



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 28, 2017 – 06:19 PM EST

PDB ID : 5NUP
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 : 2.90 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (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

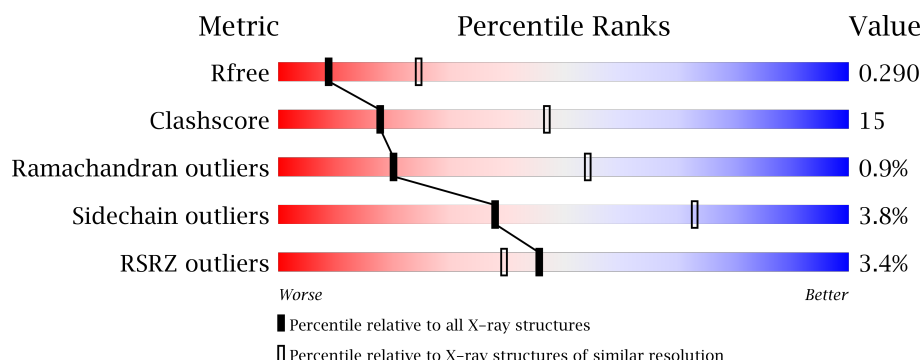
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	344	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>27%</div> <div>.</div> </div> </div>
1	B	344	<div> <div>5%</div> <div> <div></div> <div>70%</div> <div>28%</div> <div>.</div> </div> </div>
1	C	344	<div> <div>5%</div> <div> <div></div> <div>71%</div> <div>27%</div> <div>.</div> </div> </div>
2	D	236	<div> <div>0%</div> <div> <div></div> <div>55%</div> <div>26%</div> <div>..</div> <div>16%</div> </div> </div>
2	E	236	<div> <div>2%</div> <div> <div></div> <div>57%</div> <div>26%</div> <div>.</div> <div>16%</div> </div> </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
3	C8E	A	406	-	-	-	X
3	C8E	B	404	-	-	-	X
3	C8E	C	404	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13238 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 OmpK36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	0	0
			2693	1687	453	551	2			
1	B	344	Total	C	N	O	S	0	0	0
			2693	1687	453	551	2			
1	C	344	Total	C	N	O	S	0	0	0
			2693	1687	453	551	2			

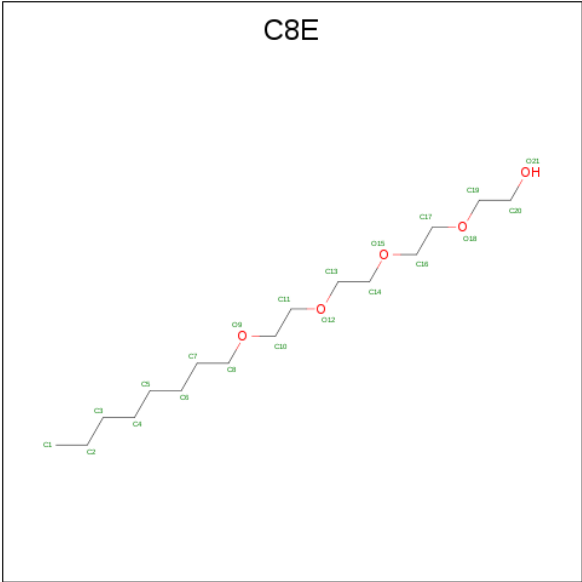
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	231	ARG	GLN	conflict	UNP D6QLY0
B	231	ARG	GLN	conflict	UNP D6QLY0
C	231	ARG	GLN	conflict	UNP D6QLY0

- 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	E	199	Total	C	N	O	S	0	0	0
			1597	1031	271	287	8			
2	F	204	Total	C	N	O	S	0	0	0
			1620	1044	276	292	8			

- Molecule 3 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: C₁₆H₃₄O₅).



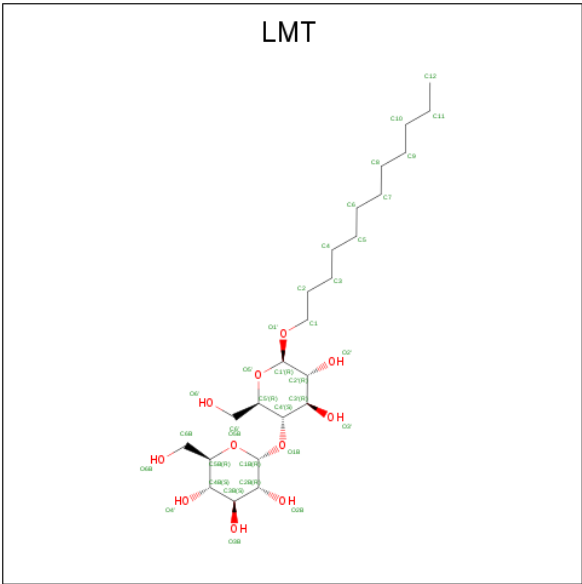
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	13	3		
3	A	1	Total	C	O	0	0
			10	9	1		
3	A	1	Total	C	O	0	0
			13	11	2		
3	A	1	Total	C	O	0	0
			9	6	3		
3	A	1	Total	C	O	0	0
			16	13	3		
3	A	1	Total	C	O	0	0
			11	10	1		
3	B	1	Total	C	O	0	0
			11	10	1		
3	B	1	Total	C	O	0	0
			18	14	4		
3	B	1	Total	C	O	0	0
			16	13	3		
3	B	1	Total	C	O	0	0
			15	12	3		
3	C	1	Total	C	O	0	0
			16	13	3		
3	C	1	Total	C	O	0	0
			21	16	5		
3	C	1	Total	C	O	0	0
			13	11	2		
3	C	1	Total	C	O	0	0
			16	13	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			13	11	2		
3	D	1	Total	C	O	0	0
			12	10	2		
3	E	1	Total	C		0	0
			8	8			
3	E	1	Total	C	O	0	0
			20	16	4		
3	F	1	Total	C	O	0	0
			7	6	1		

- Molecule 4 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).

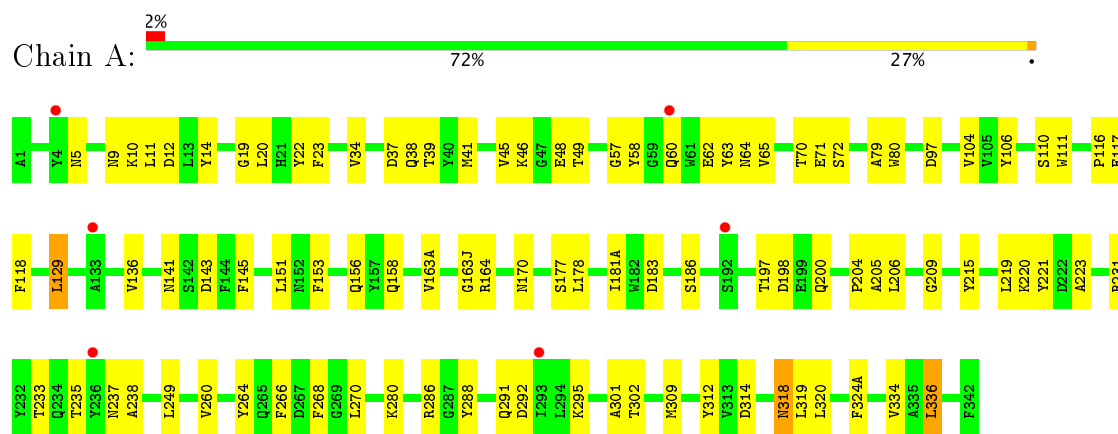


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			35	24	11		
4	B	1	Total	C	O	0	0
			25	14	11		
4	F	1	Total	C	O	0	0
			24	13	11		

