



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 19, 2016 – 02:56 PM EST

PDB ID : 5JJI
Title : Rho transcription termination factor bound to rU7 and 6 ADP-BeF3 molecules
Authors : Thomsen, N.D.; Lawson, M.R.; Witkowsky, L.B.; Qu, S.; Berger, J.M.
Deposited on : 2016-04-24
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

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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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-20028442

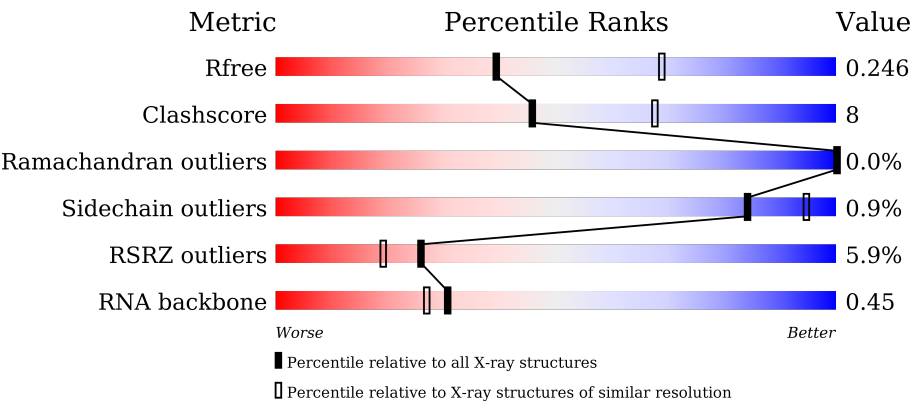
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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.



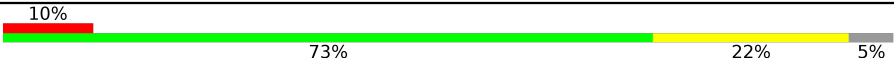


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)
RNA backbone	2183	1022 (3.00-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	420	<div><div>3%</div><div>77%</div><div>19%</div><div>.</div></div>
1	B	420	<div><div>4%</div><div>82%</div><div>15%</div><div>.</div></div>
1	C	420	<div><div>2%</div><div>81%</div><div>18%</div><div>.</div></div>
1	D	420	<div><div>4%</div><div>78%</div><div>18%</div><div>.</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	420	
1	F	420	
2	G	12	

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
4	MG	A	1001	-	-	-	X
4	MG	B	502	-	-	-	X
5	BEF	C	1002	-	-	-	X
6	MPD	B	504	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 19757 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 Transcription termination factor Rho.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	Se	0	0	0
			3181	2006	560	599	1	15			
1	B	409	Total	C	N	O	S	Se	0	0	0
			3219	2028	569	606	1	15			
1	C	417	Total	C	N	O	S	Se	0	0	0
			3280	2065	581	617	1	16			
1	D	406	Total	C	N	O	S	Se	0	0	0
			3192	2011	564	601	1	15			
1	E	400	Total	C	N	O	S	Se	0	0	0
			3142	1981	555	591	1	14			
1	F	400	Total	C	N	O	S	Se	0	0	0
			3150	1987	556	590	1	16			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MSE	-	initiating methionine	UNP P0AG32
A	-1	GLY	-	expression tag	UNP P0AG32
A	0	HIS	-	expression tag	UNP P0AG32
A	1	MSE	-	expression tag	UNP P0AG32
B	-2	MSE	-	initiating methionine	UNP P0AG32
B	-1	GLY	-	expression tag	UNP P0AG32
B	0	HIS	-	expression tag	UNP P0AG32
B	1	MSE	-	expression tag	UNP P0AG32
C	-2	MSE	-	initiating methionine	UNP P0AG32
C	-1	GLY	-	expression tag	UNP P0AG32
C	0	HIS	-	expression tag	UNP P0AG32
C	1	MSE	-	expression tag	UNP P0AG32
D	-2	MSE	-	initiating methionine	UNP P0AG32
D	-1	GLY	-	expression tag	UNP P0AG32
D	0	HIS	-	expression tag	UNP P0AG32
D	1	MSE	-	expression tag	UNP P0AG32
E	-2	MSE	-	initiating methionine	UNP P0AG32

Continued on next page...

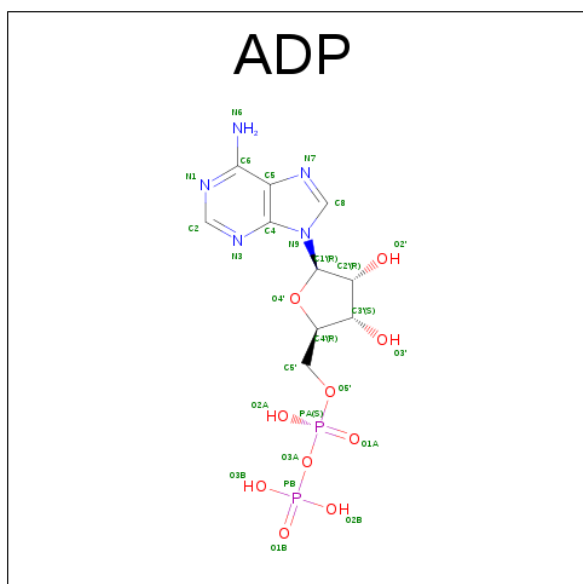
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	GLY	-	expression tag	UNP P0AG32
E	0	HIS	-	expression tag	UNP P0AG32
E	1	MSE	-	expression tag	UNP P0AG32
F	-2	MSE	-	initiating methionine	UNP P0AG32
F	-1	GLY	-	expression tag	UNP P0AG32
F	0	HIS	-	expression tag	UNP P0AG32
F	1	MSE	-	expression tag	UNP P0AG32

- Molecule 2 is a RNA chain called rU12: 5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)- 3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	7	Total	C	N	O	P	0	0	0
			141	63	14	57	7			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

Continued on next page...

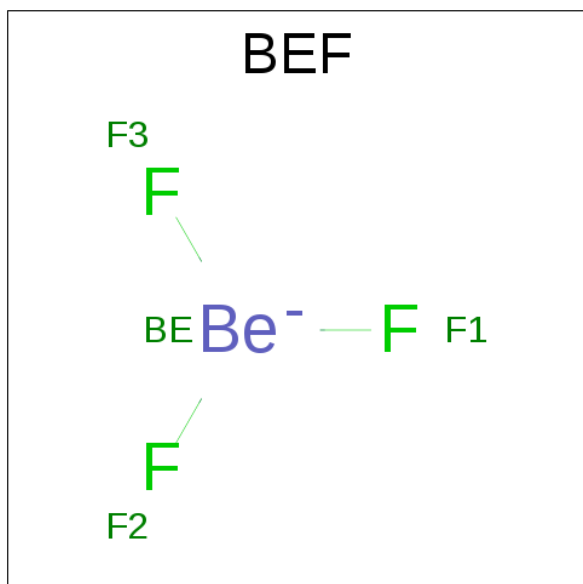
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

