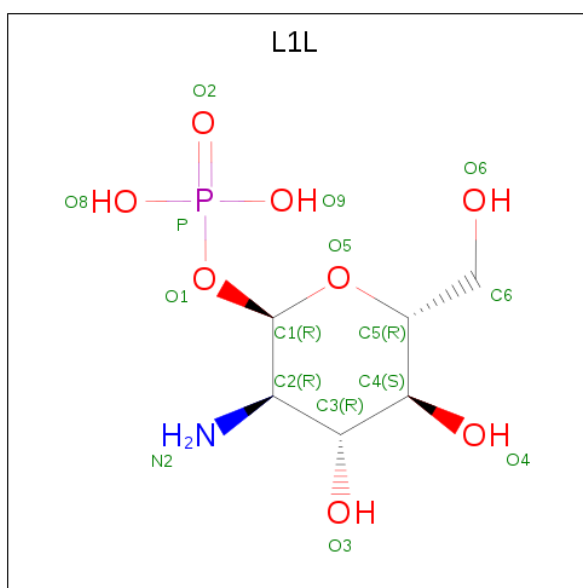
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	0	0
			16	6	1	8	1		
4	A	1	Total	C	N	O	P	0	0
			16	6	1	8	1		
4	E	1	Total	C	N	O	P	0	0
			16	6	1	8	1		

- Molecule 5 is 3-DEOXY-D-MANNO-OCT-2-ULOSONIC ACID (three-letter code: KDO) (formula:  $C_8H_{14}O_8$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			15	8	7		
5	C	1	Total	C	O	0	0
			15	8	7		
5	A	1	Total	C	O	0	0
			15	8	7		
5	A	1	Total	C	O	0	0
			15	8	7		
5	E	1	Total	C	O	0	0
			15	8	7		

- Molecule 6 is [(2R,3R,4R,5S,6R)-3-azanyl-6-(hydroxymethyl)-4,5-bis(oxidanyl)oxan-2-yl] dihydrogen phosphate (three-letter code: L1L) (formula: C<sub>6</sub>H<sub>14</sub>NO<sub>8</sub>P).



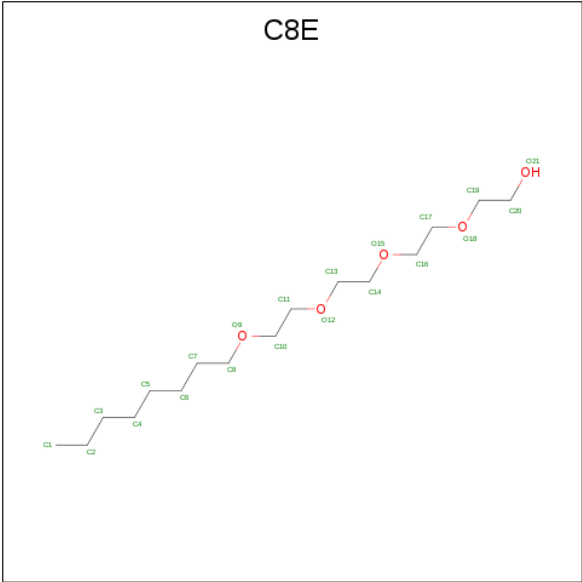
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	P	0	0
			15	6	1	7	1		
6	A	1	Total	C	N	O	P	0	0
			15	6	1	7	1		
6	E	1	Total	C	N	O	P	0	0
			15	6	1	7	1		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: C<sub>16</sub>H<sub>34</sub>O<sub>5</sub>).



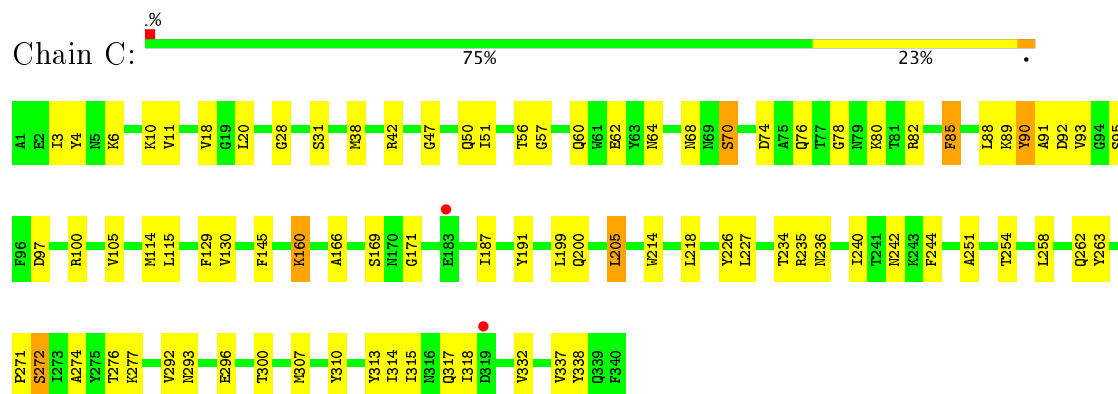
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			17	14	3		
8	A	1	Total	C	O	0	0
			21	16	5		
8	E	1	Total	C	O	0	0
			21	16	5		



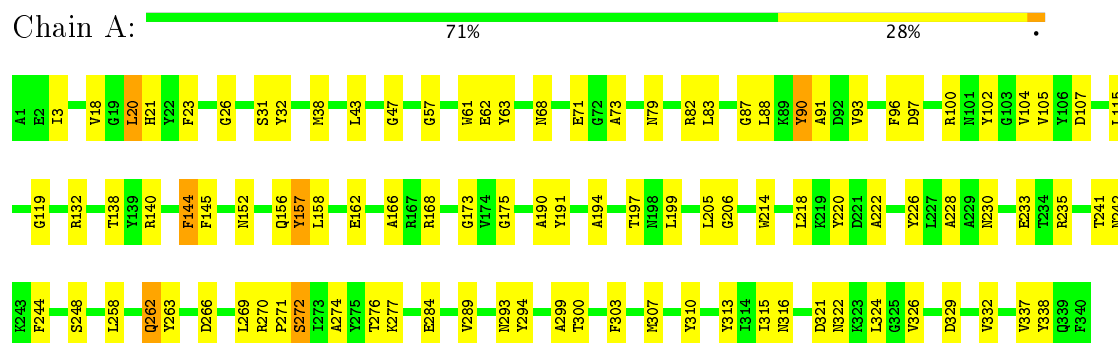
### 3 Residue-property plots [i](#)

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.

