



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 07:53 pm GMT

PDB ID : 2B8Q
Title : X-ray structure of Acanthamoeba ployphaga mimivirus nucleoside diphosphate kinase complexed with TDP
Authors : Jeudy, S.; Claverie, J.M.; Abergel, C.
Deposited on : 2005-10-10
Resolution : 2.50 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

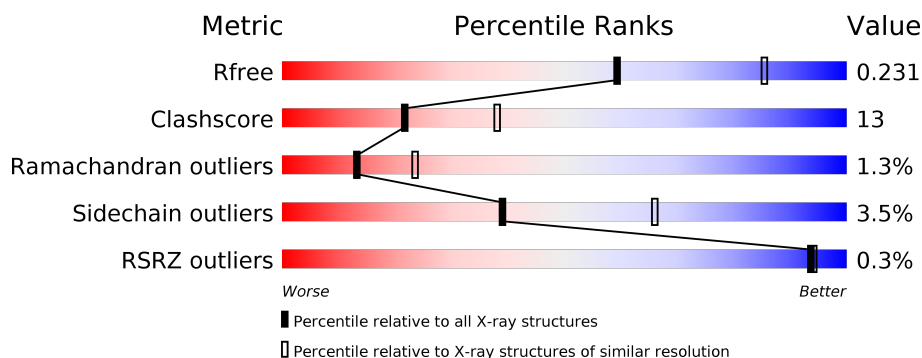
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	111664	4155 (2.50-2.50)
Clashscore	122126	4827 (2.50-2.50)
Ramachandran outliers	120053	4735 (2.50-2.50)
Sidechain outliers	120020	4737 (2.50-2.50)
RSRZ outliers	108989	4058 (2.50-2.50)

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	142	
1	B	142	
1	C	142	
1	D	142	
1	E	142	
1	F	142	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6652 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 Probable nucleoside diphosphate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	133	Total	C	N	O	S	0	0	0
			1065	673	184	204	4			
1	B	130	Total	C	N	O	S	0	0	0
			1049	664	181	200	4			
1	C	132	Total	C	N	O	S	0	0	0
			1060	670	183	203	4			
1	D	132	Total	C	N	O	S	0	0	0
			1060	670	183	203	4			
1	E	132	Total	C	N	O	S	0	0	0
			1060	670	183	203	4			
1	F	130	Total	C	N	O	S	0	0	0
			1044	661	181	198	4			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	TYR	-	EXPRESSION TAG	UNP Q5UQL3
A	-3	LYS	-	EXPRESSION TAG	UNP Q5UQL3
A	-2	LYS	-	EXPRESSION TAG	UNP Q5UQL3
A	-1	ALA	-	EXPRESSION TAG	UNP Q5UQL3
A	0	GLY	-	EXPRESSION TAG	UNP Q5UQL3
A	1	LEU	-	EXPRESSION TAG	UNP Q5UQL3
B	-4	TYR	-	EXPRESSION TAG	UNP Q5UQL3
B	-3	LYS	-	EXPRESSION TAG	UNP Q5UQL3
B	-2	LYS	-	EXPRESSION TAG	UNP Q5UQL3
B	-1	ALA	-	EXPRESSION TAG	UNP Q5UQL3
B	0	GLY	-	EXPRESSION TAG	UNP Q5UQL3
B	1	LEU	-	EXPRESSION TAG	UNP Q5UQL3
C	-4	TYR	-	EXPRESSION TAG	UNP Q5UQL3
C	-3	LYS	-	EXPRESSION TAG	UNP Q5UQL3
C	-2	LYS	-	EXPRESSION TAG	UNP Q5UQL3
C	-1	ALA	-	EXPRESSION TAG	UNP Q5UQL3
C	0	GLY	-	EXPRESSION TAG	UNP Q5UQL3