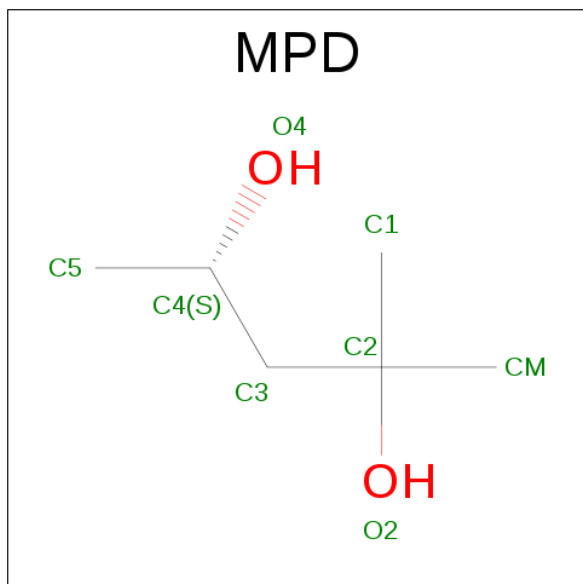
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		

- Molecule 5 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Be	F	0	0
			4	1	3		
5	B	1	Total	Be	F	0	0
			4	1	3		
5	C	1	Total	Be	F	0	0
			4	1	3		
5	D	1	Total	Be	F	0	0
			4	1	3		
5	E	1	Total	Be	F	0	0
			4	1	3		
5	F	1	Total	Be	F	0	0
			4	1	3		

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	30	Total	O	0	0
			30	30		
7	B	71	Total	O	0	0
			71	71		

Continued on next page...

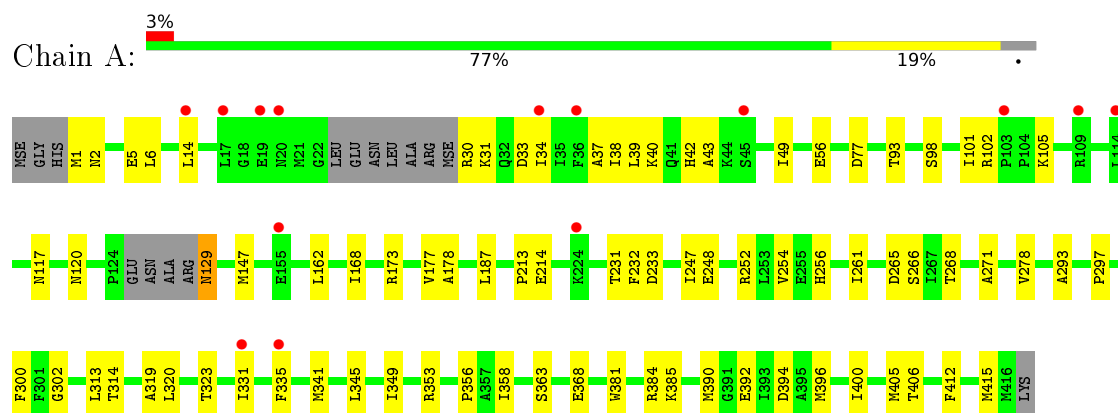
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	65	Total 65	O 65	0	0
7	D	45	Total 45	O 45	0	0
7	E	22	Total 22	O 22	0	0
7	F	8	Total 8	O 8	0	0
7	G	11	Total 11	O 11	0	0

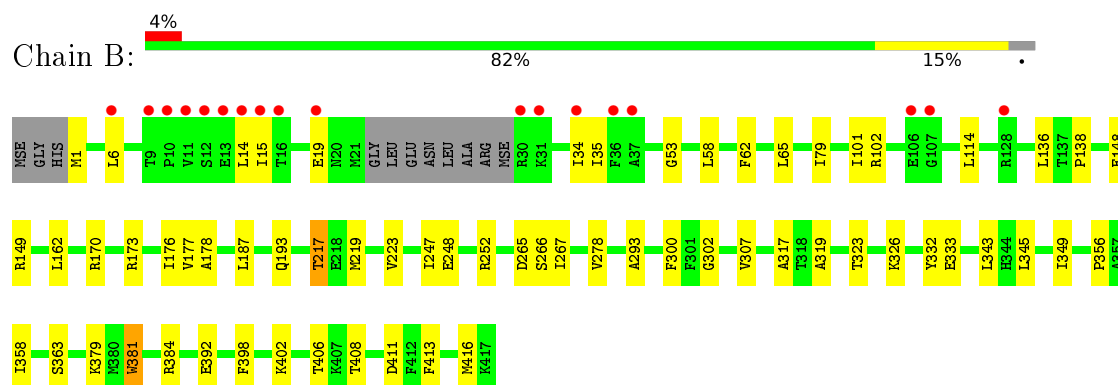
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

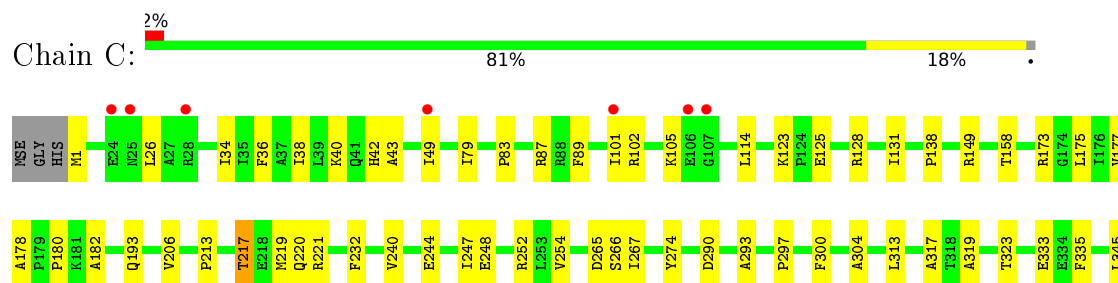
• Molecule 1: Transcription termination factor Rho

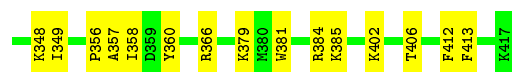


• Molecule 1: Transcription termination factor Rho

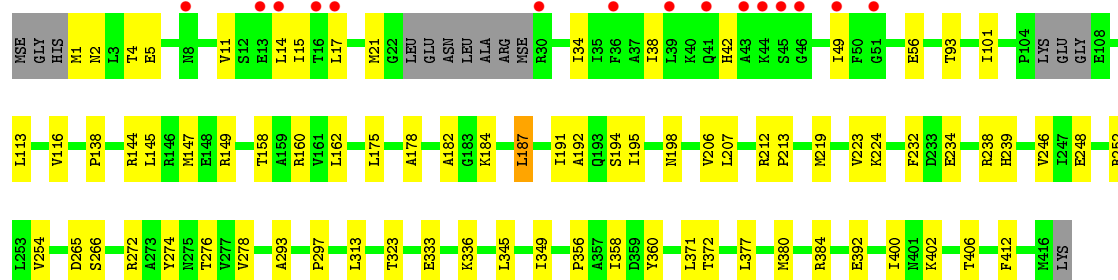
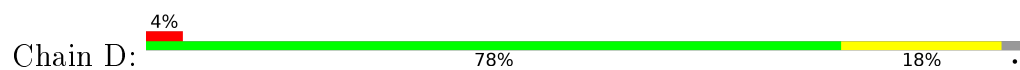