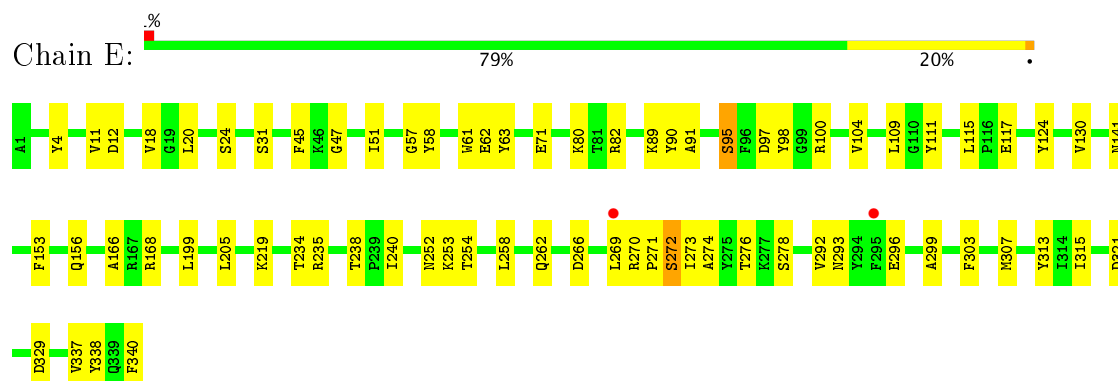
#### • Molecule 1: Outer membrane protein F



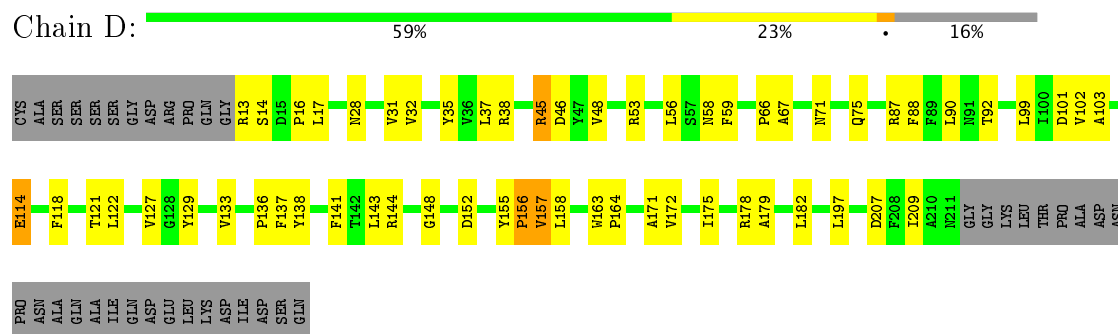
#### • Molecule 1: Outer membrane protein F



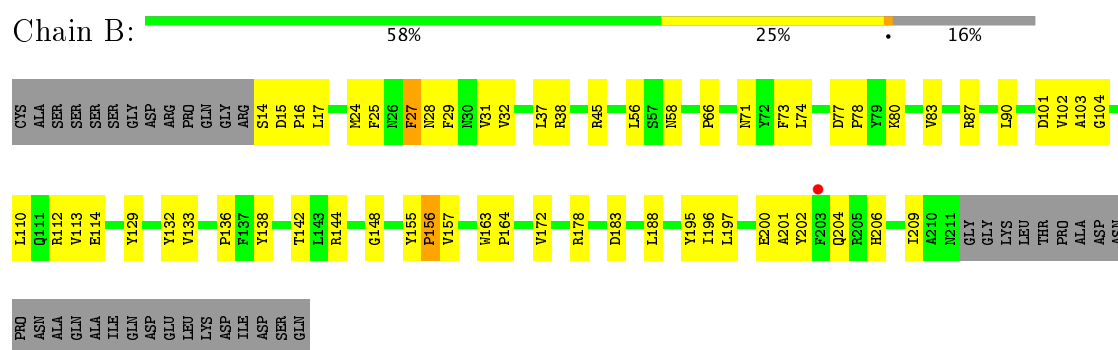
#### • Molecule 1: Outer membrane protein F



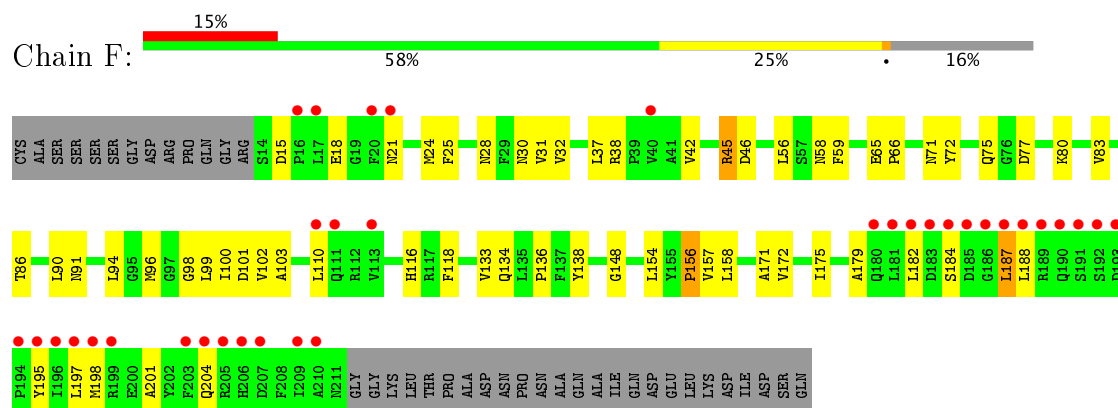
- Molecule 2: ABC transporter permease



- Molecule 2: ABC transporter permease



- Molecule 2: ABC transporter permease



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	190.55Å 179.66Å 133.39Å 90.00° 116.55° 90.00°	Depositor
Resolution (Å)	47.40 – 3.29 54.27 – 3.29	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.40-3.29) 99.4 (54.27-3.29)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 3.26Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, $R_{free}$	0.219 , 0.259 0.216 , 0.258	Depositor DCC
$R_{free}$ test set	2950 reflections (4.88%)	DCC
Wilson B-factor (Å <sup>2</sup> )	95.8	Xtriage
Anisotropy	0.672	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 81.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	12920	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: KDO, CA, Z9M, L1L, SO4, C8E

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	0.59	0/2683	0.76	1/3628 (0.0%)
1	C	0.54	0/2683	0.74	1/3628 (0.0%)
1	E	0.53	0/2683	0.73	0/3628
2	B	0.46	0/1636	0.68	0/2227
2	D	0.50	0/1647	0.72	0/2241
2	F	0.40	0/1636	0.62	1/2227 (0.0%)
All	All	0.52	0/12968	0.72	3/17579 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	154	LEU	CA-CB-CG	6.30	129.80	115.30
1	C	205	LEU	CB-CG-CD2	-5.24	102.10	111.00
1	A	43	LEU	CB-CG-CD1	-5.14	102.26	111.00

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	2627	0	2444	83	0
1	C	2627	0	2444	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2627	0	2444	57	0
2	B	1586	0	1512	33	0
2	D	1597	0	1525	40	0
2	F	1586	0	1512	41	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
4	A	16	0	10	0	0
4	C	16	0	10	1	0
4	E	16	0	10	2	0
5	A	30	0	21	1	0
5	C	30	0	21	0	0
5	E	15	0	10	0	0
6	A	15	0	0	0	0
6	C	15	0	0	0	0
6	E	15	0	0	0	0
7	A	10	0	0	0	0
7	C	15	0	0	0	0
7	E	15	0	0	2	0
8	A	38	0	61	7	0
8	E	21	0	34	4	0
All	All	12920	0	12058	300	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 12.