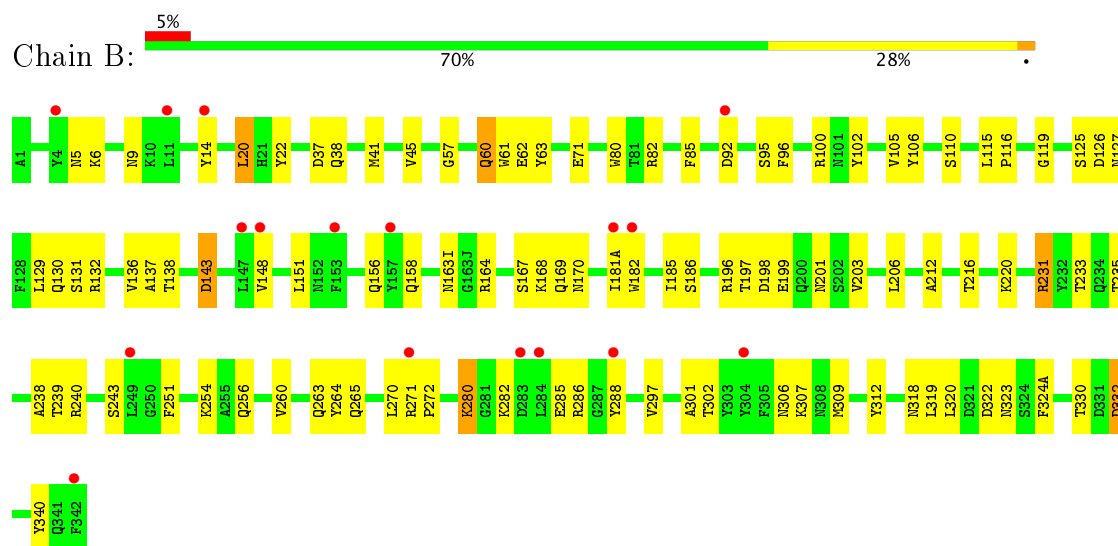
3 Residue-property plots [i](#)

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.

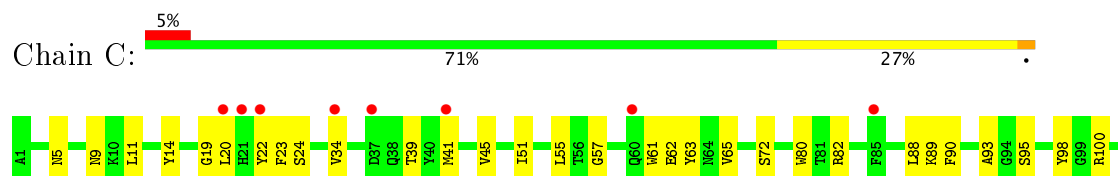
• Molecule 1: OmpK36

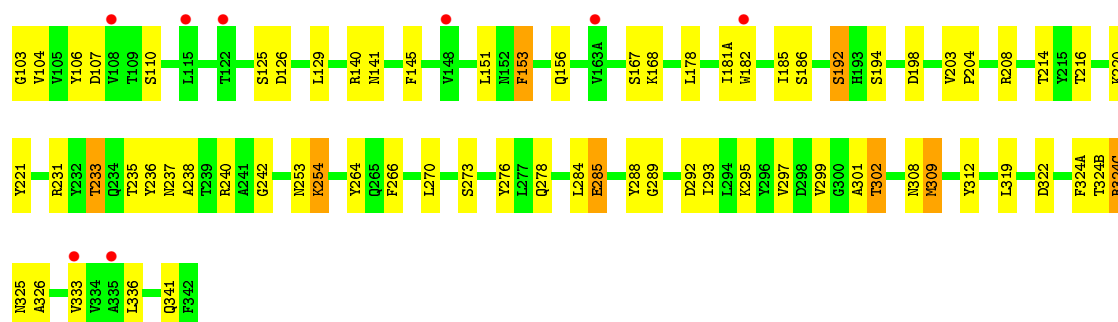


• Molecule 1: OmpK36

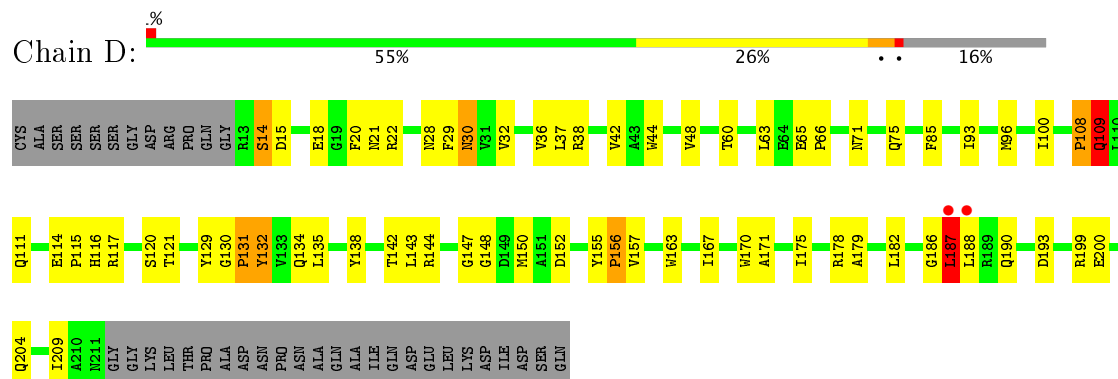


• Molecule 1: OmpK36

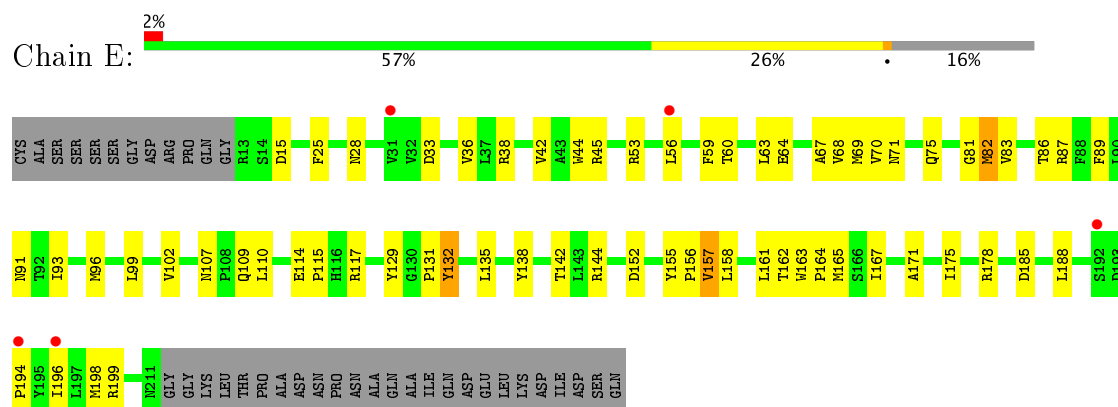




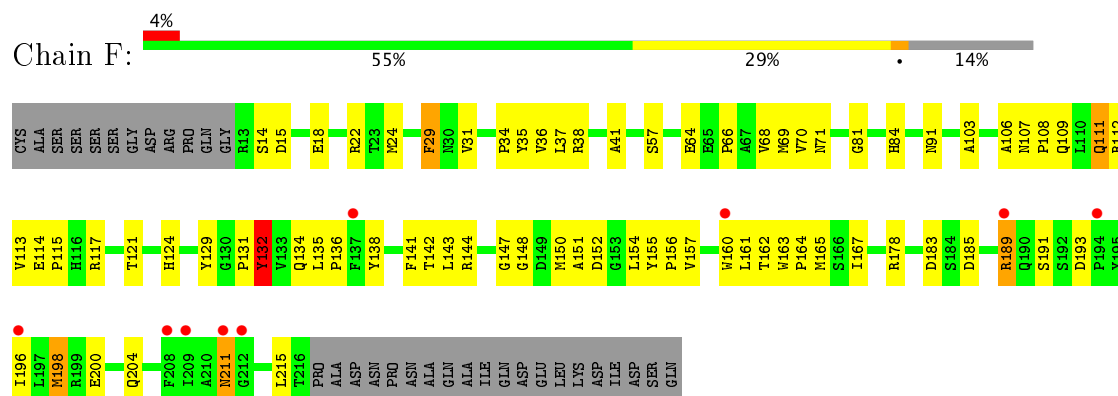
- Molecule 2: ABC transporter permease



- Molecule 2: ABC transporter permease



- Molecule 2: ABC transporter permease



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.38Å 145.24Å 232.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.38 – 2.90 123.19 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (68.38-2.90) 100.0 (123.19-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.241 , 0.290 0.238 , 0.290	Depositor DCC
R_{free} test set	3410 reflections (4.87%)	DCC
Wilson B-factor (Å ²)	60.2	Xtriage
Anisotropy	0.931	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	13238	wwPDB-VP
Average B, all atoms (Å ²)	70.0	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.*