• Molecule 1: Transcription termination factor Rho

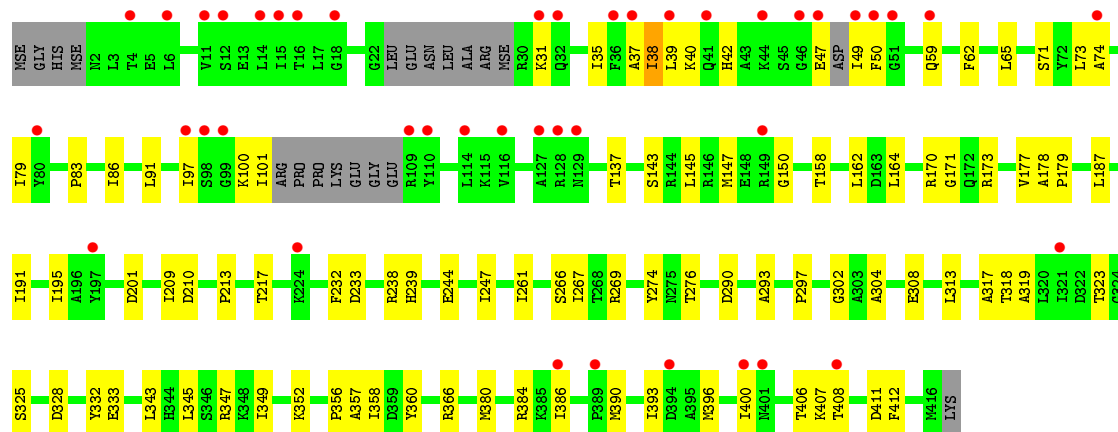
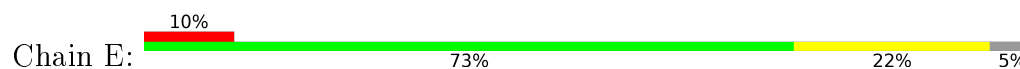




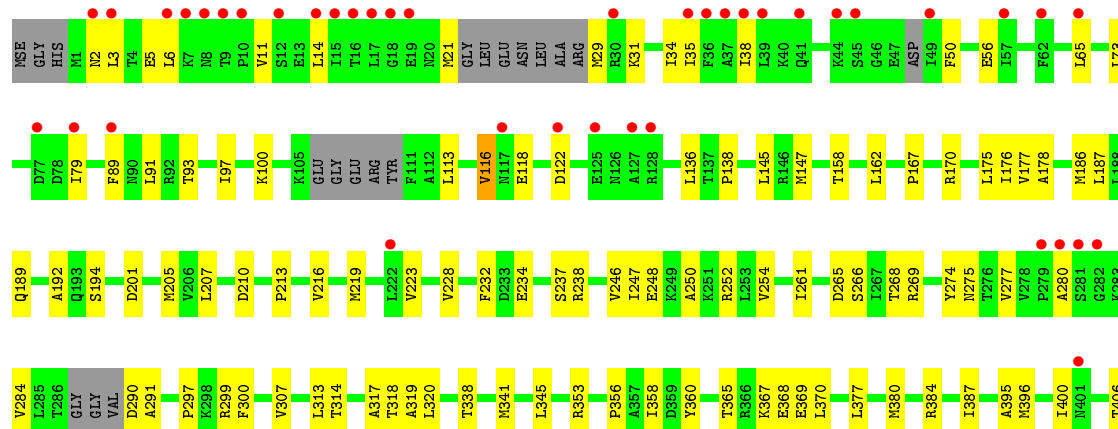
• Molecule 1: Transcription termination factor Rho



• Molecule 1: Transcription termination factor Rho



• Molecule 1: Transcription termination factor Rho





- Molecule 2: rU12: 5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)- 3'

Chain G: 42% 8% 8% 42%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.00Å 198.57Å 111.45Å 90.00° 104.36° 90.00°	Depositor
Resolution (Å)	47.42 – 2.60 47.43 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.42-2.60) 99.4 (47.43-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.61Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.219 , 0.246 0.215 , 0.246	Depositor DCC
R_{free} test set	4427 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	44.6	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	19757	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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: MG, BEF, MPD, ADP

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	0.24	0/3214	0.42	0/4304
1	B	0.24	0/3253	0.42	0/4357
1	C	0.24	0/3314	0.41	0/4438
1	D	0.24	0/3225	0.42	0/4320
1	E	0.24	0/3172	0.42	0/4246
1	F	0.24	0/3180	0.41	0/4255
2	G	0.25	0/154	1.20	3/234 (1.3%)
All	All	0.24	0/19512	0.43	3/26154 (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	G	7	U	C2-N1-C1'	7.63	126.86	117.70
2	G	7	U	N1-C2-O2	7.52	128.07	122.80
2	G	7	U	N3-C2-O2	-6.91	117.36	122.20