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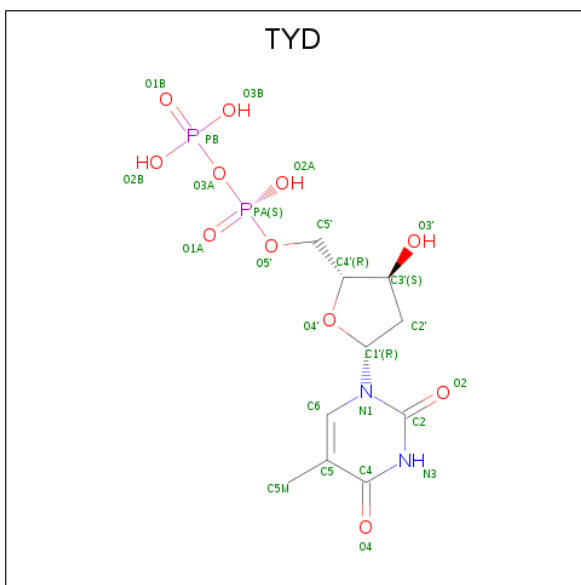
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1	LEU	-	EXPRESSION TAG	UNP Q5UQL3
D	-4	TYR	-	EXPRESSION TAG	UNP Q5UQL3
D	-3	LYS	-	EXPRESSION TAG	UNP Q5UQL3
D	-2	LYS	-	EXPRESSION TAG	UNP Q5UQL3
D	-1	ALA	-	EXPRESSION TAG	UNP Q5UQL3
D	0	GLY	-	EXPRESSION TAG	UNP Q5UQL3
D	1	LEU	-	EXPRESSION TAG	UNP Q5UQL3
E	-4	TYR	-	EXPRESSION TAG	UNP Q5UQL3
E	-3	LYS	-	EXPRESSION TAG	UNP Q5UQL3
E	-2	LYS	-	EXPRESSION TAG	UNP Q5UQL3
E	-1	ALA	-	EXPRESSION TAG	UNP Q5UQL3
E	0	GLY	-	EXPRESSION TAG	UNP Q5UQL3
E	1	LEU	-	EXPRESSION TAG	UNP Q5UQL3
F	-4	TYR	-	EXPRESSION TAG	UNP Q5UQL3
F	-3	LYS	-	EXPRESSION TAG	UNP Q5UQL3
F	-2	LYS	-	EXPRESSION TAG	UNP Q5UQL3
F	-1	ALA	-	EXPRESSION TAG	UNP Q5UQL3
F	0	GLY	-	EXPRESSION TAG	UNP Q5UQL3
F	1	LEU	-	EXPRESSION TAG	UNP Q5UQL3

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is THYMIDINE-5'-DIPHOSPHATE (three-letter code: TYD) (formula: C₁₀H₁₆N₂O₁₁P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 25	C 10	N 2	O 11	P 2	0	0
3	B	1	Total 25	C 10	N 2	O 11	P 2	0	0
3	C	1	Total 25	C 10	N 2	O 11	P 2	0	0
3	D	1	Total 25	C 10	N 2	O 11	P 2	0	0
3	E	1	Total 25	C 10	N 2	O 11	P 2	0	0
3	F	1	Total 25	C 10	N 2	O 11	P 2	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	P	0	0
			5	4	1		

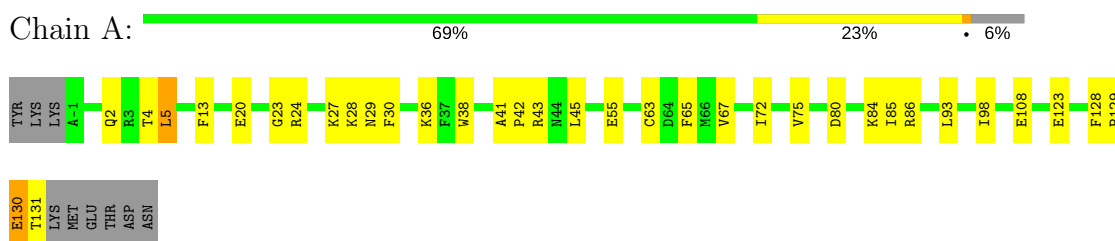
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	24	Total	O	0	0
			24	24		
5	B	19	Total	O	0	0
			19	19		
5	C	39	Total	O	0	0
			39	39		
5	D	31	Total	O	0	0
			31	31		
5	E	25	Total	O	0	0
			25	25		
5	F	15	Total	O	0	0
			15	15		

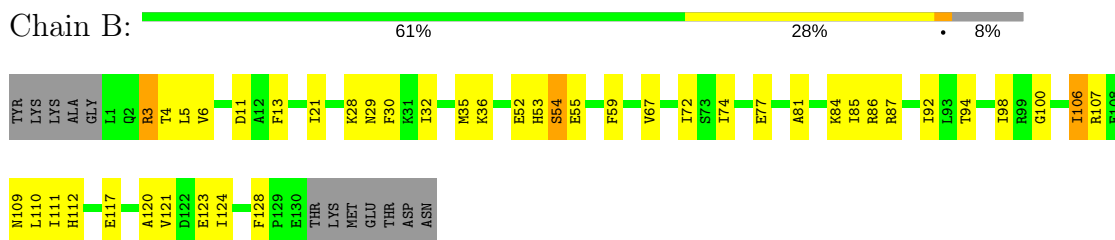
3 Residue-property plots [i](#)

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.

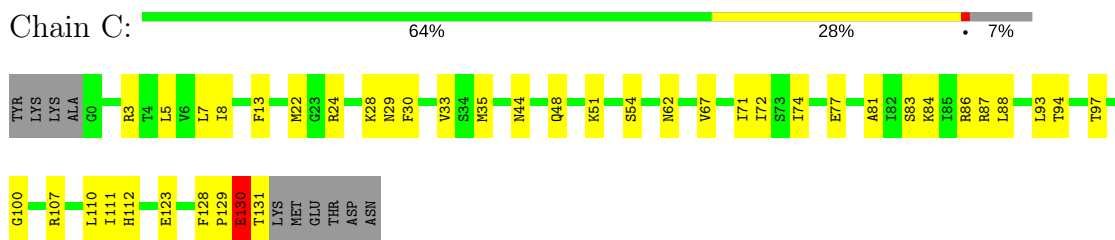
- Molecule 1: Probable nucleoside diphosphate kinase