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: LMT, 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	0.53	0/2753	0.78	2/3727 (0.1%)
1	B	0.51	0/2753	0.75	0/3727
1	C	0.50	1/2753 (0.0%)	0.75	0/3727
2	D	0.47	0/1647	0.78	4/2241 (0.2%)
2	E	0.46	0/1647	0.73	1/2241 (0.0%)
2	F	0.46	0/1670	0.71	0/2272
All	All	0.50	1/13223 (0.0%)	0.75	7/17935 (0.0%)

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
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	254	LYS	CE-NZ	6.16	1.64	1.49

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	LEU	CA-CB-CG	7.65	132.89	115.30
2	E	109	GLN	CA-CB-CG	-6.66	98.74	113.40
2	D	109	GLN	CA-CB-CG	6.36	127.38	113.40
2	D	156	PRO	C-N-CA	6.12	137.00	121.70
2	D	187	LEU	CA-CB-CG	-5.50	102.64	115.30
1	A	219	LEU	CA-CB-CG	5.26	127.39	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	108	PRO	C-N-CA	-5.14	108.84	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	92	ASP	Peptide

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	2693	0	2479	72	0
1	B	2693	0	2479	89	0
1	C	2693	0	2479	72	0
2	D	1597	0	1525	59	0
2	E	1597	0	1525	55	0
2	F	1620	0	1537	58	0
3	A	75	0	114	5	0
3	B	60	0	98	2	0
3	C	66	0	105	5	0
3	D	25	0	37	0	0
3	E	28	0	46	3	0
3	F	7	0	10	0	0
4	B	60	0	64	5	0
4	F	24	0	20	0	0
All	All	13238	0	12518	391	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 15.