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	3181	0	3252	52	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3219	0	3293	41	0
1	C	3280	0	3358	47	0
1	D	3192	0	3260	52	0
1	E	3142	0	3210	60	0
1	F	3150	0	3230	63	0
2	G	141	0	71	1	0
3	A	27	0	12	0	0
3	B	27	0	12	1	0
3	C	27	0	12	0	0
3	D	27	0	12	1	0
3	E	27	0	12	0	0
3	F	27	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
5	C	4	0	0	0	0
5	D	4	0	0	0	0
5	E	4	0	0	0	0
5	F	4	0	0	0	0
6	B	8	0	14	2	0
7	A	30	0	0	0	0
7	B	71	0	0	0	0
7	C	65	0	0	0	0
7	D	45	0	0	0	0
7	E	22	0	0	0	0
7	F	8	0	0	0	0
7	G	11	0	0	0	0
All	All	19757	0	19760	302	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 (302) 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:323:THR:HA	1:B:333:GLU:HG2	1.69	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:162:LEU:HD13	1:E:343:LEU:HD22	1.72	0.71
1:A:1:MSE:HE3	1:A:39:LEU:HD23	1.73	0.71
1:B:323:THR:HA	1:C:333:GLU:HG2	1.72	0.71
1:D:192:ALA:HB1	1:D:223:VAL:HG23	1.71	0.70
1:C:323:THR:HA	1:D:333:GLU:HG2	1.73	0.70
1:B:102:ARG:HB2	1:B:114:LEU:HD11	1.75	0.69
1:F:145:LEU:HD11	1:F:170:ARG:HG3	1.76	0.67
1:A:278:VAL:HG21	1:A:293:ALA:HB2	1.79	0.65
1:E:177:VAL:HG12	1:E:319:ALA:HB3	1.77	0.65
1:A:43:ALA:HB2	1:A:49:ILE:HD11	1.77	0.65
1:E:79:ILE:HD13	1:E:101:ILE:HG21	1.77	0.65
1:C:125:GLU:HA	1:C:128:ARG:HD3	1.78	0.64
1:D:372:THR:HG21	1:D:380:MSE:HE1	1.80	0.64
1:F:73:LEU:HD11	1:F:238:ARG:HG3	1.79	0.64
1:D:323:THR:HA	1:E:333:GLU:HG2	1.81	0.62
1:E:158:THR:HA	1:E:356:PRO:HG3	1.82	0.62
1:F:237:SER:HA	1:F:277:VAL:HG21	1.82	0.62
1:E:210:ASP:HB3	1:E:269:ARG:HD2	1.83	0.61
1:F:377:LEU:HA	1:F:380:MSE:HE2	1.82	0.60
1:A:1:MSE:HE1	1:A:38:ILE:HG22	1.82	0.60
1:C:43:ALA:HB2	1:C:49:ILE:HD11	1.84	0.60
1:F:176:ILE:HB	1:F:318:THR:HG22	1.84	0.60
1:F:6:LEU:HD23	1:F:35:ILE:HG13	1.83	0.59
1:E:356:PRO:HB2	1:E:358:ILE:HG13	1.84	0.59
1:C:89:PHE:HA	1:C:128:ARG:HG3	1.84	0.59
1:F:192:ALA:HB1	1:F:223:VAL:HG21	1.85	0.58
1:C:178:ALA:HB2	1:C:345:LEU:HB2	1.84	0.58
1:D:1:MSE:HG3	1:D:42:HIS:CE1	2.39	0.58
1:D:178:ALA:HB2	1:D:345:LEU:HB2	1.84	0.58
1:F:6:LEU:HG	1:F:14:LEU:HD11	1.85	0.58
1:B:363:SER:O	1:B:384:ARG:NH2	2.37	0.58
1:D:377:LEU:HA	1:D:380:MSE:HE2	1.85	0.58
1:B:178:ALA:HB2	1:B:345:LEU:HB2	1.85	0.57
1:E:323:THR:HG23	1:E:325:SER:H	1.69	0.57
1:F:367:LYS:HB3	1:F:370:LEU:HD13	1.86	0.57
1:F:178:ALA:HB2	1:F:345:LEU:HB2	1.87	0.57
1:D:160:ARG:HH22	1:D:406:THR:HG23	1.68	0.57
1:E:406:THR:HG23	1:E:411:ASP:HB2	1.87	0.57
1:F:234:GLU:HB3	1:F:238:ARG:HD3	1.86	0.57
1:E:178:ALA:HB2	1:E:345:LEU:HB2	1.87	0.57
3:D:1000:ADP:O2A	1:E:366:ARG:NH2	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ASN:HD21	1:A:252:ARG:HB3	1.69	0.56
1:A:177:VAL:HG22	1:A:319:ALA:HB3	1.87	0.56
1:F:369:GLU:HG2	1:F:370:LEU:HD12	1.86	0.56
1:A:349:ILE:HD11	1:A:392:GLU:HB2	1.86	0.56
1:F:268:THR:HG21	1:F:320:LEU:H	1.70	0.56
1:A:39:LEU:HD22	1:A:49:ILE:HG23	1.88	0.55
1:E:360:TYR:HE2	1:E:384:ARG:HG2	1.70	0.55
1:F:284:VAL:HA	1:F:290:ASP:HA	1.88	0.55
1:F:341:MSE:HG2	1:F:365:THR:HG22	1.87	0.55
1:A:147:MSE:HG3	1:A:162:LEU:HD22	1.88	0.55
1:C:123:LYS:HD2	1:C:125:GLU:HB2	1.88	0.55
1:E:150:GLY:HA2	1:E:408:THR:HG22	1.88	0.54
1:F:213:PRO:HD3	1:F:232:PHE:CE2	2.42	0.54
1:E:73:LEU:HD22	1:E:74:ALA:H	1.72	0.54
1:A:268:THR:HG21	1:A:320:LEU:H	1.73	0.54
1:F:113:LEU:HD21	1:F:116:VAL:HG12	1.90	0.53
1:F:147:MSE:HE3	1:F:194:SER:HB2	1.91	0.53
1:E:274:TYR:CD2	1:E:297:PRO:HG3	2.44	0.53
1:E:137:THR:HB	1:E:308:GLU:HG2	1.91	0.53
1:F:147:MSE:HG3	1:F:162:LEU:HD22	1.89	0.53
1:B:379:LYS:HD3	1:B:413:PHE:HB3	1.90	0.53
1:E:35:ILE:O	1:E:39:LEU:HD23	2.09	0.53
1:F:56:GLU:HA	1:F:93:THR:HG23	1.90	0.53
1:A:1:MSE:HG2	1:A:42:HIS:CD2	2.43	0.53
1:D:2:ASN:HB3	1:D:5:GLU:HB2	1.91	0.53
1:D:356:PRO:HB2	1:D:358:ILE:HG13	1.91	0.53
1:A:254:VAL:HG21	1:A:313:LEU:HB2	1.91	0.52
1:C:102:ARG:HB3	1:C:114:LEU:HD21	1.91	0.52
1:A:129:ASN:N	1:A:129:ASN:HD22	2.07	0.52
1:B:15:ILE:O	1:B:19:GLU:HG2	2.10	0.52
1:E:217:THR:HG21	1:F:138:PRO:HD2	1.91	0.52
1:B:102:ARG:CB	1:B:114:LEU:HD11	2.40	0.52
1:D:1:MSE:HE3	1:D:49:ILE:HD11	1.92	0.52
1:E:244:GLU:HA	1:E:247:ILE:HG22	1.91	0.52
1:C:290:ASP:HB3	1:C:293:ALA:HB2	1.92	0.52
1:C:1:MSE:HE1	1:C:38:ILE:HG22	1.92	0.51
1:D:1:MSE:HE1	1:D:38:ILE:HG22	1.91	0.51
1:E:195:ILE:HD13	1:E:261:ILE:HG21	1.92	0.51
1:F:167:PRO:O	1:F:365:THR:HG21	2.10	0.51
1:C:267:ILE:HB	1:C:317:ALA:HB1	1.92	0.51
1:D:206:VAL:HG11	1:D:219:MSE:HG2	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:276:THR:HG23	1:F:291:ALA:HB1	1.91	0.51
1:C:217:THR:O	1:C:221:ARG:HD3	2.11	0.51
1:F:247:ILE:HB	1:F:300:PHE:CE1	2.46	0.51
1:E:173:ARG:HD2	1:E:302:GLY:HA2	1.93	0.51
1:C:206:VAL:HG11	1:C:219:MSE:HG2	1.92	0.50
1:C:274:TYR:CD2	1:C:297:PRO:HG3	2.47	0.50
1:A:213:PRO:HB2	1:B:138:PRO:HG2	1.93	0.50
1:C:79:ILE:HD13	1:C:101:ILE:HG21	1.92	0.50
1:D:278:VAL:HG11	1:D:293:ALA:HA	1.94	0.50