All (300) 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:A:289:VAL:HG11	1:A:324:LEU:HD11	1.45	0.97
1:E:262:GLN:HG2	1:E:272:SER:HB2	1.58	0.84
2:F:30:ASN:O	2:F:32:VAL:N	2.10	0.83
2:B:66:PRO:HG2	2:B:157:VAL:HG21	1.60	0.83
1:A:289:VAL:HG21	1:A:324:LEU:HD12	1.62	0.81
1:A:138:THR:HG23	1:A:156:GLN:HB2	1.65	0.79
1:E:269:LEU:HD11	1:E:299:ALA:HB1	1.66	0.78
2:F:90:LEU:HB2	2:F:103:ALA:HB2	1.65	0.77
1:C:89:LYS:HG3	1:C:95:SER:HB2	1.66	0.77
1:C:262:GLN:HG2	1:C:272:SER:HB2	1.68	0.76
2:D:37:LEU:HD22	2:D:178:ARG:HG2	1.67	0.76
2:B:83:VAL:HG13	2:B:110:LEU:HD23	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:LEU:HD22	2:B:178:ARG:HG2	1.68	0.74
1:C:90:TYR:CE1	2:F:102:VAL:HG12	2.23	0.73
1:C:166:ALA:HB2	1:C:199:LEU:HD22	1.71	0.73
1:A:289:VAL:HG11	1:A:324:LEU:CD1	2.19	0.73
1:E:166:ALA:HB2	1:E:199:LEU:HD13	1.71	0.72
2:F:157:VAL:HG23	2:F:158:LEU:HD22	1.72	0.72
1:A:62:GLU:OE1	1:A:82:ARG:NH1	2.24	0.71
1:A:233:GLU:HB3	1:A:235:ARG:HH12	1.57	0.70
2:F:59:PHE:HB2	2:F:99:LEU:HD12	1.75	0.69
1:C:338:TYR:CE2	1:A:47:GLY:HA3	2.28	0.68
1:A:26:GLY:H	8:E:401:C8E:H201	1.59	0.68
1:A:82:ARG:NH2	1:A:132:ARG:HH21	1.92	0.68
1:A:166:ALA:HB2	1:A:199:LEU:HD22	1.74	0.68
1:E:234:THR:HG1	1:E:254:THR:HG1	1.42	0.67
2:D:155:TYR:HB2	2:D:156:PRO:HD2	1.77	0.67
2:D:28:ASN:HA	2:D:32:VAL:HG22	1.77	0.67
2:D:144:ARG:O	2:D:148:GLY:HA3	1.96	0.66
1:A:31:SER:HA	1:A:329:ASP:HB2	1.76	0.66
1:A:107:ASP:OD2	1:A:140:ARG:NH2	2.30	0.65
1:A:262:GLN:OE1	1:A:270:ARG:NH1	2.30	0.65
2:D:66:PRO:HG2	2:D:157:VAL:HG11	1.77	0.65
1:E:124:TYR:HE2	1:E:238:THR:HG23	1.62	0.65
1:A:20:LEU:HB3	1:A:38:MET:HB2	1.80	0.64
1:E:258:LEU:HG	1:E:276:THR:HG23	1.79	0.63
1:C:62:GLU:OE1	1:C:82:ARG:NH1	2.32	0.63
1:A:289:VAL:HG21	1:A:324:LEU:CD1	2.28	0.62
1:A:313:TYR:HD1	1:A:332:VAL:HB	1.64	0.62
1:A:307:MET:HE3	1:E:57:GLY:HA3	1.81	0.62
2:F:25:PHE:CD2	2:F:195:TYR:HD1	2.18	0.62
2:B:27:PHE:O	2:B:31:VAL:HG22	2.00	0.62
2:F:21:ASN:HB3	2:F:134:GLN:HB3	1.83	0.61
2:F:118:PHE:HB3	2:F:148:GLY:O	2.01	0.61
1:A:145:PHE:CE1	8:A:402:C8E:H162	2.36	0.61
2:D:75:GLN:HG3	2:D:121:THR:HG22	1.83	0.61
2:D:90:LEU:HB2	2:D:103:ALA:HB2	1.82	0.61
2:F:184:SER:O	2:F:187:LEU:HD22	2.01	0.61
2:F:90:LEU:HB3	2:F:102:VAL:HG23	1.82	0.61
1:C:313:TYR:HE2	1:C:315:ILE:HG12	1.66	0.60
2:F:45:ARG:NH1	2:F:46:ASP:OD1	2.34	0.60
2:B:24:MET:HE2	2:B:136:PRO:HD3	1.83	0.60
1:C:80:LYS:HG3	1:E:71:GLU:HG2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:TYR:CE2	8:E:401:C8E:H42	2.36	0.60
1:C:80:LYS:CG	1:E:71:GLU:HG2	2.32	0.59
1:C:313:TYR:CE2	1:C:315:ILE:HG12	2.38	0.59
1:A:83:LEU:HD21	1:A:102:TYR:CE1	2.38	0.58
1:C:4:TYR:OH	1:C:6:LYS:HD3	2.04	0.58
2:B:17:LEU:HD12	2:B:133:VAL:HG12	1.84	0.58
1:C:338:TYR:CZ	1:A:47:GLY:HA3	2.38	0.58
1:A:269:LEU:HD11	1:A:299:ALA:HB1	1.85	0.58
1:C:88:LEU:HD23	1:C:90:TYR:HE1	1.69	0.58
2:D:129:TYR:OH	2:D:207:ASP:OD1	2.20	0.58
2:F:66:PRO:HG2	2:F:157:VAL:HG11	1.86	0.57
1:C:169:SER:O	1:C:200:GLN:NE2	2.37	0.57
1:C:70:SER:OG	1:A:168:ARG:HD2	2.03	0.57
1:E:235:ARG:NH1	4:E:402:Z9M:O4	2.38	0.57
1:A:145:PHE:CZ	8:A:402:C8E:H162	2.40	0.57
2:B:15:ASP:OD2	2:B:195:TYR:OH	2.22	0.56
1:A:303:PHE:HB3	1:E:51:ILE:HD13	1.86	0.56
2:F:38:ARG:NH2	2:F:182:LEU:O	2.38	0.56
2:D:163:TRP:HB3	2:D:164:PRO:HD3	1.88	0.56
1:E:31:SER:HA	1:E:329:ASP:HB2	1.87	0.56
1:E:104:VAL:CG2	1:E:156:GLN:HB3	2.36	0.56
2:F:179:ALA:HA	2:F:182:LEU:HG	1.88	0.55
2:D:99:LEU:HD23	8:A:402:C8E:H191	1.89	0.55
1:A:61:TRP:CZ2	1:A:63:TYR:HB2	2.41	0.55
1:C:300:THR:HG23	1:C:310:TYR:HB3	1.88	0.55
1:C:258:LEU:HG	1:C:276:THR:HG23	1.87	0.55
1:E:124:TYR:CE2	1:E:238:THR:HG23	2.41	0.55
2:F:58:ASN:OD1	2:F:101:ASP:HB2	2.06	0.54
1:A:157:TYR:HD1	1:A:158:LEU:N	2.05	0.54
2:F:156:PRO:O	2:F:157:VAL:HG22	2.07	0.54
1:C:296:GLU:HB2	1:C:314:ILE:HD13	1.88	0.54
1:A:226:TYR:HE1	1:A:228:ALA:HB2	1.73	0.54
1:A:71:GLU:HG2	1:E:80:LYS:HG3	1.90	0.53
1:C:90:TYR:CE1	2:F:102:VAL:CG1	2.91	0.53
2:D:171:ALA:O	2:D:175:ILE:HG13	2.08	0.53
1:E:313:TYR:HE2	1:E:315:ILE:HG12	1.74	0.53
2:F:24:MET:HG3	2:F:136:PRO:HD3	1.90	0.53
2:D:87:ARG:NH1	2:D:101:ASP:OD1	2.41	0.53
2:D:99:LEU:HD23	8:A:402:C8E:H172	1.90	0.53
1:C:307:MET:HE3	1:A:57:GLY:HA3	1.91	0.53
1:C:50:GLN:HA	1:C:56:THR:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ALA:HB2	7:E:407:SO4:O4	2.09	0.53
2:B:77:ASP:CG	2:B:80:LYS:HG2	2.30	0.52
1:C:76:GLN:HE22	1:A:79:ASN:HB2	1.74	0.52
1:C:93:VAL:HG12	2:F:100:ILE:HG12	1.90	0.52