All (391) 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:216:THR:HB	1:B:233:THR:HG22	1.26	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:GLN:HE21	1:B:282:LYS:HE3	0.95	1.09
1:A:22:TYR:OH	1:A:117:GLU:OE1	1.76	1.02
1:B:256:GLN:NE2	1:B:282:LYS:HE3	1.78	0.97
2:F:29:PHE:O	2:F:189:ARG:NH1	2.02	0.92
1:B:256:GLN:HE21	1:B:282:LYS:CE	1.83	0.88
1:B:216:THR:CB	1:B:233:THR:HG22	2.06	0.84
2:F:114:GLU:HG3	2:F:115:PRO:HD2	1.59	0.84
1:A:41:MET:CE	1:A:65:VAL:HG22	2.08	0.84
2:E:178:ARG:NH2	2:E:185:ASP:OD1	2.13	0.82
1:A:20:LEU:HD23	1:A:38:GLN:HB2	1.62	0.81
1:C:103:GLY:HA2	1:C:156:GLN:HE22	1.47	0.80
1:B:105:VAL:HG11	1:B:130:GLN:OE1	1.81	0.80
1:C:270:LEU:HD11	1:C:301:ALA:HB1	1.65	0.79
1:C:55:LEU:HD12	2:F:106:ALA:HA	1.65	0.79
2:D:117:ARG:HH11	2:D:152:ASP:HB2	1.47	0.78
1:B:263:GLN:NE2	1:B:271:ARG:HE	1.81	0.78
1:C:299:VAL:HG12	3:C:401:C8E:H22	1.66	0.76
1:A:268:PHE:HB3	2:D:109:GLN:HG2	1.67	0.75
2:D:75:GLN:HE21	2:D:121:THR:HG22	1.50	0.75
2:E:33:ASP:OD1	2:E:178:ARG:NH1	2.19	0.75
1:C:302:THR:HB	1:C:312:TYR:HB3	1.68	0.75
1:B:235:THR:HG23	1:B:238:ALA:HB3	1.67	0.74
1:A:197:THR:H	1:A:200:GLN:HG3	1.52	0.73
2:D:15:ASP:HB3	2:D:18:GLU:HB2	1.70	0.72
1:A:129:LEU:O	1:A:129:LEU:HD23	1.90	0.72
2:E:188:LEU:HD23	2:E:188:LEU:O	1.90	0.72
1:A:41:MET:HE2	1:A:65:VAL:HG22	1.72	0.71
1:B:216:THR:HG22	1:B:233:THR:HB	1.73	0.71
2:F:91:ASN:HD21	2:F:103:ALA:H	1.37	0.71
1:C:276:TYR:OH	1:C:278:GLN:NE2	2.23	0.71
2:E:42:VAL:HG13	2:E:45:ARG:HH12	1.55	0.70
1:B:136:VAL:HG12	1:B:158:GLN:HB2	1.74	0.70
1:C:216:THR:HG23	1:C:233:THR:HG22	1.73	0.69
1:C:236:TYR:HE2	1:C:254:LYS:HE3	1.57	0.69
1:B:20:LEU:HD23	1:B:38:GLN:HB2	1.73	0.69
1:C:23:PHE:HE1	1:C:336:LEU:HD12	1.58	0.68
2:D:179:ALA:HA	2:D:182:LEU:HD13	1.76	0.68
1:C:19:GLY:HA2	1:C:39:THR:HG23	1.76	0.68
2:F:178:ARG:HH12	2:F:185:ASP:HB3	1.59	0.68
1:A:19:GLY:HA2	1:A:39:THR:HG23	1.75	0.67
2:F:91:ASN:ND2	2:F:103:ALA:H	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:LYS:HG2	1:B:240:ARG:HH12	1.60	0.67
2:D:156:PRO:O	2:D:157:VAL:HG22	1.94	0.67
1:A:70:THR:HG22	1:A:72:SER:N	2.10	0.67
2:D:28:ASN:HA	2:D:32:VAL:HG22	1.77	0.67
2:E:129:TYR:HD1	2:E:142:THR:HG21	1.58	0.66
1:B:265:GLN:NE2	1:B:271:ARG:HB2	2.10	0.66
2:E:15:ASP:OD2	2:E:199:ARG:NH1	2.29	0.66
2:D:129:TYR:HB3	2:D:142:THR:HG21	1.78	0.66
2:D:66:PRO:HG2	2:D:157:VAL:HG11	1.79	0.66
1:A:70:THR:HG22	1:A:72:SER:H	1.62	0.65
2:D:167:ILE:HA	2:D:170:TRP:HB3	1.77	0.65
1:C:168:LYS:HG2	1:C:240:ARG:HH12	1.61	0.65
1:C:182:TRP:HB2	1:C:185:ILE:HD13	1.79	0.64
1:C:295:LYS:HG2	1:C:319:LEU:HB2	1.79	0.64
2:D:130:GLY:H	2:D:142:THR:HG22	1.62	0.64
2:E:188:LEU:HD21	2:E:194:PRO:HB3	1.80	0.64
1:B:167:SER:O	1:B:240:ARG:NH1	2.29	0.64
1:C:242:GLY:HA3	1:C:326:ALA:HB1	1.80	0.64
2:E:82:MET:O	2:E:86:THR:HG23	1.98	0.64
1:A:57:GLY:HA3	1:C:309:MET:SD	2.37	0.64
2:E:114:GLU:HG3	2:E:115:PRO:CD	2.28	0.64
2:E:142:THR:HG22	2:E:144:ARG:H	1.62	0.63
1:A:49:THR:CG2	1:C:309:MET:HG3	2.29	0.63
1:A:23:PHE:HE1	1:A:336:LEU:HD12	1.63	0.63
1:C:270:LEU:HD22	2:E:86:THR:HG22	1.80	0.63
1:A:280:LYS:HE3	1:A:292:ASP:OD2	1.98	0.62
1:A:49:THR:HG21	1:C:309:MET:HG3	1.80	0.62
1:C:336:LEU:HD22	2:E:93:ILE:HG21	1.79	0.62
2:E:157:VAL:HG13	2:E:158:LEU:HG	1.81	0.62
2:E:83:VAL:HG13	2:E:110:LEU:HD23	1.81	0.61
1:C:23:PHE:HB3	3:E:302:C8E:H131	1.82	0.61
2:E:114:GLU:HG3	2:E:115:PRO:HD2	1.82	0.61
2:F:36:VAL:HG22	2:F:37:LEU:H	1.65	0.61
2:E:38:ARG:O	2:E:42:VAL:HG23	2.00	0.61
1:C:55:LEU:HD22	1:C:88:LEU:HD23	1.82	0.61
2:E:117:ARG:HB3	2:E:152:ASP:OD2	2.01	0.61
2:D:178:ARG:O	2:D:182:LEU:HD13	2.01	0.61
1:B:280:LYS:NZ	4:B:406:LMT:H4B	2.14	0.60
2:F:34:PRO:HG3	2:F:189:ARG:HH11	1.66	0.60
1:B:167:SER:HB2	1:B:240:ARG:HD3	1.82	0.60
2:D:147:GLY:HA2	2:D:150:MET:SD	2.42	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:187:LEU:HD22	2:D:190:GLN:HB2	1.84	0.60
2:F:117:ARG:HB3	2:F:152:ASP:OD1	2.00	0.60
2:E:129:TYR:CD1	2:E:142:THR:HG21	2.37	0.60
1:B:169:GLN:NE2	1:B:197:THR:OG1	2.34	0.60
1:B:127:ASN:HB2	1:B:240:ARG:NH2	2.16	0.59
2:E:69:MET:HG3	2:E:81:GLY:O	2.03	0.59
2:E:188:LEU:CD2	2:E:194:PRO:HB3	2.34	0.58
2:F:24:MET:HE2	2:F:136:PRO:HB3	1.85	0.58
2:F:24:MET:HG3	2:F:136:PRO:HD3	1.86	0.58
2:F:200:GLU:O	2:F:204:GLN:HG3	2.03	0.58
1:B:306:ASN:HB2	1:B:307:LYS:NZ	2.18	0.57
2:D:129:TYR:HB3	2:D:142:THR:CG2	2.34	0.57
2:E:71:ASN:O	2:E:75:GLN:HG3	2.05	0.57
2:F:71:ASN:HB3	2:F:121:THR:HG21	1.85	0.57
1:C:125:SER:O	1:C:240:ARG:NH2	2.38	0.57
2:F:142:THR:HG22	2:F:144:ARG:H	1.69	0.57
1:A:41:MET:HE2	1:A:65:VAL:CG2	2.35	0.57
1:B:158:GLN:NE2	1:B:170:ASN:OD1	2.38	0.56
2:E:87:ARG:HD2	2:E:110:LEU:O	2.05	0.56
1:A:20:LEU:HD21	1:A:22:TYR:CE1	2.40	0.56
2:F:129:TYR:HB3	2:F:142:THR:HG21	1.87	0.56
2:F:163:TRP:O	2:F:167:ILE:HG12	2.05	0.56
2:D:22:ARG:NH1	2:D:193:ASP:OD2	2.38	0.56
2:F:124:HIS:ND1	2:F:211:ASN:OD1	2.39	0.56
2:F:135:LEU:HB2	2:F:138:TYR:HB3	1.87	0.56
1:A:334:VAL:HG21	3:A:406:C8E:H102	1.88	0.56
1:B:129:LEU:HD22	1:B:156:GLN:OE1	2.06	0.56
1:B:280:LYS:HZ1	4:B:406:LMT:C3B	2.19	0.56
2:E:64:GLU:O	2:E:68:VAL:HG23	2.06	0.56
1:A:309:MET:SD	1:B:57:GLY:HA3	2.46	0.56
1:A:336:LEU:HD22	2:D:93:ILE:HG21	1.88	0.56
1:C:141:ASN:OD1	1:C:145:PHE:N	2.24	0.56
2:D:14:SER:OG	2:D:15:ASP:N	2.40	0.55
1:C:264:TYR:HB2	3:C:403:C8E:H31	1.88	0.55
2:E:135:LEU:HB2	2:E:138:TYR:HB3	1.89	0.55
1:A:58:TYR:OH	1:A:97:ASP:HB3	2.07	0.55
1:A:266:PHE:HZ	3:A:401:C8E:H102	1.72	0.55
2:E:71:ASN:ND2	2:E:117:ARG:HA	2.22	0.54
2:D:163:TRP:NE1	2:D:167:ILE:HD11	2.22	0.54
1:B:309:MET:HE3	1:C:57:GLY:HA3	1.90	0.54
2:F:69:MET:HB2	2:F:81:GLY:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:LEU:HD11	1:B:301:ALA:HB1	1.89	0.54
2:E:196:ILE:HD12	2:E:199:ARG:NH2	2.22	0.54
1:C:107:ASP:OD2	1:C:140:ARG:NH2	2.41	0.54
1:C:236:TYR:CE2	1:C:254:LYS:HE3	2.42	0.54
2:F:151:ALA:HA	2:F:154:LEU:HD13	1.89	0.54
2:F:66:PRO:HG2	2:F:157:VAL:HG22	1.88	0.54
2:D:29:PHE:HB3	2:D:30:ASN:OD1	2.07	0.54
2:D:38:ARG:O	2:D:42:VAL:HG23	2.07	0.54