1:B:162:LEU:HD13	1:B:343:LEU:HD22	1.93	0.50
1:B:1:MSE:HE2	1:B:6:LEU:HD22	1.92	0.50
1:C:149:ARG:HH21	1:C:193:GLN:HB3	1.77	0.50
1:D:147:MSE:HG3	1:D:162:LEU:HD22	1.92	0.50
1:C:175:LEU:HD11	1:C:335:PHE:HB3	1.93	0.50
1:E:179:PRO:HG2	1:E:347:ARG:HB2	1.94	0.50
1:E:39:LEU:HD13	1:E:49:ILE:HD11	1.93	0.50
1:D:17:LEU:HD22	1:D:21:MSE:HE3	1.93	0.50
1:D:187:LEU:O	1:D:191:ILE:HG12	2.11	0.49
1:F:360:TYR:CE2	1:F:384:ARG:HG2	2.48	0.49
1:A:30:ARG:HG3	1:A:33:ASP:H	1.77	0.49
1:A:356:PRO:HB2	1:A:358:ILE:HG13	1.93	0.49
1:E:37:ALA:HA	1:E:40:LYS:HE3	1.95	0.49
1:E:71:SER:HB2	1:E:238:ARG:NH2	2.26	0.49
1:E:267:ILE:HB	1:E:317:ALA:HB1	1.93	0.49
1:F:158:THR:HA	1:F:356:PRO:HG3	1.92	0.49
1:E:145:LEU:HD21	1:E:170:ARG:HG2	1.93	0.49
1:A:406:THR:HG21	1:A:412:PHE:N	2.28	0.49
1:C:1:MSE:HE2	1:C:42:HIS:HB2	1.94	0.49
3:B:501:ADP:O2A	1:C:366:ARG:NH2	2.46	0.48
1:B:278:VAL:HG11	1:B:293:ALA:HB2	1.95	0.48
1:C:36:PHE:CZ	1:C:40:LYS:HD2	2.49	0.48
1:D:178:ALA:HB1	1:D:182:ALA:HB3	1.96	0.48
1:E:233:ASP:OD2	1:F:299:ARG:HA	2.12	0.48
1:F:3:LEU:HD23	1:F:79:ILE:HD11	1.96	0.48
1:B:406:THR:HG23	1:B:411:ASP:HB2	1.95	0.48
1:A:297:PRO:HB2	1:A:335:PHE:CZ	2.48	0.48
1:A:356:PRO:HD2	1:A:400:ILE:HD11	1.96	0.48
1:F:178:ALA:CB	1:F:345:LEU:HB2	2.43	0.48
1:F:29:MSE:HE3	1:F:34:ILE:HG12	1.95	0.48
1:B:149:ARG:HH21	1:B:193:GLN:HB2	1.78	0.48
1:A:173:ARG:HD2	1:A:302:GLY:HA2	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:GLU:OE1	1:B:408:THR:HA	2.14	0.48
1:B:349:ILE:HD11	1:B:392:GLU:HB3	1.95	0.48
1:E:50:PHE:HA	1:E:100:LYS:HA	1.96	0.48
1:E:209:ILE:HG23	1:E:239:HIS:HB3	1.96	0.48
1:F:2:ASN:HB3	1:F:5:GLU:HB3	1.96	0.48
1:B:79:ILE:HD13	1:B:101:ILE:HG21	1.95	0.47
1:D:178:ALA:HB3	1:D:184:LYS:HG3	1.96	0.47
1:C:248:GLU:O	1:C:252:ARG:HG2	2.14	0.47
1:B:177:VAL:HG22	1:B:319:ALA:HB3	1.97	0.47
1:E:177:VAL:HG11	1:E:332:TYR:CD1	2.49	0.47
1:A:247:ILE:HB	1:A:300:PHE:CE1	2.50	0.47
1:C:177:VAL:HG22	1:C:319:ALA:HB3	1.96	0.47
1:E:349:ILE:HB	1:E:357:ALA:HB1	1.97	0.47
1:E:187:LEU:HD21	1:E:343:LEU:HD23	1.97	0.47
1:B:247:ILE:HB	1:B:300:PHE:CE1	2.50	0.47
1:B:356:PRO:HB2	1:B:358:ILE:HG13	1.97	0.47
1:E:290:ASP:HB3	1:E:293:ALA:HB2	1.95	0.47
1:D:356:PRO:HD2	1:D:400:ILE:HD11	1.96	0.47
1:F:205:MSE:HE1	1:F:250:ALA:HB2	1.96	0.47
1:C:83:PRO:O	1:C:87:ARG:HG3	2.15	0.46
1:D:402:LYS:HB3	1:D:412:PHE:HE1	1.79	0.46
1:C:379:LYS:HD3	1:C:413:PHE:HB3	1.96	0.46
1:C:178:ALA:CB	1:C:345:LEU:HB2	2.45	0.46
1:D:265:ASP:HA	1:D:266:SER:HA	1.57	0.46
1:C:349:ILE:HB	1:C:357:ALA:HB1	1.98	0.46
1:D:158:THR:HA	1:D:356:PRO:HG3	1.98	0.46
1:E:178:ALA:CB	1:E:345:LEU:HB2	2.44	0.46
1:F:186:MSE:HG3	3:F:1000:ADP:C8	2.50	0.46
1:E:406:THR:HG21	1:E:412:PHE:N	2.30	0.46
1:B:265:ASP:HA	1:B:266:SER:HA	1.58	0.46
1:A:49:ILE:HB	1:A:101:ILE:O	2.16	0.46
1:A:56:GLU:HA	1:A:93:THR:HG23	1.97	0.46
1:E:35:ILE:HA	1:E:38:ILE:HG22	1.98	0.46
1:E:42:HIS:CD2	1:E:47:GLU:HB2	2.50	0.46
1:F:248:GLU:O	1:F:252:ARG:HG2	2.16	0.46
1:A:147:MSE:HE3	1:A:168:ILE:HD12	1.98	0.45
1:B:219:MSE:O	1:B:223:VAL:HG12	2.17	0.45
1:C:102:ARG:NH1	1:C:105:LYS:HG3	2.31	0.45
1:D:11:VAL:O	1:D:15:ILE:HG13	2.16	0.45
1:C:158:THR:HA	1:C:356:PRO:HG3	1.98	0.45
1:E:158:THR:HG22	1:E:356:PRO:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:ILE:HG13	1:E:91:LEU:HB2	1.98	0.45
1:F:3:LEU:HD12	1:F:35:ILE:HD11	1.98	0.45
1:B:398:PHE:O	1:B:402:LYS:HG2	2.16	0.45
1:E:164:LEU:HA	1:E:380:MSE:HE2	1.99	0.45
1:F:50:PHE:CD1	1:F:100:LYS:HG2	2.51	0.45
1:A:102:ARG:NH1	1:A:105:LYS:HG3	2.32	0.45
1:B:248:GLU:O	1:B:252:ARG:HG2	2.17	0.45
1:F:207:LEU:HD13	1:F:246:VAL:HG21	1.98	0.45
1:F:387:ILE:HG23	1:F:395:ALA:HB1	1.97	0.45
1:F:2:ASN:O	1:F:6:LEU:HB2	2.17	0.45
1:A:368:GLU:OE2	1:F:353:ARG:NH1	2.49	0.45
1:B:217:THR:HG21	1:C:138:PRO:O	2.17	0.44
1:F:210:ASP:HB3	1:F:269:ARG:HB3	1.99	0.44
1:F:265:ASP:HA	1:F:266:SER:HA	1.65	0.44
1:A:265:ASP:HA	1:A:266:SER:HA	1.59	0.44
1:A:37:ALA:HA	1:A:40:LYS:HE2	1.98	0.44
1:D:191:ILE:O	1:D:195:ILE:HG12	2.17	0.44
1:A:231:THR:HG22	1:A:233:ASP:H	1.82	0.44
1:D:21:MSE:SE	1:D:38:ILE:HG23	2.67	0.44
1:D:254:VAL:HG21	1:D:313:LEU:HB2	1.99	0.44
1:C:180:PRO:HB2	1:D:336:LYS:HD3	1.99	0.44
1:A:2:ASN:HB3	1:A:5:GLU:HB3	2.00	0.44
1:C:173:ARG:NH1	1:C:304:ALA:O	2.50	0.44
1:F:177:VAL:HG22	1:F:319:ALA:HB3	1.99	0.44
1:D:272:ARG:O	1:D:276:THR:HG23	2.17	0.44
1:E:396:MSE:O	1:E:400:ILE:HG12	2.18	0.44
1:E:232:PHE:CZ	1:F:338:THR:HG23	2.53	0.44
1:A:271:ALA:HB1	1:A:331:ILE:HG21	1.99	0.44
1:A:37:ALA:HA	1:A:40:LYS:HG2	2.00	0.44
1:D:56:GLU:HA	1:D:93:THR:HG23	2.00	0.44
1:E:173:ARG:NH1	1:E:304:ALA:O	2.51	0.44
1:F:356:PRO:HB2	1:F:358:ILE:HG13	1.99	0.44
1:C:360:TYR:HE2	1:C:384:ARG:HG2	1.83	0.44
1:F:21:MSE:SE	1:F:38:ILE:HG23	2.68	0.44
1:F:406:THR:HG21	1:F:412:PHE:N	2.33	0.44
1:A:248:GLU:O	1:A:252:ARG:HG2	2.18	0.43
1:C:247:ILE:HB	1:C:300:PHE:CE1	2.53	0.43