1:C:160:LYS:HB2	1:C:171:GLY:HA2	1.91	0.52
1:E:262:GLN:OE1	1:E:270:ARG:NH1	2.42	0.52
2:B:90:LEU:HB3	2:B:102:VAL:HG23	1.91	0.52
1:A:104:VAL:HG21	1:A:156:GLN:HB3	1.91	0.51
1:A:18:VAL:HG13	1:A:337:VAL:HG22	1.92	0.51
1:E:141:ASN:HB3	1:E:153:PHE:CE1	2.45	0.51
1:E:18:VAL:HG13	1:E:337:VAL:HG22	1.91	0.51
1:A:115:LEU:HD11	1:A:274:ALA:HB2	1.92	0.51
1:A:157:TYR:CE2	8:A:401:C8E:H72	2.46	0.51
1:A:156:GLN:N	1:A:175:GLY:O	2.38	0.51
2:B:196:ILE:O	2:B:200:GLU:HB2	2.11	0.51
1:E:234:THR:OG1	1:E:254:THR:OG1	2.23	0.51
1:A:338:TYR:CZ	1:E:47:GLY:HA3	2.46	0.51
2:D:156:PRO:O	2:D:157:VAL:HG22	2.10	0.51
2:D:56:LEU:HD23	2:D:172:VAL:HG11	1.92	0.51
1:C:57:GLY:HA3	1:E:307:MET:HE3	1.93	0.51
2:D:45:ARG:NH1	2:D:46:ASP:OD1	2.44	0.50
1:C:38:MET:HA	1:C:68:ASN:HD22	1.76	0.50
1:E:104:VAL:HG21	1:E:156:GLN:HB3	1.93	0.50
1:E:253:LYS:NZ	4:E:402:Z9M:O8	2.26	0.50
1:A:88:LEU:HD23	1:A:90:TYR:HE1	1.75	0.50
1:C:234:THR:HG1	1:C:254:THR:HG1	1.55	0.50
2:F:66:PRO:HD2	2:F:157:VAL:HG21	1.93	0.50
5:A:406:KDO:O6	5:A:406:KDO:O8	2.22	0.50
1:A:32:TYR:HB2	1:A:316:ASN:ND2	2.27	0.50
1:A:93:VAL:HG11	8:A:402:C8E:O12	2.12	0.50
2:B:25:PHE:HD2	2:B:195:TYR:HB2	1.76	0.50
2:B:25:PHE:CE2	2:B:195:TYR:HA	2.47	0.49
2:D:13:ARG:HA	2:D:13:ARG:HE	1.77	0.49
2:D:90:LEU:HB3	2:D:102:VAL:HG23	1.94	0.49
2:F:77:ASP:HB3	2:F:80:LYS:HG2	1.93	0.49
1:C:205:LEU:HD23	1:C:240:ILE:HG13	1.95	0.49
1:A:322:ASN:OD1	1:A:326:VAL:HB	2.12	0.49
1:C:234:THR:OG1	1:C:254:THR:OG1	2.26	0.49
2:D:67:ALA:O	2:D:71:ASN:ND2	2.29	0.49
1:C:114:MET:HG3	1:C:226:TYR:CE2	2.48	0.49
1:A:90:TYR:HB2	1:A:93:VAL:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:56:LEU:HD23	2:F:172:VAL:HG11	1.95	0.49
1:E:269:LEU:HD22	2:F:86:THR:OG1	2.13	0.49
2:B:14:SER:O	2:B:16:PRO:HD3	2.13	0.49
1:C:191:TYR:HD2	1:C:214:TRP:HB3	1.77	0.49
1:C:18:VAL:HG13	1:C:337:VAL:HG22	1.94	0.48
2:B:201:ALA:O	2:B:204:GLN:HB3	2.13	0.48
1:A:157:TYR:CD1	1:A:158:LEU:N	2.81	0.48
1:A:277:LYS:HD2	1:A:293:ASN:OD1	2.14	0.48
1:A:38:MET:HA	1:A:68:ASN:ND2	2.29	0.48
1:A:258:LEU:HG	1:A:276:THR:HG23	1.95	0.48
1:C:20:LEU:HB3	1:C:38:MET:HB2	1.94	0.48
1:E:89:LYS:HG3	1:E:95:SER:HB2	1.95	0.48
1:C:235:ARG:NH1	4:C:402:Z9M:O4	2.47	0.48
1:C:115:LEU:HD11	1:C:274:ALA:HB2	1.94	0.48
1:E:62:GLU:OE1	1:E:82:ARG:NH1	2.45	0.48
1:A:21:HIS:HD2	1:A:23:PHE:CE1	2.31	0.48
1:A:162:GLU:OE2	1:A:197:THR:HB	2.14	0.47
1:A:313:TYR:CE2	1:A:315:ILE:HG12	2.49	0.47
2:B:144:ARG:O	2:B:148:GLY:HA3	2.14	0.47
2:D:59:PHE:HB2	2:D:99:LEU:HD12	1.96	0.47
1:E:24:SER:HB3	1:E:31:SER:OG	2.14	0.47
1:A:263:TYR:O	1:A:271:PRO:HD2	2.13	0.47
1:C:105:VAL:HB	1:C:130:VAL:HG12	1.97	0.47
2:B:28:ASN:HA	2:B:32:VAL:CG1	2.44	0.47
2:D:14:SER:O	2:D:16:PRO:HD3	2.15	0.47
2:F:96:MET:HB2	2:F:100:ILE:HD12	1.97	0.47
1:A:266:ASP:N	1:A:266:ASP:OD1	2.48	0.47
2:B:73:PHE:CE1	2:B:78:PRO:HA	2.50	0.47
1:E:4:TYR:HB3	1:E:11:VAL:HB	1.97	0.47
1:C:51:ILE:HD13	1:E:303:PHE:HB3	1.97	0.47
2:F:195:TYR:O	2:F:198:MET:HB3	2.14	0.46
1:C:313:TYR:HD1	1:C:332:VAL:HB	1.80	0.46
2:D:66:PRO:HD2	2:D:157:VAL:HG21	1.97	0.46
1:A:82:ARG:CZ	1:A:132:ARG:HH21	2.28	0.46
1:C:92:ASP:O	1:C:145:PHE:HA	2.15	0.46
1:C:97:ASP:N	1:C:97:ASP:OD1	2.48	0.46
2:D:114:GLU:HG3	2:D:209:ILE:HG13	1.97	0.46
1:E:111:TYR:CD2	1:E:219:LYS:HB3	2.49	0.46
1:A:226:TYR:CE1	1:A:228:ALA:HB2	2.50	0.46
2:B:87:ARG:HA	2:B:103:ALA:CB	2.46	0.46
1:C:11:VAL:HG21	1:E:340:PHE:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:VAL:HA	1:A:190:ALA:CB	2.46	0.46
1:A:173:GLY:HA3	1:A:194:ALA:HB2	1.97	0.46
2:D:58:ASN:OD1	2:D:101:ASP:HB2	2.15	0.46
1:A:119:GLY:HA2	1:A:294:TYR:OH	2.15	0.46
1:A:321:ASP:OD1	1:A:321:ASP:N	2.46	0.46
1:C:242:ASN:OD1	1:C:244:PHE:HB2	2.15	0.46
2:D:31:VAL:O	2:D:35:TYR:HB2	2.16	0.46
1:A:218:LEU:HD23	1:A:218:LEU:HA	1.67	0.45
1:C:240:ILE:HG21	1:C:251:ALA:HB2	1.99	0.45
1:C:42:ARG:HE	1:C:64:ASN:HD22	1.63	0.45
1:A:220:TYR:CE1	1:A:222:ALA:HB3	2.51	0.45
2:D:122:LEU:O	2:D:127:VAL:HG22	2.17	0.45
1:E:20:LEU:HD11	1:E:117:GLU:CD	2.36	0.45
1:C:28:GLY:HA2	1:C:31:SER:OG	2.16	0.45
1:C:64:ASN:HB2	1:C:82:ARG:HD2	1.99	0.45
1:E:278:SER:HB3	1:E:292:VAL:HG23	1.99	0.45
1:A:313:TYR:CD1	1:A:332:VAL:HB	2.47	0.45
1:A:26:GLY:N	8:E:401:C8E:H201	2.31	0.45
1:E:12:ASP:O	1:E:45:PHE:HA	2.17	0.45
1:A:105:VAL:HA	1:A:190:ALA:HB1	1.99	0.44
1:A:289:VAL:CG1	1:A:324:LEU:CD1	2.94	0.44
1:C:313:TYR:CD1	1:C:332:VAL:HB	2.52	0.44
1:A:38:MET:HA	1:A:68:ASN:HD22	1.81	0.44
1:A:115:LEU:HD22	1:A:119:GLY:HA3	1.99	0.44