2:F:36:VAL:O	2:F:38:ARG:N	2.41	0.54
1:C:5:ASN:HA	1:C:9:ASN:O	2.06	0.53
2:D:36:VAL:O	2:D:38:ARG:N	2.40	0.53
2:F:112:ARG:HG2	2:F:113:VAL:N	2.22	0.53
2:F:29:PHE:CE2	2:F:189:ARG:NH2	2.76	0.53
1:B:82:ARG:O	1:B:100:ARG:HD3	2.08	0.53
2:D:117:ARG:HB3	2:D:152:ASP:OD1	2.08	0.53
1:A:5:ASN:HA	1:A:9:ASN:O	2.08	0.53
1:C:129:LEU:HD22	1:C:156:GLN:NE2	2.23	0.53
1:A:104:VAL:HG22	1:A:156:GLN:HE21	1.74	0.53
2:D:60:THR:HA	2:D:63:LEU:HD12	1.91	0.53
2:E:156:PRO:O	2:E:157:VAL:HG12	2.09	0.53
1:A:46:LYS:HG2	1:A:60:GLN:HG3	1.91	0.53
1:B:280:LYS:HZ1	4:B:406:LMT:H4B	1.73	0.53
1:B:260:VAL:HG13	4:B:405:LMT:H122	1.91	0.53
2:E:60:THR:HA	2:E:63:LEU:CD1	2.39	0.53
2:F:162:THR:HB	2:F:164:PRO:HD2	1.90	0.52
2:E:45:ARG:HB3	2:E:45:ARG:HH11	1.75	0.52
2:E:67:ALA:HA	2:E:70:VAL:HG12	1.89	0.52
1:C:297:VAL:HG23	1:C:319:LEU:HD11	1.90	0.52
1:A:136:VAL:HG12	1:A:158:GLN:HB2	1.91	0.52
1:A:264:TYR:HB2	3:A:404:C8E:H191	1.92	0.52
1:B:288:TYR:CD1	1:B:324(A):PHE:HB2	2.44	0.52
2:D:71:ASN:O	2:D:75:GLN:HG3	2.09	0.52
1:C:167:SER:O	1:C:240:ARG:NH1	2.42	0.52
1:C:24:SER:HB2	1:C:333:VAL:HG22	1.92	0.52
1:B:307:LYS:H	1:B:307:LYS:HE2	1.75	0.52
1:A:104:VAL:HG22	1:A:129:LEU:HD21	1.91	0.52
3:A:406:C8E:H22	2:D:85:PHE:CZ	2.45	0.51
1:B:196:ARG:NH1	1:B:201:ASN:OD1	2.36	0.51
2:D:171:ALA:O	2:D:175:ILE:HG13	2.09	0.51
2:D:44:TRP:O	2:D:48:VAL:HG22	2.10	0.51
1:B:96:PHE:CE1	1:B:137:ALA:HB1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:TYR:OH	1:C:62:GLU:HB2	2.10	0.51
1:B:265:GLN:HE22	1:B:271:ARG:HB2	1.74	0.51
2:F:134:GLN:HE22	2:F:198:MET:HE3	1.75	0.51
1:A:318:ASN:ND2	1:A:320:LEU:H	2.09	0.51
1:C:324(C):ARG:HG3	1:C:325:ASN:N	2.26	0.51
1:A:163(A):VAL:HA	1:A:163(J):GLY:HA3	1.93	0.50
2:F:129:TYR:HB3	2:F:142:THR:CG2	2.42	0.50
2:F:71:ASN:HB3	2:F:121:THR:CG2	2.41	0.50
1:A:270:LEU:HD11	1:A:301:ALA:HB1	1.92	0.50
1:C:90:PHE:HB2	1:C:93:ALA:HB3	1.92	0.50
2:F:29:PHE:CD2	2:F:189:ARG:NH2	2.79	0.50
1:C:266:PHE:HZ	3:C:402:C8E:H51	1.77	0.50
1:C:141:ASN:HB3	1:C:153:PHE:CE1	2.47	0.50
2:F:161:LEU:HD12	2:F:165:MET:HB3	1.92	0.50
2:E:45:ARG:HB3	2:E:45:ARG:NH1	2.26	0.50
1:B:116:PRO:HB3	1:B:302:THR:HG22	1.93	0.50
1:A:104:VAL:H	1:A:156:GLN:NE2	2.10	0.50
1:A:37:ASP:HB3	1:B:163(I):ASN:ND2	2.27	0.50
1:A:14:TYR:OH	1:A:62:GLU:HB2	2.12	0.50
1:A:71:GLU:HB3	1:B:80:TRP:CD1	2.47	0.50
1:B:216:THR:HB	1:B:233:THR:CG2	2.18	0.50
2:F:135:LEU:HD23	2:F:141:PHE:HB3	1.93	0.50
1:A:295:LYS:HG2	1:A:319:LEU:HB2	1.94	0.49
1:B:127:ASN:HB2	1:B:240:ARG:HH21	1.75	0.49
2:E:107:ASN:HB3	2:E:110:LEU:HD12	1.94	0.49
2:D:132:TYR:CE2	2:D:199:ARG:HG3	2.47	0.49
2:D:167:ILE:HG23	2:D:170:TRP:HD1	1.77	0.49
1:A:104:VAL:N	1:A:156:GLN:HE22	2.10	0.49
1:A:205:ALA:HB1	1:A:286:ARG:NH1	2.27	0.49
1:B:167:SER:HA	1:B:251:PHE:CZ	2.48	0.49
1:C:192:SER:HB3	1:C:214:THR:OG1	2.12	0.49
2:F:114:GLU:HG3	2:F:115:PRO:CD	2.38	0.49
1:A:235:THR:HB	1:A:238:ALA:HB3	1.94	0.49
1:C:288:TYR:CD1	1:C:324(A):PHE:HB2	2.46	0.49
2:E:132:TYR:CE1	2:E:199:ARG:HG3	2.48	0.49
1:B:100:ARG:NH2	1:B:126:ASP:OD1	2.45	0.49
1:B:125:SER:HA	1:B:131:SER:HB3	1.94	0.49
2:F:152:ASP:HA	2:F:155:TYR:CE1	2.48	0.49
1:A:23:PHE:CE1	1:A:336:LEU:HD12	2.46	0.49
1:B:20:LEU:CD1	1:B:312:TYR:OH	2.61	0.49
1:C:23:PHE:CE1	1:C:336:LEU:HD12	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:VAL:HG12	1:A:79:ALA:CB	2.43	0.49
2:D:144:ARG:O	2:D:148:GLY:HA3	2.13	0.49
2:F:18:GLU:OE1	2:F:22:ARG:NH2	2.45	0.49
1:C:308:ASN:ND2	1:C:341:GLN:O	2.37	0.49
2:D:96:MET:HB2	2:D:100:ILE:HD12	1.94	0.49
1:A:116:PRO:HB3	1:A:302:THR:HG22	1.95	0.48
2:D:28:ASN:HA	2:D:32:VAL:CG2	2.42	0.48
1:A:104:VAL:HG13	1:A:156:GLN:NE2	2.28	0.48
1:B:307:LYS:H	1:B:307:LYS:CE	2.26	0.48
1:C:22:TYR:HD2	1:C:34:VAL:HG12	1.77	0.48
2:D:108:PRO:O	2:D:111:GLN:HG3	2.14	0.48
1:A:209:GLY:HA3	1:A:237:ASN:ND2	2.28	0.48
1:C:41:MET:HG3	1:C:65:VAL:HB	1.95	0.48
2:D:18:GLU:OE1	2:D:22:ARG:NH2	2.47	0.48
3:E:302:C8E:H41	3:E:302:C8E:H13	1.61	0.48
1:B:169:GLN:HB3	1:B:197:THR:HG21	1.95	0.48
2:E:91:ASN:OD1	2:E:102:VAL:N	2.47	0.48
1:A:10:LYS:NZ	1:A:48:GLU:OE1	2.25	0.47
1:B:306:ASN:HB2	1:B:307:LYS:HZ3	1.79	0.47
1:B:323:ASN:HB2	1:B:324(A):PHE:H	1.78	0.47
1:C:151:LEU:HD11	1:C:178:LEU:HD11	1.96	0.47
1:C:106:TYR:O	1:C:110:SER:HB3	2.14	0.47
1:C:126:ASP:HB3	1:C:168:LYS:HB3	1.96	0.47
2:D:200:GLU:O	2:D:204:GLN:HG3	2.13	0.47
2:E:44:TRP:CD1	2:E:53:ARG:HD3	2.48	0.47
1:C:203:VAL:HG12	1:C:204:PRO:HD3	1.97	0.47
1:A:206:LEU:HD22	1:A:249:LEU:HB3	1.97	0.47
1:A:186:SER:HB2	1:A:220:LYS:HG2	1.96	0.47
1:A:11:LEU:HD11	1:A:45:VAL:CG2	2.44	0.47
1:C:100:ARG:NH1	1:C:126:ASP:OD2	2.47	0.47
1:A:197:THR:N	1:A:200:GLN:HG3	2.23	0.47
1:A:41:MET:HE3	1:A:65:VAL:HG22	1.90	0.47
1:C:186:SER:HB2	1:C:220:LYS:HG2	1.97	0.47
1:A:106:TYR:O	1:A:110:SER:HB3	2.13	0.47
2:E:171:ALA:O	2:E:175:ILE:HG13	2.15	0.47
2:F:64:GLU:O	2:F:68:VAL:HG23	2.14	0.47
1:A:116:PRO:HB2	1:A:314:ASP:HB2	1.97	0.47
1:A:141:ASN:OD1	1:A:145:PHE:N	2.45	0.46
1:B:143:ASP:OD1	1:B:143:ASP:N	2.48	0.46
2:D:147:GLY:HA2	2:D:150:MET:HG3	1.97	0.46
2:E:70:VAL:HG11	2:E:155:TYR:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:28:ASN:ND2	2:E:135:LEU:O	2.46	0.46
1:B:235:THR:HG21	1:B:239:THR:H	1.80	0.46
1:B:264:TYR:O	1:B:272:PRO:HD2	2.16	0.46
1:B:309:MET:HE3	1:B:309:MET:HB2	1.76	0.46
1:C:270:LEU:HD22	2:E:86:THR:CG2	2.45	0.46
2:F:147:GLY:HA2	2:F:150:MET:HG3	1.96	0.46
1:C:284:LEU:HB2	1:C:288:TYR:O	2.15	0.46
2:F:144:ARG:O	2:F:148:GLY:HA3	2.16	0.46
1:C:293:ILE:HD13	1:C:324(A):PHE:CZ	2.51	0.46
2:D:152:ASP:HA	2:D:155:TYR:CE1	2.50	0.46
1:B:20:LEU:HD21	1:B:22:TYR:CE1	2.49	0.46
1:A:318:ASN:HD21	1:A:320:LEU:HD13	1.81	0.46
1:B:186:SER:HB2	1:B:220:LYS:HG2	1.98	0.46
2:D:186:GLY:C	2:D:188:LEU:H	2.18	0.46
1:B:318:ASN:OD1	1:B:320:LEU:CD2	2.64	0.46
2:D:116:HIS:CE1	2:D:209:ILE:HG23	2.51	0.46
1:A:104:VAL:HB	1:A:177:SER:HB3	1.98	0.45
1:B:309:MET:CE	1:B:340:TYR:HD1	2.29	0.45
2:E:163:TRP:O	2:E:167:ILE:HG13	2.15	0.45