1:C:265:ASP:HA	1:C:266:SER:HA	1.55	0.43
1:C:356:PRO:HB2	1:C:358:ILE:HG13	1.99	0.43
1:D:234:GLU:HB2	1:D:239:HIS:CE1	2.53	0.43
1:E:323:THR:HG21	1:E:328:ASP:OD2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:LEU:HD21	1:D:116:VAL:HG12	2.00	0.43
1:D:207:LEU:HD13	1:D:246:VAL:HG21	2.00	0.43
1:D:49:ILE:HG23	1:D:101:ILE:HG13	2.00	0.43
1:E:407:LYS:HG2	1:E:408:THR:HG23	2.01	0.43
1:F:118:GLU:HG3	1:F:122:ASP:O	2.18	0.43
1:C:213:PRO:HD3	1:C:232:PHE:CZ	2.54	0.43
1:A:213:PRO:HD2	1:A:214:GLU:OE2	2.19	0.43
1:A:178:ALA:HB2	1:A:345:LEU:HB2	2.00	0.43
1:A:405:MSE:SE	1:A:415:MSE:HE1	2.68	0.43
1:B:14:LEU:HB3	1:B:34:ILE:HG21	1.99	0.43
1:D:392:GLU:H	1:D:392:GLU:HG2	1.62	0.43
1:A:381:TRP:O	1:A:385:LYS:HG3	2.18	0.43
1:E:143:SER:HB3	1:E:170:ARG:HG3	2.00	0.43
1:C:381:TRP:CZ2	1:C:385:LYS:HE3	2.53	0.43
1:D:147:MSE:HE3	1:D:194:SER:HB2	2.00	0.43
1:E:65:LEU:HD21	1:E:97:ILE:HD12	2.00	0.43
1:F:189:GLN:HG2	1:F:219:MSE:SE	2.69	0.43
1:D:2:ASN:OD1	1:D:4:THR:HG22	2.19	0.43
1:D:144:ARG:HD2	1:D:371:LEU:O	2.19	0.43
1:F:274:TYR:CD2	1:F:297:PRO:HG3	2.54	0.43
1:A:353:ARG:HB3	1:B:381:TRP:CZ2	2.54	0.43
1:C:217:THR:HA	1:C:220:GLN:HG2	2.01	0.43
1:C:217:THR:HG21	1:D:138:PRO:O	2.19	0.43
1:D:213:PRO:HD3	1:D:232:PHE:CZ	2.54	0.43
1:F:365:THR:OG1	1:F:368:GLU:HB3	2.19	0.43
1:D:349:ILE:HD11	1:D:392:GLU:HB2	2.01	0.42
1:B:416:MSE:HE3	1:B:416:MSE:HB2	1.89	0.42
1:C:175:LEU:HA	1:C:317:ALA:O	2.19	0.42
1:A:261:ILE:HG12	1:A:314:THR:HB	2.01	0.42
1:B:406:THR:CG2	1:B:411:ASP:HB2	2.49	0.42
1:B:6:LEU:HD23	1:B:35:ILE:HG23	2.01	0.42
1:E:31:LYS:HE2	1:E:31:LYS:HB3	1.89	0.42
1:E:62:PHE:N	1:E:62:PHE:CD2	2.87	0.42
1:A:297:PRO:HB2	1:A:335:PHE:CE2	2.55	0.42
1:B:58:LEU:HD12	1:B:62:PHE:CE1	2.54	0.42
1:D:194:SER:O	1:D:198:ASN:HB2	2.19	0.42
1:D:274:TYR:CD2	1:D:297:PRO:HG3	2.54	0.42
1:E:386:ILE:HG22	1:E:390:MSE:HE3	2.02	0.42
1:A:168:ILE:HD11	1:A:341:MSE:HE3	2.00	0.42
1:A:396:MSE:O	1:A:400:ILE:HG12	2.20	0.42
1:D:178:ALA:CB	1:D:345:LEU:HB2	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:VAL:HG11	1:B:332:TYR:CE1	2.54	0.42
1:B:267:ILE:HB	1:B:317:ALA:HB1	2.00	0.42
1:A:98:SER:O	1:A:117:ASN:N	2.51	0.42
1:B:170:ARG:HD2	6:B:504:MPD:H4	2.02	0.42
1:C:178:ALA:HB1	1:C:182:ALA:HB3	2.01	0.42
1:C:254:VAL:HG21	1:C:313:LEU:HB2	2.01	0.42
1:D:14:LEU:HD12	1:D:34:ILE:HD12	2.02	0.42
1:A:120:ASN:HD22	1:A:256:HIS:CD2	2.37	0.42
1:D:224:LYS:HD3	1:D:224:LYS:HA	1.90	0.42
1:D:406:THR:HG21	1:D:412:PHE:HB2	2.01	0.42
1:E:147:MSE:HE1	1:E:191:ILE:HA	2.02	0.42
1:A:213:PRO:HG3	1:A:231:THR:HG21	2.01	0.42
1:A:6:LEU:HG	1:A:14:LEU:HD11	2.01	0.42
1:E:171:GLY:HA2	1:E:313:LEU:O	2.19	0.42
1:F:254:VAL:HG21	1:F:313:LEU:HB2	2.01	0.42
1:A:77:ASP:N	1:A:77:ASP:OD1	2.53	0.41
6:B:504:MPD:H53	6:B:504:MPD:HM1	2.01	0.41
1:B:53:GLY:HA3	1:B:65:LEU:HB3	2.02	0.41
1:D:248:GLU:O	1:D:252:ARG:HG2	2.19	0.41
1:F:136:LEU:HB3	1:F:307:VAL:HG13	2.01	0.41
1:F:201:ASP:N	1:F:201:ASP:OD2	2.52	0.41
1:A:363:SER:O	1:A:384:ARG:NH2	2.53	0.41
1:D:212:ARG:HA	1:D:232:PHE:CE2	2.55	0.41
1:F:50:PHE:HD1	1:F:100:LYS:HG2	1.85	0.41
1:C:131:ILE:HG12	1:C:131:ILE:H	1.67	0.41
1:C:240:VAL:O	1:C:244:GLU:HG2	2.19	0.41
1:D:234:GLU:HB2	1:D:239:HIS:HE1	1.86	0.41
1:E:62:PHE:N	1:E:62:PHE:HD2	2.18	0.41
1:D:234:GLU:HB3	1:D:238:ARG:HD3	2.02	0.41
1:E:266:SER:HB2	1:E:318:THR:O	2.21	0.41
1:F:207:LEU:HA	1:F:228:VAL:O	2.21	0.41
1:F:31:LYS:O	1:F:35:ILE:HG22	2.20	0.41
1:F:65:LEU:HD21	1:F:97:ILE:HD12	2.03	0.41
1:B:326:LYS:NZ	2:G:6:U:O2	2.52	0.41
1:F:261:ILE:HG12	1:F:314:THR:HB	2.03	0.41
1:B:136:LEU:HB3	1:B:307:VAL:HG13	2.03	0.41
1:B:178:ALA:CB	1:B:345:LEU:HB2	2.50	0.41
1:B:176:ILE:HD12	1:B:343:LEU:HD23	2.02	0.41
1:D:360:TYR:HE2	1:D:384:ARG:HD2	1.85	0.41
1:E:266:SER:OG	1:E:269:ARG:HG3	2.20	0.41
1:A:31:LYS:HA	1:A:34:ILE:HG22	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:175:LEU:HA	1:F:317:ALA:O	2.21	0.41
1:F:266:SER:HB2	1:F:318:THR:O	2.20	0.41
1:F:396:MSE:O	1:F:400:ILE:HG12	2.21	0.41
1:A:390:MSE:HE2	1:A:394:ASP:HB3	2.03	0.40
1:B:413:PHE:HA	1:B:416:MSE:HE3	2.02	0.40
1:E:62:PHE:CD2	1:E:83:PRO:HG3	2.55	0.40
1:F:89:PHE:HB2	1:F:91:LEU:HG	2.03	0.40
1:B:173:ARG:HD2	1:B:302:GLY:HA2	2.03	0.40
1:C:402:LYS:HB3	1:C:412:PHE:HE1	1.87	0.40
1:C:348:LYS:HE3	1:C:348:LYS:HB2	1.85	0.40
1:C:26:LEU:O	1:C:34:ILE:HD11	2.22	0.40
1:E:213:PRO:HD3	1:E:232:PHE:CE2	2.57	0.40
1:A:213:PRO:HD3	1:A:232:PHE:CZ	2.57	0.40
1:E:352:LYS:HD3	1:E:393:ILE:HG21	2.03	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	399/420 (95%)	390 (98%)	9 (2%)	0	100	100
1	B	405/420 (96%)	399 (98%)	6 (2%)	0	100	100
1	C	415/420 (99%)	408 (98%)	7 (2%)	0	100	100
1	D	400/420 (95%)	391 (98%)	9 (2%)	0	100	100
1	E	392/420 (93%)	385 (98%)	7 (2%)	0	100	100
1	F	390/420 (93%)	385 (99%)	4 (1%)	1 (0%)	46	72
All	All	2401/2520 (95%)	2358 (98%)	42 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	280	ALA