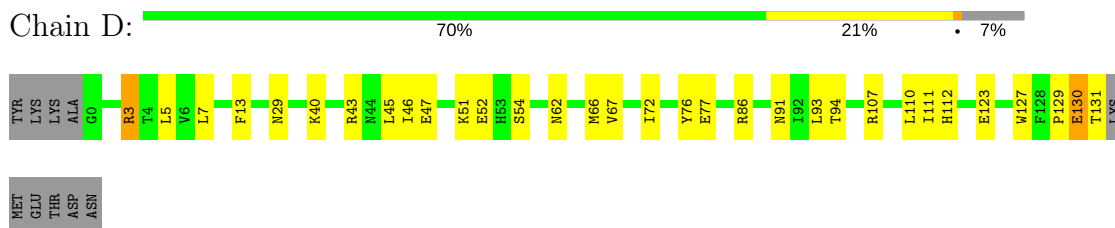
- Molecule 1: Probable nucleoside diphosphate kinase



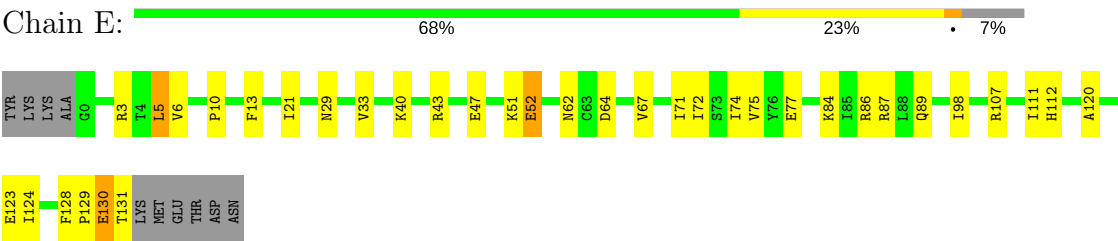
- Molecule 1: Probable nucleoside diphosphate kinase



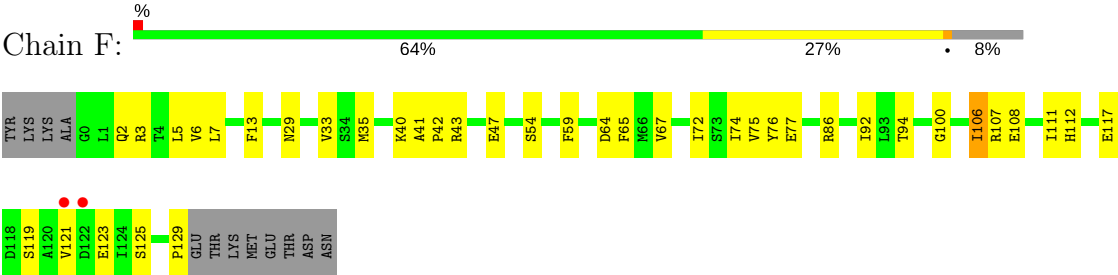
- Molecule 1: Probable nucleoside diphosphate kinase



- Molecule 1: Probable nucleoside diphosphate kinase



- Molecule 1: Probable nucleoside diphosphate kinase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	80.39Å 153.35Å 185.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.55 – 2.50 59.10 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.55-2.50) 99.9 (59.10-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.07 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.199 , 0.231 0.199 , 0.231	Depositor DCC
R_{free} test set	2003 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6652	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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: TYD, PO4, MG

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	0.36	0/1085	0.62	0/1464
1	B	0.40	0/1069	0.62	0/1442
1	C	0.38	0/1080	0.62	0/1457
1	D	0.38	0/1080	0.63	0/1457
1	E	0.36	0/1080	0.62	0/1457
1	F	0.38	0/1064	0.62	0/1435
All	All	0.38	0/6458	0.62	0/8712

There are no bond length outliers.

There are no bond angle outliers.

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	1065	0	1060	23	0
1	B	1049	0	1045	34	0
1	C	1060	0	1055	34	0
1	D	1060	0	1055	22	0
1	E	1060	0	1055	25	0
1	F	1044	0	1042	26	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	25	0	13	1	0
3	B	25	0	13	2	0
3	C	25	0	13	3	0
3	D	25	0	13	1	0
3	E	25	0	13	3	0
3	F	25	0	13	3	0
4	C	5	0	0	0	0
5	A	24	0	0	0	0
5	B	19	0	0	0	0
5	C	39	0	0	2	0
5	D	31	0	0	1	0
5	E	25	0	0	1	0
5	F	15	0	0	0	0
All	All	6652	0	6390	165	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 13.