2:F:171:ALA:O	2:F:175:ILE:HG13	2.16	0.44
2:F:38:ARG:NH1	2:F:182:LEU:HD22	2.32	0.44
2:B:163:TRP:HB3	2:B:164:PRO:HD3	1.99	0.44
2:D:197:LEU:HA	2:D:197:LEU:HD23	1.72	0.44
1:E:109:LEU:HA	1:E:109:LEU:HD23	1.73	0.44
2:F:28:ASN:HA	2:F:32:VAL:HG12	1.98	0.44
2:D:102:VAL:HG11	1:A:90:TYR:CE1	2.53	0.44
2:B:114:GLU:HG3	2:B:209:ILE:HD11	2.00	0.44
1:C:4:TYR:O	1:C:10:LYS:HA	2.17	0.44
2:F:71:ASN:O	2:F:75:GLN:HG3	2.18	0.44
2:B:132:TYR:HA	2:B:142:THR:HG22	1.99	0.43
1:C:218:LEU:HD23	1:C:218:LEU:HA	1.70	0.43
1:A:157:TYR:HD1	1:A:158:LEU:H	1.66	0.43
1:A:206:GLY:H	1:A:284:GLU:CD	2.22	0.43
1:A:262:GLN:HB3	1:A:272:SER:HB2	2.00	0.43
1:C:70:SER:HB3	1:C:74:ASP:OD1	2.18	0.43
2:D:133:VAL:HG23	2:D:141:PHE:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:VAL:CG1	2:F:100:ILE:HG12	2.48	0.43
1:A:93:VAL:HG12	1:A:145:PHE:HD1	1.83	0.43
2:F:83:VAL:HG13	2:F:110:LEU:HD23	2.01	0.43
2:D:157:VAL:HG23	2:D:158:LEU:N	2.33	0.43
1:E:61:TRP:CZ2	1:E:63:TYR:HB2	2.54	0.43
1:C:226:TYR:O	1:C:227:LEU:HD23	2.19	0.43
1:C:293:ASN:HB3	1:C:318:ILE:HD12	2.00	0.43
1:A:71:GLU:HG2	1:E:80:LYS:CG	2.48	0.43
1:A:191:TYR:HD2	1:A:214:TRP:HB3	1.84	0.43
1:A:241:THR:HA	1:A:248:SER:HA	2.01	0.43
2:B:29:PHE:HE1	2:B:188:LEU:HD23	1.84	0.43
1:C:236:ASN:OD1	1:C:236:ASN:N	2.51	0.43
1:C:293:ASN:ND2	1:C:317:GLN:HB2	2.34	0.43
2:B:112:ARG:HG3	2:B:113:VAL:N	2.33	0.43
1:C:88:LEU:HD23	1:C:90:TYR:CE1	2.53	0.43
2:F:188:LEU:HD13	2:F:197:LEU:HD11	2.00	0.43
1:C:60:GLN:HB3	1:C:85:PHE:CE1	2.54	0.42
2:D:118:PHE:HB2	2:D:152:ASP:OD1	2.18	0.42
2:F:94:LEU:O	2:F:96:MET:N	2.50	0.42
2:B:77:ASP:OD1	2:B:80:LYS:HG2	2.18	0.42
1:C:18:VAL:HG22	1:C:337:VAL:HG22	2.00	0.42
1:E:307:MET:HE2	1:E:338:TYR:HD1	1.84	0.42
2:F:38:ARG:O	2:F:42:VAL:HG23	2.20	0.42
2:B:71:ASN:HA	2:B:74:LEU:HB2	2.01	0.42
1:C:105:VAL:HG23	1:C:129:PHE:HB3	2.02	0.42
2:B:56:LEU:HD23	2:B:172:VAL:CG1	2.49	0.42
2:F:201:ALA:HA	2:F:204:GLN:HB2	2.02	0.42
2:F:91:ASN:HB3	2:F:98:GLY:HA2	2.00	0.42
1:A:313:TYR:HE2	1:A:315:ILE:HG12	1.85	0.42
2:B:58:ASN:OD1	2:B:101:ASP:HB2	2.20	0.42
1:C:3:ILE:HG21	1:A:3:ILE:HD12	2.00	0.42
2:D:17:LEU:HD12	2:D:133:VAL:HG12	2.02	0.42
2:D:157:VAL:HG23	2:D:158:LEU:H	1.84	0.42
1:E:109:LEU:HD12	1:E:130:VAL:CG2	2.50	0.42
1:E:269:LEU:HG	1:E:271:PRO:HD3	2.02	0.42
2:F:28:ASN:HA	2:F:32:VAL:CG1	2.50	0.42
2:D:143:LEU:HA	2:D:143:LEU:HD23	1.74	0.42
1:E:205:LEU:HD23	1:E:240:ILE:HG13	2.02	0.42
1:A:144:PHE:HD1	1:A:145:PHE:CD2	2.37	0.42
1:C:187:ILE:HD12	1:C:218:LEU:HD21	2.01	0.42
1:E:58:TYR:CE2	1:E:97:ASP:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:GLY:HA3	1:E:338:TYR:CZ	2.55	0.41
1:C:78:GLY:O	1:C:80:LYS:HD3	2.20	0.41
2:F:65:GLU:HB2	2:F:66:PRO:HD3	2.01	0.41
1:A:242:ASN:OD1	1:A:244:PHE:HB2	2.20	0.41
2:F:24:MET:HE2	2:F:136:PRO:HB3	2.02	0.41
1:E:266:ASP:N	1:E:266:ASP:OD1	2.52	0.41
2:F:15:ASP:HB3	2:F:18:GLU:OE1	2.20	0.41
2:D:114:GLU:HG2	2:D:114:GLU:O	2.20	0.41
2:D:136:PRO:HB2	2:D:137:PHE:CD2	2.56	0.41
1:E:18:VAL:HG22	1:E:337:VAL:HG13	2.03	0.41
1:A:87:GLY:HA3	1:A:97:ASP:HB3	2.03	0.41
1:A:262:GLN:NE2	1:A:272:SER:HB2	2.35	0.41
1:C:277:LYS:HA	1:C:292:VAL:O	2.21	0.41
1:A:300:THR:HG23	1:A:310:TYR:HB3	2.03	0.41
2:D:48:VAL:HG12	2:D:53:ARG:HG3	2.02	0.41
2:D:66:PRO:HG2	2:D:157:VAL:CG1	2.49	0.41
1:E:115:LEU:HD11	1:E:274:ALA:HB2	2.03	0.41
1:E:104:VAL:HG23	1:E:156:GLN:HB3	2.01	0.41
1:A:276:THR:O	1:A:293:ASN:HA	2.20	0.41
2:B:87:ARG:NH1	2:B:101:ASP:OD1	2.54	0.41
1:C:20:LEU:HA	1:C:20:LEU:HD23	1.66	0.41
2:D:179:ALA:HA	2:D:182:LEU:HG	2.02	0.41
1:E:20:LEU:HA	1:E:20:LEU:HD23	1.73	0.41
1:E:168:ARG:NH1	7:E:408:SO4:O1	2.49	0.41
1:E:58:TYR:HE2	1:E:97:ASP:HB3	1.86	0.41
2:F:21:ASN:ND2	2:F:133:VAL:HA	2.36	0.41
2:B:129:TYR:N	2:B:129:TYR:CD1	2.89	0.40
1:C:263:TYR:O	1:C:271:PRO:HD2	2.21	0.40
2:D:88:PHE:O	2:D:92:THR:OG1	2.27	0.40
1:E:321:ASP:N	1:E:321:ASP:OD1	2.51	0.40
1:A:205:LEU:HB2	1:A:248:SER:O	2.22	0.40
2:B:155:TYR:HB2	2:B:156:PRO:HD2	2.03	0.40
1:C:47:GLY:HA3	1:E:338:TYR:CE2	2.56	0.40
1:A:96:PHE:HA	1:A:138:THR:O	2.22	0.40
2:B:197:LEU:HA	2:B:197:LEU:HD23	1.91	0.40
8:E:401:C8E:H202	8:E:401:C8E:H171	1.87	0.40
2:B:202:TYR:CE2	2:B:206:HIS:NE2	2.90	0.40
2:B:25:PHE:CE1	2:B:29:PHE:HB2	2.56	0.40
1:E:273:ILE:HA	1:E:296:GLU:O	2.22	0.40
1:C:80:LYS:CB	1:E:71:GLU:HG2	2.51	0.40
8:A:402:C8E:H42	8:A:402:C8E:H13	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:276:THR:O	1:E:293:ASN:HA	2.22	0.40