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	347/342 (102%)	345 (99%)	2 (1%)	90	97
1	B	351/342 (103%)	348 (99%)	3 (1%)	84	95
1	C	357/342 (104%)	355 (99%)	2 (1%)	90	97
1	D	348/342 (102%)	344 (99%)	4 (1%)	80	93
1	E	342/342 (100%)	339 (99%)	3 (1%)	84	95
1	F	345/342 (101%)	340 (99%)	5 (1%)	74	90
All	All	2090/2052 (102%)	2071 (99%)	19 (1%)	84	95

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	ASN
1	A	187	LEU
1	B	187	LEU
1	B	217	THR
1	B	381	TRP
1	C	217	THR
1	C	406	THR
1	D	145	LEU
1	D	149	ARG
1	D	175	LEU
1	D	187	LEU
1	E	38	ILE
1	E	59	GLN
1	E	201	ASP
1	F	11	VAL
1	F	116	VAL
1	F	187	LEU
1	F	216	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	275	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	HIS
1	B	41	GLN
1	D	32	GLN
1	E	388	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	G	6/12 (50%)	1 (16%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	G	7	U

There are no RNA pucker outliers to report.

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 19 ligands modelled in this entry, 6 are monoatomic - leaving 13 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
3	ADP	A	1000	5,4	24,29,29	0.99	1 (4%)	23,45,45	1.76	2 (8%)
5	BEF	A	1002	3	0,3,3	0.00	-	0,3,3	0.00	-
3	ADP	B	501	5,4	24,29,29	1.00	1 (4%)	23,45,45	1.78	2 (8%)
5	BEF	B	503	3	0,3,3	0.00	-	0,3,3	0.00	-
6	MPD	B	504	-	6,7,7	0.37	0	6,10,10	0.78	0
3	ADP	C	1000	5,4	24,29,29	1.00	1 (4%)	23,45,45	1.77	2 (8%)
5	BEF	C	1002	3	0,3,3	0.00	-	0,3,3	0.00	-
3	ADP	D	1000	5,4	24,29,29	1.00	1 (4%)	23,45,45	1.82	2 (8%)
5	BEF	D	1002	3	0,3,3	0.00	-	0,3,3	0.00	-
3	ADP	E	1000	5,4	24,29,29	0.99	1 (4%)	23,45,45	1.72	1 (4%)
5	BEF	E	1002	3	0,3,3	0.00	-	0,3,3	0.00	-
3	ADP	F	1000	5,4	24,29,29	0.98	1 (4%)	23,45,45	1.75	1 (4%)
5	BEF	F	1002	3	0,3,3	0.00	-	0,3,3	0.00	-

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	ADP	A	1000	5,4	-	0/12/32/32	0/3/3/3
5	BEF	A	1002	3	-	0/0/0/0	0/0/0/0
3	ADP	B	501	5,4	-	0/12/32/32	0/3/3/3
5	BEF	B	503	3	-	0/0/0/0	0/0/0/0
6	MPD	B	504	-	-	0/5/5/5	0/0/0/0
3	ADP	C	1000	5,4	-	0/12/32/32	0/3/3/3
5	BEF	C	1002	3	-	0/0/0/0	0/0/0/0
3	ADP	D	1000	5,4	-	0/12/32/32	0/3/3/3
5	BEF	D	1002	3	-	0/0/0/0	0/0/0/0
3	ADP	E	1000	5,4	-	0/12/32/32	0/3/3/3
5	BEF	E	1002	3	-	0/0/0/0	0/0/0/0
3	ADP	F	1000	5,4	-	0/12/32/32	0/3/3/3
5	BEF	F	1002	3	-	0/0/0/0	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1000	ADP	C5-C4	3.05	1.47	1.40
3	D	1000	ADP	C5-C4	3.05	1.47	1.40
3	C	1000	ADP	C5-C4	3.10	1.47	1.40
3	F	1000	ADP	C5-C4	3.10	1.47	1.40
3	B	501	ADP	C5-C4	3.11	1.47	1.40
3	E	1000	ADP	C5-C4	3.13	1.47	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1000	ADP	N3-C2-N1	-6.69	123.62	128.87
3	B	501	ADP	N3-C2-N1	-6.68	123.63	128.87
3	A	1000	ADP	N3-C2-N1	-6.64	123.65	128.87
3	C	1000	ADP	N3-C2-N1	-6.57	123.71	128.87
3	F	1000	ADP	N3-C2-N1	-6.57	123.71	128.87
3	E	1000	ADP	N3-C2-N1	-6.55	123.72	128.87
3	C	1000	ADP	C2'-C1'-N9	-2.93	105.63	113.47
3	D	1000	ADP	C2'-C1'-N9	-2.78	106.01	113.47
3	B	501	ADP	C2'-C1'-N9	-2.72	106.17	113.47
3	A	1000	ADP	C2'-C1'-N9	-2.52	106.71	113.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	ADP	1	0
6	B	504	MPD	2	0
3	D	1000	ADP	1	0
3	F	1000	ADP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	390/420 (92%)	-0.04	14 (3%) 46 38	33, 60, 113, 138	0
1	B	394/420 (93%)	-0.09	18 (4%) 36 29	23, 44, 113, 140	0
1	C	401/420 (95%)	-0.10	7 (1%) 73 68	24, 46, 99, 123	0
1	D	391/420 (93%)	-0.03	15 (3%) 44 36	28, 56, 108, 127	0
1	E	386/420 (91%)	0.47	43 (11%) 7 4	46, 78, 121, 136	0
1	F	384/420 (91%)	0.56	41 (10%) 8 4	65, 81, 127, 136	0
2	G	7/12 (58%)	-0.33	0 100 100	44, 48, 62, 80	0
All	All	2353/2532 (92%)	0.12	138 (5%) 26 19	23, 64, 115, 140	0