2:E:96:MET:O	2:E:99:LEU:HD23	2.16	0.45
2:F:84:HIS:HE1	2:F:113:VAL:HG12	1.81	0.45
1:B:280:LYS:HZ1	4:B:406:LMT:C4B	2.30	0.45
2:D:30:ASN:N	2:D:30:ASN:OD1	2.50	0.45
2:F:114:GLU:H	2:F:215:LEU:CB	2.29	0.45
2:D:188:LEU:HA	2:D:188:LEU:HD12	1.80	0.45
2:F:193:ASP:OD2	2:F:196:ILE:HG12	2.17	0.45
1:B:148:VAL:HG13	1:B:151:LEU:HB3	1.98	0.45
1:C:299:VAL:CG1	3:C:401:C8E:H22	2.42	0.45
2:F:141:PHE:CZ	2:F:143:LEU:HD12	2.51	0.45
2:D:28:ASN:HD22	2:D:134:GLN:HE21	1.65	0.45
1:B:14:TYR:OH	1:B:62:GLU:HB3	2.17	0.45
1:B:196:ARG:HD2	1:B:212:ALA:HB2	1.99	0.45
1:B:231:ARG:HE	1:B:233:THR:CG2	2.30	0.45
2:F:14:SER:HB2	2:F:15:ASP:H	1.58	0.45
1:A:288:TYR:CD1	1:A:324(A):PHE:HB2	2.51	0.45
2:E:161:LEU:HD23	2:E:165:MET:HB3	1.98	0.45
1:C:322:ASP:HA	1:C:324(B):THR:HG21	1.99	0.45
2:E:178:ARG:HH22	2:E:185:ASP:CG	2.20	0.45
2:F:64:GLU:OE1	2:F:115:PRO:HG3	2.17	0.45
1:B:235:THR:HG21	1:B:239:THR:OG1	2.17	0.45
2:D:36:VAL:HG22	2:D:37:LEU:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:132:TYR:OH	2:F:198:MET:SD	2.74	0.45
2:D:15:ASP:OD1	2:D:199:ARG:NH1	2.46	0.44
2:E:158:LEU:HA	2:E:161:LEU:CD1	2.47	0.44
1:A:266:PHE:CZ	3:A:401:C8E:H102	2.52	0.44
2:D:114:GLU:HG3	2:D:115:PRO:HD2	1.99	0.44
2:F:134:GLN:HE22	2:F:198:MET:CE	2.30	0.44
1:A:151:LEU:HD11	1:A:178:LEU:HD11	1.98	0.44
1:B:199:GLU:O	1:B:203:VAL:HG12	2.17	0.44
2:D:179:ALA:CA	2:D:182:LEU:HD13	2.46	0.44
1:A:111:TRP:CD2	1:A:220:LYS:HD3	2.53	0.44
1:A:12:ASP:HB3	1:A:46:LYS:HB2	1.98	0.44
2:F:156:PRO:HB3	2:F:160:TRP:NE1	2.33	0.44
1:A:64:ASN:ND2	1:A:80:TRP:CZ2	2.86	0.44
1:B:254:LYS:HD3	1:B:282:LYS:HD2	1.99	0.44
2:F:31:VAL:O	2:F:35:TYR:HB2	2.18	0.44
2:F:57:SER:O	2:F:112:ARG:NH2	2.51	0.44
1:B:158:GLN:HE21	1:B:170:ASN:CG	2.21	0.44
1:C:185:ILE:HG13	1:C:221:TYR:HD2	1.82	0.44
1:B:264:TYR:HE2	3:B:404:C8E:H51	1.83	0.44
1:A:221:TYR:CZ	1:A:223:ALA:HB3	2.53	0.43
1:A:22:TYR:HD2	1:A:34:VAL:HG12	1.82	0.43
1:B:102:TYR:CE1	1:B:132:ARG:HG3	2.53	0.43
1:B:182:TRP:HB2	1:B:185:ILE:HD13	2.00	0.43
2:D:187:LEU:HD13	2:D:187:LEU:HA	1.61	0.43
1:B:185:ILE:HA	1:B:220:LYS:O	2.18	0.43
1:C:266:PHE:CZ	3:C:402:C8E:H51	2.53	0.43
2:F:108:PRO:HA	2:F:111:GLN:HE21	1.83	0.43
2:F:24:MET:CE	2:F:136:PRO:HB3	2.48	0.43
1:B:167:SER:HA	1:B:251:PHE:HZ	1.82	0.43
2:F:22:ARG:NH1	2:F:193:ASP:OD2	2.51	0.43
1:A:11:LEU:HD12	1:A:11:LEU:HA	1.73	0.43
1:C:100:ARG:HH12	1:C:126:ASP:CG	2.22	0.43
1:C:285:GLU:HG2	1:C:285:GLU:H	1.58	0.43
1:A:118:PHE:CD2	1:A:314:ASP:OD2	2.72	0.42
1:B:231:ARG:HE	1:B:233:THR:HG23	1.84	0.42
2:E:89:PHE:HB2	3:E:302:C8E:H11	2.01	0.42
1:B:216:THR:HG22	1:B:233:THR:CB	2.46	0.42
1:B:60:GLN:HG2	1:B:85:PHE:CZ	2.55	0.42
2:D:21:ASN:ND2	2:D:132:TYR:O	2.50	0.42
2:D:60:THR:HA	2:D:63:LEU:CD1	2.49	0.42
1:B:126:ASP:HB3	1:B:168:LYS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:ASP:OD1	1:B:332:ASP:N	2.52	0.42
2:E:161:LEU:HB3	2:E:165:MET:HB2	2.01	0.42
1:A:302:THR:HB	1:A:312:TYR:HB3	2.02	0.42
1:B:138:THR:OG1	1:B:156:GLN:NE2	2.50	0.42
1:C:20:LEU:HD13	1:C:312:TYR:OH	2.19	0.42
1:B:71:GLU:HB3	1:C:80:TRP:CD1	2.55	0.42
2:E:152:ASP:HA	2:E:155:TYR:CE1	2.54	0.42
1:C:11:LEU:HD12	1:C:11:LEU:HA	1.87	0.42
2:D:163:TRP:CE2	2:D:167:ILE:HD11	2.54	0.42
1:A:65:VAL:HG12	1:A:79:ALA:HB1	2.01	0.42
2:D:178:ARG:O	2:D:182:LEU:CD1	2.67	0.42
2:E:36:VAL:O	2:E:38:ARG:N	2.51	0.42
1:B:182:TRP:HE3	1:B:185:ILE:HD13	1.85	0.42
1:B:20:LEU:HD13	1:B:312:TYR:OH	2.19	0.42
2:D:129:TYR:CD1	2:D:142:THR:HG21	2.55	0.42
1:B:297:VAL:HG23	1:B:319:LEU:HD11	2.01	0.42
1:B:37:ASP:OD1	1:C:98:TYR:OH	2.30	0.42
1:C:276:TYR:CE2	1:C:278:GLN:NE2	2.88	0.42
2:D:147:GLY:HA2	2:D:150:MET:CG	2.50	0.42
2:E:157:VAL:HG13	2:E:158:LEU:N	2.35	0.42
2:E:38:ARG:NE	2:E:185:ASP:OD2	2.38	0.42
2:F:107:ASN:ND2	2:F:109:GLN:OE1	2.48	0.42
1:B:322:ASP:HA	1:B:330:THR:HG21	2.02	0.41
1:B:45:VAL:HG22	1:B:61:TRP:HE3	1.84	0.41
1:B:5:ASN:HA	1:B:9:ASN:O	2.20	0.41
1:C:55:LEU:HA	1:C:55:LEU:HD23	1.82	0.41
2:D:135:LEU:HB2	2:D:138:TYR:HB3	2.01	0.41
2:D:143:LEU:HD23	2:D:143:LEU:HA	1.78	0.41
1:A:215:TYR:O	1:A:233:THR:HA	2.20	0.41
1:C:208:ARG:HH11	1:C:208:ARG:HG2	1.84	0.41
1:C:11:LEU:HD11	1:C:45:VAL:CG1	2.50	0.41
2:E:25:PHE:CD1	2:E:198:MET:HE2	2.55	0.41
1:C:235:THR:HB	1:C:238:ALA:HB3	2.01	0.41
2:F:37:LEU:O	2:F:41:ALA:N	2.52	0.41
1:A:117:GLU:HB2	1:A:312:TYR:CE1	2.55	0.41
1:B:100:ARG:NH1	1:B:132:ARG:HB3	2.34	0.41
1:C:51:ILE:HB	1:C:55:LEU:HB3	2.02	0.41
3:B:402:C8E:H172	3:B:402:C8E:H141	1.80	0.41
1:B:41:MET:HE1	1:C:61:TRP:CE3	2.56	0.41
1:A:204:PRO:O	1:A:205:ALA:HB3	2.20	0.41
1:B:206:LEU:HD22	1:B:285:GLU:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:LEU:HD22	1:B:119:GLY:HA3	2.03	0.41
2:E:56:LEU:HA	2:E:56:LEU:HD12	1.68	0.41
2:F:69:MET:CG	2:F:70:VAL:N	2.83	0.41
2:D:131:PRO:HB2	2:D:132:TYR:H	1.61	0.41
2:E:161:LEU:HD12	2:E:161:LEU:N	2.36	0.41
2:F:129:TYR:HD1	2:F:142:THR:HG21	1.85	0.41
1:B:216:THR:CG2	1:B:233:THR:CG2	2.99	0.41
2:E:162:THR:HB	2:E:164:PRO:HD2	2.02	0.41
2:E:59:PHE:O	2:E:63:LEU:HD12	2.21	0.41
1:A:158:GLN:HE21	1:A:170:ASN:CG	2.23	0.40
1:B:309:MET:HE1	1:B:340:TYR:HD1	1.86	0.40
2:D:37:LEU:HD13	2:D:178:ARG:HG2	2.02	0.40
2:D:120:SER:OG	2:D:209:ILE:HG22	2.21	0.40
1:C:237:ASN:ND2	1:C:253:ASN:HA	2.36	0.40
1:B:106:TYR:O	1:B:110:SER:HB3	2.22	0.40
1:C:104:VAL:H	1:C:156:GLN:NE2	2.19	0.40
1:C:62:GLU:OE1	1:C:82:ARG:NE	2.51	0.40
2:F:147:GLY:HA2	2:F:150:MET:SD	2.61	0.40
2:F:38:ARG:HH11	2:F:185:ASP:CG	2.24	0.40
1:A:288:TYR:HB3	1:A:291:GLN:HG3	2.03	0.40
2:F:129:TYR:CD1	2:F:142:THR:HG21	2.57	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	342/344 (99%)	313 (92%)	27 (8%)	2 (1%)	28 64
1	B	342/344 (99%)	316 (92%)	25 (7%)	1 (0%)	44 77
1	C	342/344 (99%)	317 (93%)	23 (7%)	2 (1%)	28 64
2	D	197/236 (84%)	179 (91%)	15 (8%)	3 (2%)	12 39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	197/236 (84%)	175 (89%)	19 (10%)	3 (2%)	12	39
2	F	202/236 (86%)	182 (90%)	16 (8%)	4 (2%)	9	31
All	All	1622/1740 (93%)	1482 (91%)	125 (8%)	15 (1%)	20	54