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	A	338/340 (99%)	315 (93%)	22 (6%)	1 (0%)	44	76
1	C	338/340 (99%)	316 (94%)	21 (6%)	1 (0%)	44	76
1	E	338/340 (99%)	317 (94%)	20 (6%)	1 (0%)	44	76
2	B	196/236 (83%)	175 (89%)	19 (10%)	2 (1%)	18	53
2	D	197/236 (84%)	173 (88%)	22 (11%)	2 (1%)	18	53
2	F	196/236 (83%)	175 (89%)	19 (10%)	2 (1%)	18	53
All	All	1603/1728 (93%)	1471 (92%)	123 (8%)	9 (1%)	28	63

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	91	ALA
1	A	91	ALA
1	E	91	ALA
2	F	31	VAL
2	D	156	PRO
2	B	156	PRO
2	F	156	PRO
2	D	157	VAL
2	B	104	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	263/263 (100%)	254 (97%)	9 (3%)	42	73
1	C	263/263 (100%)	257 (98%)	6 (2%)	56	79
1	E	263/263 (100%)	258 (98%)	5 (2%)	62	81
2	B	167/197 (85%)	162 (97%)	5 (3%)	46	75
2	D	168/197 (85%)	164 (98%)	4 (2%)	54	79
2	F	167/197 (85%)	161 (96%)	6 (4%)	40	72
All	All	1291/1380 (94%)	1256 (97%)	35 (3%)	50	77