All (165) 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:D:40:LYS:HE3	1:D:67:VAL:HG13	1.51	0.93
1:F:106:ILE:HD13	1:F:106:ILE:H	1.36	0.91
1:C:35:MET:HE2	1:C:74:ILE:HG12	1.66	0.78
1:D:5:LEU:HD22	1:D:123:GLU:HB3	1.69	0.75
1:B:117:GLU:O	1:B:121:VAL:HG23	1.88	0.73
1:A:129:PRO:C	1:A:131:THR:H	1.93	0.71
1:D:3:ARG:HD3	1:D:77:GLU:OE1	1.90	0.71
1:B:54:SER:HA	1:B:59:PHE:CD2	2.31	0.65
1:A:13:PHE:HZ	1:A:72:ILE:HG13	1.62	0.64
1:E:43:ARG:NH2	1:E:64:ASP:OD1	2.30	0.64
1:C:13:PHE:HZ	1:C:72:ILE:HG13	1.63	0.63
1:D:5:LEU:CD2	1:D:123:GLU:HB3	2.30	0.62
1:C:44:ASN:O	1:C:48:GLN:HG3	2.00	0.62
1:E:5:LEU:HD22	1:E:123:GLU:HB3	1.82	0.62
1:D:129:PRO:C	1:D:131:THR:H	2.03	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:ARG:HD3	1:C:77:GLU:OE1	2.00	0.61
1:E:51:LYS:HG3	1:E:52:GLU:N	2.15	0.61
1:A:93:LEU:HD23	1:C:84:LYS:HE2	1.83	0.60
1:E:51:LYS:HG3	1:E:52:GLU:H	1.67	0.59
1:C:93:LEU:HD23	1:E:84:LYS:HE2	1.83	0.59
1:F:106:ILE:H	1:F:106:ILE:CD1	2.14	0.59
1:F:119:SER:O	1:F:123:GLU:HG3	2.02	0.59
1:E:89:GLN:HG3	1:E:111:ILE:HG23	1.84	0.59
1:E:10:PRO:HD3	1:E:71:ILE:HG22	1.85	0.59
1:E:13:PHE:HZ	1:E:72:ILE:HG13	1.68	0.58
1:B:84:LYS:HE2	1:F:92:ILE:HG22	1.86	0.57
1:B:52:GLU:HG3	1:B:52:GLU:O	2.05	0.57
1:E:5:LEU:HG	1:E:6:VAL:N	2.20	0.56
1:A:5:LEU:HD22	1:A:123:GLU:HB3	1.87	0.56
1:D:111:ILE:HG12	1:D:112:HIS:N	2.19	0.56
1:B:32:ILE:HD13	1:B:35:MET:HE1	1.87	0.56
1:B:13:PHE:HZ	1:B:72:ILE:HG13	1.71	0.55
1:C:24:ARG:HD3	5:C:1019:HOH:O	2.06	0.55
1:D:13:PHE:HZ	1:D:72:ILE:HG13	1.71	0.55
1:B:106:ILE:H	1:B:106:ILE:CD1	2.20	0.55
1:B:5:LEU:HD22	1:B:123:GLU:HB3	1.88	0.55
1:D:91:ASN:OD1	1:D:94:THR:HG23	2.07	0.55
1:C:129:PRO:C	1:C:131:THR:H	2.09	0.54
1:C:7:LEU:HB2	1:C:112:HIS:HB3	1.89	0.54
1:F:94:THR:O	1:F:100:GLY:HA3	2.07	0.54
3:B:161:TYD:H5'2	3:B:161:TYD:O1B	2.07	0.54
1:B:3:ARG:NH2	1:B:77:GLU:OE1	2.41	0.54
1:A:65:PHE:CE2	1:A:108:GLU:HG2	2.42	0.54
1:F:43:ARG:NH2	1:F:64:ASP:OD1	2.41	0.54
1:C:62:ASN:ND2	3:C:162:TYD:H1'	2.23	0.54
1:A:24:ARG:HD2	1:A:98:ILE:HG12	1.91	0.53
1:B:36:LYS:HE2	1:B:128:PHE:CE1	2.43	0.53
1:A:129:PRO:O	1:A:131:THR:N	2.40	0.53
1:A:129:PRO:C	1:A:131:THR:N	2.60	0.53
1:B:106:ILE:H	1:B:106:ILE:HD13	1.72	0.53
1:B:72:ILE:HG22	1:B:74:ILE:HG13	1.91	0.53
1:E:72:ILE:HG22	1:E:74:ILE:HG13	1.91	0.52
1:C:93:LEU:O	1:E:87:ARG:HD3	2.10	0.52
1:B:107:ARG:HA	3:B:161:TYD:H2'2	1.92	0.52
1:E:3:ARG:HD3	1:E:77:GLU:OE1	2.10	0.52
1:F:13:PHE:HZ	1:F:72:ILE:HG13	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:LEU:HD22	1:C:123:GLU:HB3	1.92	0.51