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	181(A)	ILE
1	A	183	ASP
2	D	131	PRO
2	E	132	TYR
2	F	131	PRO
1	B	181(A)	ILE
2	D	132	TYR
2	E	131	PRO
2	F	191	SER
2	F	211	ASN
1	C	181(A)	ILE
1	C	289	GLY
2	D	187	LEU
2	F	132	TYR
2	E	157	VAL

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	276/276 (100%)	267 (97%)	9 (3%)	43	77
1	B	276/276 (100%)	263 (95%)	13 (5%)	30	65
1	C	276/276 (100%)	260 (94%)	16 (6%)	23	56
2	D	168/197 (85%)	163 (97%)	5 (3%)	46	80
2	E	168/197 (85%)	167 (99%)	1 (1%)	89	97
2	F	168/197 (85%)	162 (96%)	6 (4%)	40	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1332/1419 (94%)	1282 (96%)	50 (4%)	38 73

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	TYR
1	A	143	ASP
1	A	153	PHE
1	A	164	ARG
1	A	198	ASP
1	A	231	ARG
1	A	260	VAL
1	A	318	ASN
1	A	336	LEU
1	B	6	LYS
1	B	20	LEU
1	B	60	GLN
1	B	63	TYR
1	B	95	SER
1	B	143	ASP
1	B	164	ARG
1	B	198	ASP
1	B	231	ARG
1	B	243	SER
1	B	280	LYS
1	B	286	ARG
1	B	332	ASP
1	C	63	TYR
1	C	72	SER
1	C	89	LYS
1	C	95	SER
1	C	153	PHE
1	C	192	SER
1	C	194	SER
1	C	198	ASP
1	C	231	ARG
1	C	233	THR
1	C	273	SER
1	C	285	GLU
1	C	292	ASP
1	C	302	THR
1	C	309	MET

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Mol	Chain	Res	Type
1	C	324(C)	ARG
2	D	14	SER
2	D	20	PHE
2	D	30	ASN
2	D	65	GLU
2	D	109	GLN
2	E	82	MET
2	F	29	PHE
2	F	111	GLN
2	F	132	TYR
2	F	183	ASP
2	F	189	ARG
2	F	198	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	GLN
1	A	158	GLN
1	A	291	GLN
1	A	318	ASN
1	B	158	GLN
1	B	169	GLN
1	B	211	ASN
1	B	256	GLN
1	B	257	ASN
1	B	263	GLN
1	B	265	GLN
1	B	291	GLN
1	C	127	ASN
1	C	130	GLN
1	C	156	GLN
1	C	237	ASN
1	C	253	ASN
1	C	257	ASN
1	C	278	GLN
2	D	75	GLN
2	E	30	ASN
2	F	91	ASN
2	F	111	GLN
2	F	180	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

22 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	C8E	A	401	-	15,15,20	0.35	0	14,14,19	0.45	0
3	C8E	A	402	-	9,9,20	0.31	0	8,8,19	0.46	0
3	C8E	A	403	-	11,11,20	0.41	0	8,9,19	0.34	0
3	C8E	A	404	-	8,8,20	0.55	0	7,7,19	0.31	0
3	C8E	A	405	-	15,15,20	0.50	0	14,14,19	0.55	0
3	C8E	A	406	-	10,10,20	0.46	0	9,9,19	0.68	0
3	C8E	B	401	-	10,10,20	0.37	0	9,9,19	0.66	0
3	C8E	B	402	-	17,17,20	0.43	0	16,16,19	0.35	0
3	C8E	B	403	-	15,15,20	0.47	0	14,14,19	0.67	0
3	C8E	B	404	-	14,14,20	0.39	0	13,13,19	0.37	0
4	LMT	B	405	-	36,36,36	1.12	4 (11%)	47,47,47	1.09	4 (8%)
4	LMT	B	406	-	25,25,36	1.33	3 (12%)	36,36,47	1.44	6 (16%)
3	C8E	C	401	-	15,15,20	0.38	0	14,14,19	0.61	0
3	C8E	C	402	-	20,20,20	0.45	0	19,19,19	0.52	0
3	C8E	C	403	-	12,12,20	0.46	0	11,11,19	0.36	0
3	C8E	C	404	-	15,15,20	0.46	0	14,14,19	0.60	0
3	C8E	D	301	-	12,12,20	0.34	0	11,11,19	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	C8E	D	302	-	11,11,20	0.47	0	10,10,19	0.54	0
3	C8E	E	301	-	7,7,20	0.39	0	6,6,19	0.27	0
3	C8E	E	302	-	19,19,20	0.42	0	18,18,19	0.33	0
3	C8E	F	301	-	6,6,20	0.35	0	5,5,19	0.27	0
4	LMT	F	302	-	25,25,36	1.27	3 (12%)	36,36,47	1.30	4 (11%)