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	41	GLN	7.6
1	D	14	LEU	6.8
1	F	6	LEU	6.7
1	E	14	LEU	5.8
1	A	19	GLU	5.4
1	E	98	SER	5.3
1	B	14	LEU	5.2
1	E	127	ALA	5.1
1	F	16	THR	5.0
1	B	9	THR	5.0
1	E	114	LEU	4.9
1	D	46	GLY	4.9
1	E	51	GLY	4.9
1	E	99	GLY	4.8
1	F	15	ILE	4.6
1	F	12	SER	4.6
1	E	49	ILE	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	31	LYS	4.6
1	A	14	LEU	4.5
1	F	14	LEU	4.4
1	B	10	PRO	4.3
1	E	110	TYR	4.3
1	E	41	GLN	4.2
1	B	19	GLU	4.2
1	F	128	ARG	4.2
1	F	35	ILE	4.1
1	E	50	PHE	4.1
1	D	13	GLU	4.1
1	C	49	ILE	3.9
1	E	149	ARG	3.9
1	F	17	LEU	3.8
1	F	45	SER	3.8
1	B	6	LEU	3.7
1	E	36	PHE	3.7
1	A	34	ILE	3.7
1	E	80	TYR	3.7
1	F	49	ILE	3.7
1	F	62	PHE	3.6
1	A	109	ARG	3.6
1	F	89	PHE	3.6
1	D	41	GLN	3.6
1	F	77	ASP	3.5
1	F	3	LEU	3.5
1	E	39	LEU	3.5
1	D	36	PHE	3.5
1	B	106	GLU	3.5
1	F	19	GLU	3.2
1	D	49	ILE	3.2
1	B	30	ARG	3.2
1	E	129	ASN	3.2
1	F	10	PRO	3.1
1	E	116	VAL	3.1
1	E	6	LEU	3.0
1	F	8	ASN	3.0
1	C	24	GLU	3.0
1	F	282	GLY	3.0
1	E	128	ARG	3.0
1	B	36	PHE	3.0
1	D	43	ALA	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	74	ALA	2.9
1	B	13	GLU	2.9
1	E	97	ILE	2.9
1	E	400	ILE	2.9
1	D	39	LEU	2.9
1	F	222	LEU	2.8
1	E	44	LYS	2.8
1	E	386	ILE	2.8
1	E	59	GLN	2.8
1	F	57	ILE	2.8
1	A	103	PRO	2.8
1	E	18	GLY	2.7
1	E	197	TYR	2.7
1	B	31	LYS	2.7
1	F	39	LEU	2.7
1	E	389	PRO	2.7
1	F	125	GLU	2.7
1	E	12	SER	2.7
1	F	401	ASN	2.7
1	A	155	GLU	2.6
1	F	18	GLY	2.6
1	F	44	LYS	2.6
1	F	65	LEU	2.6
1	D	8	ASN	2.6
1	D	17	LEU	2.6
1	B	107	GLY	2.6
1	F	280	ALA	2.6
1	C	25	ASN	2.5
1	F	9	THR	2.5
1	A	17	LEU	2.5
1	C	28	ARG	2.5
1	A	20	ASN	2.5
1	F	38	ILE	2.5
1	E	32	GLN	2.5
1	F	30	ARG	2.4
1	E	394	ASP	2.4
1	F	117	ASN	2.4
1	D	51	GLY	2.4
1	A	45	SER	2.4
1	F	36	PHE	2.4
1	E	321	ILE	2.4
1	E	401	ASN	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	16	THR	2.4
1	A	114	LEU	2.3
1	D	16	THR	2.3
1	B	15	ILE	2.3
1	D	30	ARG	2.3
1	F	79	ILE	2.3
1	F	127	ALA	2.3
1	C	101	ILE	2.3
1	F	122	ASP	2.3
1	E	4	THR	2.3
1	B	128	ARG	2.3
1	B	37	ALA	2.3
1	B	34	ILE	2.3
1	F	279	PRO	2.2
1	E	109	ARG	2.2
1	E	224	LYS	2.2
1	E	11	VAL	2.2
1	E	37	ALA	2.2
1	A	335	PHE	2.2
1	C	106	GLU	2.2
1	F	2	ASN	2.2
1	F	7	LYS	2.2
1	E	46	GLY	2.2
1	A	224	LYS	2.2
1	E	408	THR	2.2
1	E	15	ILE	2.1
1	E	47	GLU	2.1
1	C	107	GLY	2.1
1	B	11	VAL	2.1
1	F	37	ALA	2.1
1	B	12	SER	2.1
1	A	331	ILE	2.1
1	B	16	THR	2.1
1	D	45	SER	2.1
1	A	36	PHE	2.1
1	F	281	SER	2.0
1	D	44	LYS	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
6	MPD	B	504	8/8	0.74	0.30	5.08	47,78,89,96	0
4	MG	A	1001	1/1	0.93	0.21	2.97	45,45,45,45	0
4	MG	B	502	1/1	0.96	0.24	2.80	38,38,38,38	0
5	BEF	C	1002	4/4	0.97	0.26	2.07	30,32,35,53	0
4	MG	C	1001	1/1	0.97	0.20	0.86	45,45,45,45	0
5	BEF	E	1002	4/4	0.94	0.20	0.82	63,63,63,71	0
3	ADP	A	1000	27/27	0.97	0.17	0.20	31,39,48,54	0
3	ADP	C	1000	27/27	0.96	0.16	0.02	29,39,49,58	0
3	ADP	B	501	27/27	0.97	0.17	-0.28	25,30,36,43	0
3	ADP	F	1000	27/27	0.92	0.17	-0.32	66,71,75,82	0
3	ADP	D	1000	27/27	0.97	0.15	-0.95	40,54,62,74	0
5	BEF	B	503	4/4	0.98	0.17	-1.00	20,23,29,30	0
5	BEF	F	1002	4/4	0.91	0.17	-1.00	66,66,66,67	0
5	BEF	A	1002	4/4	0.94	0.14	-1.50	30,32,33,36	0
3	ADP	E	1000	27/27	0.92	0.13	-1.52	66,76,83,85	0
4	MG	E	1001	1/1	0.96	0.12	-2.58	63,63,63,63	0
4	MG	F	1001	1/1	0.89	0.15	-2.58	67,67,67,67	0
4	MG	D	1001	1/1	0.98	0.12	-3.72	46,46,46,46	0
5	BEF	D	1002	4/4	0.94	0.11	-5.18	39,42,44,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.