1:E:21:ILE:HG23	1:E:98:ILE:HD13	1.93	0.51
1:B:4:THR:HG21	1:B:85:ILE:HD12	1.92	0.50
1:B:94:THR:O	1:B:100:GLY:HA3	2.11	0.50
1:E:129:PRO:O	1:E:131:THR:N	2.44	0.50
1:A:28:LYS:HG3	1:A:28:LYS:O	2.11	0.50
1:C:8:ILE:HD11	1:C:22:MET:HG3	1.92	0.50
1:B:35:MET:CE	1:B:74:ILE:HG12	2.42	0.50
1:C:129:PRO:O	1:C:131:THR:N	2.34	0.49
1:F:65:PHE:CE2	1:F:108:GLU:HG2	2.47	0.49
1:F:117:GLU:O	1:F:121:VAL:HG23	2.12	0.49
1:B:120:ALA:O	1:B:124:ILE:HG13	2.12	0.49
1:C:62:ASN:HD22	1:C:107:ARG:HG3	1.77	0.49
1:C:28:LYS:HG2	1:C:30:PHE:HE1	1.77	0.49
1:A:42:PRO:HB2	1:A:45:LEU:HD13	1.95	0.49
1:C:129:PRO:HD2	1:C:130:GLU:OE2	2.13	0.49
1:C:30:PHE:CE2	1:C:81:ALA:HA	2.48	0.49
1:D:62:ASN:HA	1:D:107:ARG:HD2	1.94	0.49
1:D:62:ASN:HD22	1:D:107:ARG:HG3	1.76	0.49
1:D:3:ARG:HA	1:D:76:TYR:O	2.13	0.49
1:B:30:PHE:CE2	1:B:81:ALA:HA	2.49	0.48
1:B:109:ASN:O	1:B:111:ILE:N	2.42	0.48
3:F:165:TYD:H5'2	3:F:165:TYD:O1B	2.13	0.48
1:A:75:VAL:HG23	1:A:128:PHE:CE2	2.47	0.48
1:B:28:LYS:HG3	1:B:28:LYS:O	2.14	0.48
1:E:111:ILE:HG12	1:E:112:HIS:N	2.29	0.48
1:C:128:PHE:HA	1:C:130:GLU:OE2	2.14	0.48
1:B:53:HIS:O	1:B:55:GLU:N	2.47	0.47
1:C:111:ILE:HG12	1:C:112:HIS:N	2.27	0.47
1:F:107:ARG:HA	3:F:165:TYD:H2'2	1.96	0.47
1:B:36:LYS:HE2	1:B:128:PHE:CD1	2.50	0.47
1:D:7:LEU:HB2	1:D:112:HIS:HB3	1.97	0.47
1:D:51:LYS:HG3	1:D:52:GLU:N	2.29	0.47
1:F:5:LEU:HG	1:F:6:VAL:N	2.29	0.47
1:C:8:ILE:CD1	1:C:22:MET:HG3	2.46	0.46
1:F:35:MET:HE2	1:F:74:ILE:HG12	1.98	0.46
1:A:130:GLU:N	1:A:130:GLU:OE1	2.39	0.46
1:B:106:ILE:HD13	1:B:106:ILE:N	2.30	0.46
1:A:23:GLY:O	1:A:27:LYS:HG2	2.15	0.46
1:C:5:LEU:CD2	1:C:123:GLU:HB3	2.46	0.46
1:F:33:VAL:HB	1:F:75:VAL:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:162:TYD:O2B	3:C:162:TYD:O1A	2.34	0.46
1:F:3:ARG:HA	1:F:76:TYR:O	2.16	0.46
1:E:130:GLU:HB2	5:E:219:HOH:O	2.16	0.46
3:E:164:TYD:O1B	3:E:164:TYD:H5'2	2.15	0.46
1:F:6:VAL:HA	1:F:112:HIS:O	2.16	0.45
1:F:40:LYS:CE	1:F:67:VAL:HG22	2.47	0.45
1:F:125:SER:O	1:F:129:PRO:HG3	2.17	0.45
1:F:54:SER:HA	1:F:59:PHE:CD2	2.52	0.45
1:C:88:LEU:O	1:C:97:THR:HB	2.17	0.45
1:A:20:GLU:O	1:A:24:ARG:HG3	2.17	0.45
1:F:7:LEU:HB2	1:F:112:HIS:HB3	1.99	0.45
1:B:111:ILE:HG12	1:B:112:HIS:N	2.31	0.45
1:E:107:ARG:HA	3:E:164:TYD:H2'2	1.99	0.45
1:C:28:LYS:HG3	1:C:28:LYS:O	2.16	0.44
3:D:163:TYD:H5'2	3:D:163:TYD:O1B	2.17	0.44
1:E:120:ALA:O	1:E:124:ILE:HG13	2.17	0.44
1:F:33:VAL:HG21	1:F:77:GLU:HB2	1.99	0.44
1:F:107:ARG:HG3	3:F:165:TYD:O2	2.17	0.44