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	C8E	A	401	-	-	0/13/13/18	0/0/0/0
3	C8E	A	402	-	-	0/7/7/18	0/0/0/0
3	C8E	A	403	-	-	0/7/7/18	0/0/0/0
3	C8E	A	404	-	-	0/6/6/18	0/0/0/0
3	C8E	A	405	-	-	0/13/13/18	0/0/0/0
3	C8E	A	406	-	-	0/8/8/18	0/0/0/0
3	C8E	B	401	-	-	0/8/8/18	0/0/0/0
3	C8E	B	402	-	-	0/15/15/18	0/0/0/0
3	C8E	B	403	-	-	0/13/13/18	0/0/0/0
3	C8E	B	404	-	-	0/12/12/18	0/0/0/0
4	LMT	B	405	-	-	0/21/61/61	0/2/2/2
4	LMT	B	406	-	-	0/10/50/61	0/2/2/2
3	C8E	C	401	-	-	0/13/13/18	0/0/0/0
3	C8E	C	402	-	-	0/18/18/18	0/0/0/0
3	C8E	C	403	-	-	0/10/10/18	0/0/0/0
3	C8E	C	404	-	-	0/13/13/18	0/0/0/0
3	C8E	D	301	-	-	0/10/10/18	0/0/0/0
3	C8E	D	302	-	-	0/9/9/18	0/0/0/0
3	C8E	E	301	-	-	0/5/5/18	0/0/0/0
3	C8E	E	302	-	-	0/17/17/18	0/0/0/0
3	C8E	F	301	-	-	0/4/4/18	0/0/0/0
4	LMT	F	302	-	-	0/10/50/61	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	406	LMT	O2'-C2'	-2.94	1.36	1.43
4	F	302	LMT	O2'-C2'	-2.82	1.36	1.43
4	B	405	LMT	O3B-C3B	-2.56	1.37	1.43
4	B	406	LMT	O3B-C3B	-2.48	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	302	LMT	O3'-C3'	-2.46	1.37	1.43
4	F	302	LMT	O2B-C2B	-2.42	1.37	1.43
4	B	405	LMT	O3'-C3'	-2.41	1.37	1.43
4	B	406	LMT	O3'-C3'	-2.36	1.37	1.43
4	B	405	LMT	O4'-C4B	-2.12	1.38	1.43
4	B	405	LMT	O2'-C2'	-2.02	1.38	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	406	LMT	O1B-C4'-C5'	-2.56	103.04	109.34
4	B	405	LMT	C3B-C4B-C5B	-2.46	105.88	110.22
4	B	405	LMT	C1'-O5'-C5'	-2.37	109.25	113.72
4	B	405	LMT	C3'-C4'-C5'	-2.32	105.95	110.88
4	B	406	LMT	O5'-C1'-C2'	-2.18	106.08	110.30
4	F	302	LMT	O5B-C5B-C6B	2.06	111.34	106.41
4	B	406	LMT	O1'-C1'-C2'	2.20	110.76	108.14
4	F	302	LMT	O5'-C5'-C6'	2.29	111.89	106.41
4	B	406	LMT	O5B-C5B-C6B	2.43	112.24	106.41
4	B	405	LMT	O1'-C1'-C2'	2.46	112.24	108.23
4	B	406	LMT	O5B-C5B-C4B	2.78	114.79	109.66
4	F	302	LMT	O1'-C1'-C2'	2.89	111.58	108.14
4	F	302	LMT	O5'-C5'-C4'	3.02	115.94	109.75
4	B	406	LMT	O5'-C5'-C4'	3.90	117.72	109.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	C8E	2	0
3	A	404	C8E	1	0
3	A	406	C8E	2	0
3	B	402	C8E	1	0
3	B	404	C8E	1	0
4	B	405	LMT	1	0
4	B	406	LMT	4	0
3	C	401	C8E	2	0
3	C	402	C8E	2	0
3	C	403	C8E	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	302	C8E	3	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 ⓘ

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, 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	344/344 (100%)	0.52	6 (1%) 70 68	48, 58, 83, 140	0
1	B	344/344 (100%)	0.60	17 (4%) 30 26	48, 61, 91, 155	0
1	C	344/344 (100%)	0.63	16 (4%) 32 28	50, 68, 103, 153	0
2	D	199/236 (84%)	0.29	2 (1%) 82 81	46, 71, 98, 165	0
2	E	199/236 (84%)	0.34	5 (2%) 58 53	56, 75, 102, 152	0
2	F	204/236 (86%)	0.26	9 (4%) 35 30	55, 80, 124, 159	0
All	All	1634/1740 (93%)	0.48	55 (3%) 46 39	46, 67, 102, 165	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	182	TRP	5.7
2	F	211	ASN	4.6
1	B	288	TYR	4.2
1	B	92	ASP	3.6
2	F	194	PRO	3.4
1	C	108	VAL	3.4
2	F	189	ARG	3.4
1	C	182	TRP	3.1
2	D	187	LEU	3.0
2	F	212	GLY	3.0
1	B	284	LEU	3.0
2	E	194	PRO	2.8
1	B	249	LEU	2.8
1	C	85	PHE	2.8
1	B	283	ASP	2.7
2	F	208	PHE	2.7
1	C	335	ALA	2.7
1	B	14	TYR	2.6
1	A	293	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	188	LEU	2.6
1	C	21	HIS	2.5
1	B	147	LEU	2.5
1	B	11	LEU	2.5
2	F	196	ILE	2.5
1	A	60	GLN	2.4
1	A	236	TYR	2.4
1	C	20	LEU	2.4
2	F	160	TRP	2.4
1	C	22	TYR	2.4
2	E	31	VAL	2.4
1	A	192	SER	2.4
1	A	4	TYR	2.3
1	B	304	TYR	2.3
1	C	60	GLN	2.3
1	C	333	VAL	2.3
1	C	34	VAL	2.3
1	B	157	TYR	2.3
1	C	163(A)	VAL	2.3
2	E	56	LEU	2.3
1	B	342	PHE	2.3
1	B	181(A)	ILE	2.2
1	C	115	LEU	2.2
1	B	4	TYR	2.2
1	B	148	VAL	2.2
2	E	196	ILE	2.2
2	F	209	ILE	2.2
1	C	41	MET	2.2
1	B	153	PHE	2.1
2	F	137	PHE	2.1
1	C	37	ASP	2.1
2	E	192	SER	2.1
1	A	133	ALA	2.1
1	C	148	VAL	2.1
1	B	271	ARG	2.0
1	C	122	THR	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 [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, 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	LLDF	B-factors(Å ²)	Q<0.9
3	C8E	C	404	16/21	0.82	0.47	3.85	26,51,104,105	0
3	C8E	B	404	15/21	0.69	0.40	3.06	65,75,85,85	0
3	C8E	A	406	11/21	0.90	0.29	2.50	44,48,54,55	0
3	C8E	E	302	20/21	0.89	0.38	1.97	55,69,104,105	0
3	C8E	C	403	13/21	0.89	0.26	1.22	50,77,96,98	0
3	C8E	B	403	16/21	0.86	0.26	1.12	49,59,74,76	0
3	C8E	A	405	16/21	0.81	0.34	0.94	33,70,89,90	0
3	C8E	B	401	11/21	0.94	0.26	0.79	47,52,60,62	0
3	C8E	A	401	16/21	0.91	0.22	0.47	49,52,73,78	0
3	C8E	A	403	13/21	0.85	0.32	0.41	51,63,69,71	0
3	C8E	C	402	21/21	0.90	0.23	0.12	33,63,100,103	0
4	LMT	B	405	35/35	0.94	0.24	-0.18	37,83,101,106	0
4	LMT	B	406	25/35	0.88	0.22	-0.20	54,85,102,107	0
3	C8E	F	301	7/21	0.83	0.20	-0.23	57,59,65,70	0
3	C8E	B	402	18/21	0.86	0.21	-0.26	49,82,89,91	0
3	C8E	C	401	16/21	0.92	0.22	-0.84	43,66,82,82	0
3	C8E	E	301	8/21	0.91	0.19	-0.91	46,58,72,72	0
3	C8E	A	402	10/21	0.89	0.18	-3.10	62,66,77,81	0
3	C8E	A	404	9/21	0.93	0.18	-3.99	62,66,72,72	0
4	LMT	F	302	24/35	0.80	0.31	-	66,109,116,131	0
3	C8E	D	301	13/21	0.83	0.29	-	53,70,75,78	0
3	C8E	D	302	12/21	0.81	0.21	-	52,62,73,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.