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	70	SER
1	C	85	PHE
1	C	90	TYR
1	C	100	ARG
1	C	160	LYS
1	C	272	SER
2	D	38	ARG
2	D	45	ARG
2	D	114	GLU
2	D	138	TYR
1	A	20	LEU
1	A	90	TYR
1	A	100	ARG
1	A	144	PHE
1	A	152	ASN
1	A	157	TYR
1	A	230	ASN
1	A	262	GLN
1	A	272	SER
2	B	27	PHE
2	B	38	ARG
2	B	45	ARG

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Mol	Chain	Res	Type
2	B	138	TYR
2	B	183	ASP
1	E	90	TYR
1	E	95	SER
1	E	100	ARG
1	E	252	ASN
1	E	272	SER
2	F	37	LEU
2	F	45	ARG
2	F	72	TYR
2	F	116	HIS
2	F	138	TYR
2	F	187	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	64	ASN
1	C	66	GLN
2	F	75	GLN

### 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](#)

Of 25 ligands modelled in this entry, 3 are monoatomic - leaving 22 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	$\# Z  > 2$
8	C8E	A	401	-	16,16,20	0.65	0	15,15,19	0.88	0
8	C8E	A	402	-	20,20,20	0.49	0	19,19,19	0.58	0
4	Z9M	A	404	5,6	16,16,16	2.21	3 (18%)	21,24,24	1.24	2 (9%)
5	KDO	A	405	5,4	12,15,16	1.66	4 (33%)	13,21,24	1.71	2 (15%)
5	KDO	A	406	3,5	12,15,16	1.46	2 (16%)	13,21,24	1.93	2 (15%)
6	L1L	A	407	4	14,15,16	2.20	5 (35%)	21,23,24	2.42	7 (33%)
7	SO4	A	408	-	4,4,4	0.14	0	6,6,6	0.23	0
7	SO4	A	409	-	4,4,4	0.24	0	6,6,6	0.68	0
4	Z9M	C	402	5,6	16,16,16	2.30	3 (18%)	21,24,24	1.05	1 (4%)
5	KDO	C	403	5,4	12,15,16	1.73	2 (16%)	13,21,24	1.20	2 (15%)
5	KDO	C	404	3,5	12,15,16	1.63	4 (33%)	13,21,24	1.95	4 (30%)
6	L1L	C	405	4	14,15,16	1.90	5 (35%)	21,23,24	1.44	2 (9%)
7	SO4	C	406	-	4,4,4	0.19	0	6,6,6	0.27	0
7	SO4	C	407	-	4,4,4	0.19	0	6,6,6	0.28	0
7	SO4	C	408	-	4,4,4	0.18	0	6,6,6	0.70	0
8	C8E	E	401	-	20,20,20	0.47	0	19,19,19	0.41	0
4	Z9M	E	402	5,6	16,16,16	2.12	3 (18%)	21,24,24	1.15	3 (14%)
5	KDO	E	403	3,4	12,15,16	1.52	3 (25%)	13,21,24	3.48	6 (46%)
6	L1L	E	404	4	14,15,16	2.05	6 (42%)	21,23,24	2.10	7 (33%)
7	SO4	E	406	-	4,4,4	0.17	0	6,6,6	0.18	0
7	SO4	E	407	-	4,4,4	0.22	0	6,6,6	0.42	0
7	SO4	E	408	-	4,4,4	0.10	0	6,6,6	0.30	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
8	C8E	A	401	-	-	0/14/14/18	0/0/0/0
8	C8E	A	402	-	-	0/18/18/18	0/0/0/0
4	Z9M	A	404	5,6	-	0/7/27/27	0/1/1/1
5	KDO	A	405	5,4	-	0/6/26/30	0/1/1/1
5	KDO	A	406	3,5	-	0/6/26/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	L1L	A	407	4	1/1/6/6	0/4/25/27	0/1/1/1
7	SO4	A	408	-	-	0/0/0/0	0/0/0/0
7	SO4	A	409	-	-	0/0/0/0	0/0/0/0
4	Z9M	C	402	5,6	-	0/7/27/27	0/1/1/1
5	KDO	C	403	5,4	-	0/6/26/30	0/1/1/1
5	KDO	C	404	3,5	-	0/6/26/30	0/1/1/1
6	L1L	C	405	4	1/1/6/6	0/4/25/27	0/1/1/1
7	SO4	C	406	-	-	0/0/0/0	0/0/0/0
7	SO4	C	407	-	-	0/0/0/0	0/0/0/0
7	SO4	C	408	-	-	0/0/0/0	0/0/0/0
8	C8E	E	401	-	-	0/18/18/18	0/0/0/0
4	Z9M	E	402	5,6	-	0/7/27/27	0/1/1/1
5	KDO	E	403	3,4	-	0/6/26/30	0/1/1/1
6	L1L	E	404	4	1/1/6/6	0/4/25/27	0/1/1/1
7	SO4	E	406	-	-	0/0/0/0	0/0/0/0
7	SO4	E	407	-	-	0/0/0/0	0/0/0/0
7	SO4	E	408	-	-	0/0/0/0	0/0/0/0

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	405	L1L	C3-C2	-3.31	1.49	1.53
6	A	407	L1L	C3-C2	-3.21	1.49	1.53
4	E	402	Z9M	C3-C2	-3.16	1.49	1.53
4	C	402	Z9M	C3-C2	-3.06	1.49	1.53
5	C	403	KDO	C3-C4	-2.99	1.48	1.52
6	E	404	L1L	C3-C2	-2.98	1.49	1.53
5	C	404	KDO	C3-C4	-2.63	1.48	1.52
5	A	405	KDO	C3-C4	-2.24	1.49	1.52
5	E	403	KDO	O7-C7	-2.21	1.38	1.43
5	C	404	KDO	O7-C7	-2.07	1.38	1.43
5	A	406	KDO	C3-C4	-2.04	1.49	1.52
5	A	405	KDO	O7-C7	-2.04	1.38	1.43
5	C	404	KDO	C4-C5	-2.02	1.49	1.52
6	E	404	L1L	C1-C2	2.05	1.56	1.52
6	A	407	L1L	C2-N2	2.09	1.50	1.47
5	E	403	KDO	O6-C6	2.11	1.47	1.43
6	C	405	L1L	C2-N2	2.13	1.50	1.47
5	A	405	KDO	O6-C6	2.15	1.47	1.43
6	C	405	L1L	O3-C3	2.31	1.48	1.43
6	E	404	L1L	C2-N2	2.40	1.50	1.47
4	A	404	Z9M	C1-C2	2.53	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	406	KDO	O6-C2	2.64	1.50	1.43
6	C	405	L1L	O5-C1	2.73	1.48	1.41
6	E	404	L1L	O5-C1	2.78	1.48	1.41
6	A	407	L1L	O3-C3	2.79	1.49	1.43
6	A	407	L1L	O5-C1	2.81	1.48	1.41
6	E	404	L1L	O3-C3	2.81	1.49	1.43
5	E	403	KDO	O6-C2	3.05	1.51	1.43
5	A	405	KDO	O6-C2	3.14	1.52	1.43
5	C	404	KDO	O6-C2	3.17	1.52	1.43
5	C	403	KDO	O6-C2	3.58	1.53	1.43
6	C	405	L1L	P-O1	3.86	1.66	1.59
6	E	404	L1L	P-O1	4.26	1.67	1.59
4	E	402	Z9M	O5-C1	4.76	1.51	1.43
4	C	402	Z9M	O5-C1	4.80	1.51	1.43
4	A	404	Z9M	O5-C1	4.85	1.52	1.43
6	A	407	L1L	P-O1	5.24	1.68	1.59
4	E	402	Z9M	P1-O4	5.41	1.69	1.59
4	A	404	Z9M	P1-O4	5.68	1.69	1.59
4	C	402	Z9M	P1-O4	6.16	1.70	1.59