1:A:45:LEU:HD12	1:A:45:LEU:N	2.32	0.44
1:B:11:ASP:OD1	1:B:11:ASP:N	2.50	0.44
1:F:41:ALA:HA	1:F:42:PRO:HD3	1.90	0.44
1:A:28:LYS:HG2	1:A:30:PHE:HE1	1.83	0.44
1:A:36:LYS:HD2	1:A:38:TRP:CZ2	2.52	0.44
1:D:43:ARG:O	1:D:47:GLU:HG3	2.17	0.44
1:B:35:MET:HE2	1:B:74:ILE:CD1	2.48	0.44
1:E:128:PHE:N	1:E:129:PRO:HD3	2.33	0.44
1:C:130:GLU:O	1:C:131:THR:HB	2.18	0.43
1:C:83:SER:O	1:C:87:ARG:HG3	2.17	0.43
1:D:130:GLU:OE1	1:D:130:GLU:N	2.38	0.43
1:D:46:ILE:HD12	1:D:66:MET:HB3	1.99	0.43
1:F:111:ILE:HG12	1:F:112:HIS:N	2.33	0.43
1:D:91:ASN:OD1	1:D:93:LEU:HB2	2.19	0.43
1:B:35:MET:HE3	1:B:74:ILE:HG12	2.01	0.43
1:E:40:LYS:HE2	1:E:67:VAL:HG22	2.00	0.42
1:B:21:ILE:HG23	1:B:98:ILE:HD13	2.00	0.42
1:A:41:ALA:HA	1:A:42:PRO:HD3	1.88	0.42
1:C:48:GLN:O	1:C:51:LYS:HG2	2.19	0.42
1:E:75:VAL:HG23	1:E:128:PHE:CE2	2.55	0.42
1:F:33:VAL:CG2	1:F:77:GLU:HB2	2.48	0.42
1:C:7:LEU:HD22	1:C:71:ILE:HD13	2.01	0.42
1:C:3:ARG:HD2	1:C:33:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:LEU:HD23	1:E:84:LYS:CE	2.48	0.42
1:F:2:GLN:O	1:F:77:GLU:HA	2.20	0.42
3:A:160:TYD:O1B	3:A:160:TYD:H5'2	2.20	0.42
1:A:63:CYS:O	1:A:67:VAL:HG22	2.19	0.42
1:C:129:PRO:C	1:C:131:THR:N	2.71	0.42
1:D:13:PHE:CZ	1:D:72:ILE:HG13	2.53	0.42
1:A:80:ASP:OD2	1:A:84:LYS:HE3	2.19	0.42
1:C:94:THR:O	1:C:100:GLY:HA3	2.20	0.42
1:F:43:ARG:O	1:F:47:GLU:HG3	2.19	0.42
1:D:5:LEU:HD21	1:D:127:TRP:CD1	2.55	0.41
1:B:5:LEU:HG	1:B:6:VAL:N	2.34	0.41
1:E:43:ARG:O	1:E:47:GLU:HG3	2.20	0.41
1:E:62:ASN:CG	3:E:164:TYD:H1'	2.40	0.41
1:D:129:PRO:C	1:D:131:THR:N	2.69	0.41
1:D:43:ARG:HD3	5:D:213:HOH:O	2.20	0.41
1:B:67:VAL:HG13	1:B:67:VAL:O	2.20	0.41
3:C:162:TYD:H2'1	5:C:1018:HOH:O	2.20	0.41
1:E:33:VAL:HG21	1:E:77:GLU:HB2	2.02	0.41
1:A:93:LEU:HD23	1:C:84:LYS:CE	2.50	0.41
1:B:87:ARG:HG2	1:B:87:ARG:NH1	2.36	0.41
1:A:4:THR:CG2	1:A:85:ILE:HD12	2.50	0.41
1:B:111:ILE:CG1	1:B:112:HIS:N	2.84	0.41
1:B:28:LYS:HG2	1:B:30:PHE:HE1	1.86	0.41
1:D:111:ILE:CG1	1:D:112:HIS:N	2.82	0.41
1:A:28:LYS:CG	1:A:30:PHE:HE1	2.34	0.40
1:B:92:ILE:O	1:B:92:ILE:HG22	2.21	0.40
1:C:111:ILE:CG1	1:C:112:HIS:N	2.84	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	131/142 (92%)	126 (96%)	4 (3%)	1 (1%)	21	37
1	B	128/142 (90%)	120 (94%)	6 (5%)	2 (2%)	11	19
1	C	130/142 (92%)	124 (95%)	3 (2%)	3 (2%)	7	11
1	D	130/142 (92%)	124 (95%)	3 (2%)	3 (2%)	7	11
1	E	130/142 (92%)	123 (95%)	6 (5%)	1 (1%)	21	37
1	F	128/142 (90%)	126 (98%)	2 (2%)	0	100	100
All	All	777/852 (91%)	743 (96%)	24 (3%)	10 (1%)	13	23

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	54	SER
1	B	110	LEU
1	D	54	SER
1	E	130	GLU
1	C	54	SER
1	C	110	LEU
1	C	130	GLU
1	D	110	LEU
1	A	130	GLU
1	D	130	GLU

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	118/127 (93%)	112 (95%)	6 (5%)	26	48
1	B	117/127 (92%)	113 (97%)	4 (3%)	40	67
1	C	118/127 (93%)	114 (97%)	4 (3%)	40	67
1	D	118/127 (93%)	114 (97%)	4 (3%)	40	67
1	E	118/127 (93%)	114 (97%)	4 (3%)	40	67
1	F	116/127 (91%)	113 (97%)	3 (3%)	49	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	705/762 (92%)	680 (96%)	25 (4%)	39 66

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	5	LEU
1	A	29	ASN
1	A	43	ARG
1	A	55	GLU
1	A	86	ARG
1	B	3	ARG
1	B	29	ASN
1	B	86	ARG
1	B	106	ILE
1	C	29	ASN
1	C	67	VAL
1	C	86	ARG
1	C	130	GLU
1	D	3	ARG
1	D	29	ASN
1	D	45	LEU
1	D	86	ARG
1	E	5	LEU
1	E	29	ASN
1	E	52	GLU
1	E	86	ARG
1	F	29	ASN
1	F	86	ARG
1	F	106	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	B	29	ASN
1	B	62	ASN
1	C	29	ASN
1	C	44	ASN
1	C	48	GLN
1	C	62	ASN

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Mol	Chain	Res	Type
1	D	29	ASN
1	D	62	ASN
1	E	29	ASN
1	E	62	ASN
1	F	29	ASN
1	F	48	GLN
1	F	62	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 6 are monoatomic - leaving 7 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	TYD	A	160	2	24,26,26	1.72	4 (16%)	30,40,40	1.97	9 (30%)
3	TYD	B	161	2	24,26,26	1.71	4 (16%)	30,40,40	1.95	9 (30%)
4	PO4	C	1001	-	4,4,4	0.87	0	6,6,6	0.40	0
3	TYD	C	162	2	24,26,26	1.71	4 (16%)	30,40,40	1.92	10 (33%)
3	TYD	D	163	2	24,26,26	1.71	4 (16%)	30,40,40	1.97	10 (33%)
3	TYD	E	164	2	24,26,26	1.72	4 (16%)	30,40,40	1.96	9 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TYD	F	165	2	24,26,26	1.72	4 (16%)	30,40,40	2.02	10 (33%)

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	TYD	A	160	2	-	0/16/28/28	0/2/2/2
3	TYD	B	161	2	-	0/16/28/28	0/2/2/2
4	PO4	C	1001	-	-	0/0/0/0	0/0/0/0
3	TYD	C	162	2	-	0/16/28/28	0/2/2/2
3	TYD	D	163	2	-	0/16/28/28	0/2/2/2
3	TYD	E	164	2	-	0/16/28/28	0/2/2/2
3	TYD	F	165	2	-	0/16/28/28	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	165	TYD	C6-N1	-4.79	1.40	1.46
3	A	160	TYD	C6-N1	-4.76	1.40	1.46
3	E	164	TYD	C6-N1	-4.76	1.40	1.46
3	D	163	TYD	C6-N1	-4.74	1.40	1.46
3	B	161	TYD	C6-N1	-4.71	1.40	1.46
3	C	162	TYD	C6-N1	-4.69	1.40	1.46
3	B	161	TYD	C6-C5	-3.86	1.39	1.51
3	C	162	TYD	C6-C5	-3.86	1.39	1.51
3	D	163	TYD	C6-C5	-3.84	1.39	1.51
3	E	164	TYD	C6-C5	-3.82	1.39	1.51
3	A	160	TYD	C6-C5	-3.82	1.39	1.51
3	F	165	TYD	C6-C5	-3.80	1.39	1.51
3	C	162	TYD	C1'-N1	2.10	1.48	1.45
3	B	161	TYD	C1'-N1	2.12	1.48	1.45
3	D	163	TYD	C1'-N1	2.20	1.48	1.45
3	A	160	TYD	C1'-N1	2.26	1.48	1.45
3	F	165	TYD	C1'-N1	2.27	1.48	1.45
3	E	164	TYD	C1'-N1	2.29	1.48	1.45
3	D	163	TYD	C2-N1	3.37	1.40	1.35
3	F	165	TYD	C2-N1	3.39	1.40	1.35
3	C	162	TYD	C2-N1	3.43	1.40	1.35
3	E	164	TYD	C2-N1	3.48	1.40	1.35
3	A	160	TYD	C2-N1	3.49	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	161	TYD	C2-N1	3.52	1.40	1.35