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	404	L1L	C6-C5-C4	-2.51	108.59	113.07
5	C	404	KDO	O5-C5-C4	-2.05	106.30	110.02
5	E	403	KDO	O4-C4-C5	-2.04	106.16	110.17
6	A	407	L1L	C1-O5-C5	2.07	117.34	113.67
4	E	402	Z9M	C1-C2-C3	2.13	113.40	110.60
5	C	403	KDO	C3-C4-C5	2.13	113.37	110.59
5	C	403	KDO	O4-C4-C5	2.26	114.61	110.17
6	C	405	L1L	C1-C2-C3	2.28	116.30	109.96
5	A	405	KDO	C4-C3-C2	2.28	114.02	109.75
4	C	402	Z9M	O5-C5-C4	2.31	114.47	109.75
5	C	404	KDO	C3-C4-C5	2.31	113.60	110.59
4	E	402	Z9M	O5-C1-C2	2.34	112.24	109.51
4	A	404	Z9M	C1-C2-C3	2.52	113.92	110.60
6	E	404	L1L	C1-O5-C5	2.55	118.17	113.67
6	E	404	L1L	O1-C1-C2	2.59	113.09	108.40
4	E	402	Z9M	O5-C5-C6	2.67	112.79	106.41
6	E	404	L1L	O5-C1-C2	2.75	116.24	110.06
6	A	407	L1L	O5-C1-C2	2.76	116.27	110.06
6	A	407	L1L	O5-C5-C4	2.95	114.49	109.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	404	L1L	C1-C2-C3	2.97	118.22	109.96
5	C	404	KDO	O6-C2-C3	2.97	115.17	109.82
6	A	407	L1L	C1-C2-C3	3.10	118.58	109.96
4	A	404	Z9M	O1-C1-C2	3.29	115.75	108.96
6	A	407	L1L	O5-C5-C6	3.37	113.83	106.69
5	A	406	KDO	O6-C2-C3	3.66	116.41	109.82
5	E	403	KDO	C4-C5-C6	3.76	118.09	110.47
6	E	404	L1L	O5-C5-C4	3.92	116.08	109.62
5	A	406	KDO	C3-C4-C5	4.21	116.09	110.59
5	E	403	KDO	C4-C3-C2	4.33	117.87	109.75
6	A	407	L1L	O5-C1-O1	4.34	117.04	111.36
6	C	405	L1L	C3-C4-C5	4.54	116.82	109.68
5	C	404	KDO	C4-C3-C2	4.58	118.35	109.75
5	A	405	KDO	O6-C6-C5	4.71	115.02	108.00
5	E	403	KDO	O6-C2-C3	5.23	119.24	109.82
6	E	404	L1L	C3-C4-C5	5.88	118.92	109.68
5	E	403	KDO	C3-C4-C5	6.19	118.68	110.59
5	E	403	KDO	O6-C6-C5	6.99	118.41	108.00
6	A	407	L1L	C3-C4-C5	7.03	120.73	109.68

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	407	L1L	C3
6	E	404	L1L	C3
6	C	405	L1L	C3

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	401	C8E	1	0
8	A	402	C8E	6	0
5	A	406	KDO	1	0
4	C	402	Z9M	1	0
8	E	401	C8E	4	0
4	E	402	Z9M	2	0
7	E	407	SO4	1	0
7	E	408	SO4	1	0

## 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	340/340 (100%)	-0.07	0 100 100	79, 99, 130, 147	0
1	C	340/340 (100%)	0.10	2 (0%) 89 88	85, 110, 148, 179	0
1	E	340/340 (100%)	0.07	2 (0%) 89 88	87, 109, 136, 153	0
2	B	198/236 (83%)	0.11	1 (0%) 90 90	112, 135, 156, 216	0
2	D	199/236 (84%)	-0.14	0 100 100	103, 126, 147, 206	0
2	F	198/236 (83%)	0.73	35 (17%) 2 1	104, 160, 227, 276	0
All	All	1615/1728 (93%)	0.11	40 (2%) 58 54	79, 116, 171, 276	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	192	SER	6.6
2	F	187	LEU	6.0
2	F	193	ASP	5.4
2	F	195	TYR	4.9
2	F	196	ILE	4.8
2	F	181	LEU	4.6
2	F	209	ILE	4.4
2	F	182	LEU	4.3
2	F	184	SER	4.2
2	F	188	LEU	3.8
2	F	190	GLN	3.6
2	F	110	LEU	3.6
2	F	203	PHE	3.5
2	F	206	HIS	3.4
2	F	199	ARG	3.4
2	F	204	GLN	3.4
2	F	191	SER	3.3
2	F	197	LEU	3.3
2	F	207	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
2	F	113	VAL	3.0
2	F	21	ASN	2.9
2	F	194	PRO	2.8
2	F	205	ARG	2.8
2	F	180	GLN	2.8
2	F	17	LEU	2.8
2	F	20	PHE	2.7
2	F	198	MET	2.7
2	F	210	ALA	2.5
2	F	186	GLY	2.5
2	F	16	PRO	2.5
1	C	183	GLU	2.4
2	B	203	PHE	2.4
1	E	295	PHE	2.3
2	F	40	VAL	2.3
2	F	185	ASP	2.3
2	F	183	ASP	2.1
2	F	111	GLN	2.1
1	C	319	ASP	2.1
1	E	269	LEU	2.0
2	F	189	ARG	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 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. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
8	C8E	A	402	21/21	0.69	0.38	5.25	103,115,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	C8E	A	401	17/21	0.82	0.32	1.30	90,108,118,118	0
5	KDO	C	404	15/16	0.81	0.44	0.96	222,228,229,229	0
5	KDO	A	406	15/16	0.91	0.34	0.68	157,165,169,171	0
8	C8E	E	401	21/21	0.87	0.25	0.41	83,121,129,131	0
7	SO4	C	408	5/5	0.97	0.20	-0.21	91,93,94,96	0
7	SO4	E	407	5/5	0.97	0.19	-1.13	97,97,99,104	0
7	SO4	A	409	5/5	0.99	0.17	-2.66	94,94,99,99	0
3	CA	A	403	1/1	0.96	0.08	-	149,149,149,149	0
7	SO4	C	407	5/5	0.83	0.42	-	172,173,174,175	0
5	KDO	C	403	15/16	0.63	0.43	-	222,226,228,228	0
4	Z9M	E	402	16/16	0.80	0.14	-	165,183,193,202	0
7	SO4	C	406	5/5	0.89	0.36	-	171,173,174,176	0
5	KDO	A	405	15/16	0.81	0.32	-	160,167,174,174	0
6	L1L	A	407	15/16	0.82	0.19	-	148,152,153,155	0
7	SO4	E	408	5/5	0.81	0.39	-	191,192,193,194	0
3	CA	E	405	1/1	0.71	0.28	-	237,237,237,237	0
7	SO4	E	406	5/5	0.93	0.43	-	161,162,163,165	0
4	Z9M	C	402	16/16	0.66	0.20	-	182,194,208,215	0
6	L1L	E	404	15/16	0.82	0.23	-	165,169,175,177	0
4	Z9M	A	404	16/16	0.75	0.18	-	150,158,165,168	0
3	CA	C	401	1/1	0.76	0.13	-	207,207,207,207	0
5	KDO	E	403	15/16	0.72	0.26	-	199,205,214,223	0
7	SO4	A	408	5/5	0.95	0.30	-	177,180,180,181	0
6	L1L	C	405	15/16	0.84	0.18	-	194,198,202,202	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.