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	163	TYD	C4-N3-C2	-5.35	120.32	126.86
3	A	160	TYD	C4-N3-C2	-5.31	120.37	126.86
3	F	165	TYD	C4-N3-C2	-5.30	120.38	126.86
3	C	162	TYD	C4-N3-C2	-5.27	120.41	126.86
3	E	164	TYD	C4-N3-C2	-5.20	120.50	126.86
3	B	161	TYD	C4-N3-C2	-5.18	120.53	126.86
3	F	165	TYD	C2'-C1'-N1	-3.89	110.85	115.61
3	D	163	TYD	C2'-C1'-N1	-3.59	111.22	115.61
3	A	160	TYD	C2'-C1'-N1	-3.55	111.27	115.61
3	E	164	TYD	C2'-C1'-N1	-3.38	111.48	115.61
3	B	161	TYD	C2'-C1'-N1	-3.34	111.53	115.61
3	F	165	TYD	PA-O3A-PB	-3.13	122.10	132.63
3	F	165	TYD	C2'-C3'-C4'	-2.93	96.55	102.76
3	C	162	TYD	C2'-C1'-N1	-2.91	112.05	115.61
3	B	161	TYD	PA-O3A-PB	-2.91	122.86	132.63
3	E	164	TYD	C2'-C3'-C4'	-2.90	96.63	102.76
3	A	160	TYD	C2'-C3'-C4'	-2.71	97.01	102.76
3	D	163	TYD	PA-O3A-PB	-2.70	123.56	132.63
3	B	161	TYD	C2'-C3'-C4'	-2.70	97.05	102.76
3	D	163	TYD	C2'-C3'-C4'	-2.69	97.06	102.76
3	E	164	TYD	PA-O3A-PB	-2.66	123.69	132.63
3	C	162	TYD	PA-O3A-PB	-2.63	123.79	132.63
3	A	160	TYD	PA-O3A-PB	-2.60	123.87	132.63
3	C	162	TYD	C2'-C3'-C4'	-2.60	97.25	102.76
3	C	162	TYD	O2-C2-N1	-2.29	120.30	123.12
3	F	165	TYD	O2-C2-N1	-2.13	120.49	123.12
3	D	163	TYD	O2-C2-N1	-2.06	120.58	123.12
3	B	161	TYD	N3-C2-N1	2.48	119.18	116.73
3	F	165	TYD	N3-C2-N1	2.56	119.25	116.73
3	E	164	TYD	N3-C2-N1	2.56	119.26	116.73
3	D	163	TYD	N3-C2-N1	2.58	119.27	116.73
3	C	162	TYD	N3-C2-N1	2.64	119.34	116.73
3	A	160	TYD	N3-C2-N1	2.70	119.39	116.73
3	B	161	TYD	C6-C5-C4	2.76	119.46	111.53
3	D	163	TYD	C6-C5-C4	2.77	119.47	111.53
3	E	164	TYD	C6-C5-C4	2.80	119.58	111.53
3	A	160	TYD	C6-C5-C4	2.80	119.58	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	165	TYD	C6-C5-C4	2.82	119.62	111.53
3	C	162	TYD	C6-C5-C4	2.82	119.63	111.53
3	D	163	TYD	O2B-PB-O1B	2.86	121.75	110.60
3	F	165	TYD	O2B-PB-O1B	2.92	121.97	110.60
3	B	161	TYD	O2B-PB-O1B	2.92	121.99	110.60
3	F	165	TYD	O3B-PB-O1B	2.94	122.07	110.60
3	E	164	TYD	O3B-PB-O1B	2.94	122.07	110.60
3	C	162	TYD	O3B-PB-O1B	2.98	122.23	110.60
3	C	162	TYD	O2B-PB-O1B	2.99	122.26	110.60
3	A	160	TYD	O2B-PB-O1B	2.99	122.27	110.60
3	E	164	TYD	O2B-PB-O1B	3.00	122.30	110.60
3	D	163	TYD	O3B-PB-O1B	3.00	122.31	110.60
3	B	161	TYD	O3B-PB-O1B	3.02	122.37	110.60
3	A	160	TYD	O3B-PB-O1B	3.04	122.47	110.60
3	F	165	TYD	C5M-C5-C6	3.41	119.76	112.41
3	B	161	TYD	C5M-C5-C6	3.45	119.83	112.41
3	C	162	TYD	C5M-C5-C6	3.46	119.87	112.41
3	D	163	TYD	C5M-C5-C6	3.47	119.88	112.41
3	E	164	TYD	C5M-C5-C6	3.53	120.01	112.41
3	A	160	TYD	C5M-C5-C6	3.54	120.03	112.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	160	TYD	1	0
3	B	161	TYD	2	0
3	C	162	TYD	3	0
3	D	163	TYD	1	0
3	E	164	TYD	3	0
3	F	165	TYD	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	133/142 (93%)	-0.03	0	100 100	29, 42, 62, 77	0
1	B	130/142 (91%)	0.07	0	100 100	28, 47, 69, 75	0
1	C	132/142 (92%)	-0.09	0	100 100	27, 40, 53, 76	0
1	D	132/142 (92%)	-0.02	0	100 100	27, 43, 57, 74	0
1	E	132/142 (92%)	-0.02	0	100 100	31, 43, 64, 80	0
1	F	130/142 (91%)	0.16	2 (1%)	73 75	29, 42, 65, 74	0
All	All	789/852 (92%)	0.01	2 (0%)	93 94	27, 43, 62, 80	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	121	VAL	2.9
1	F	122	ASP	2.9

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. 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	B-factors(\AA^2)	Q<0.9
2	MG	F	205	1/1	0.68	0.29	77,77,77,77	0
2	MG	D	204	1/1	0.74	0.25	72,72,72,72	0
2	MG	B	202	1/1	0.83	0.17	66,66,66,66	0
2	MG	A	201	1/1	0.87	0.23	65,65,65,65	0
2	MG	E	206	1/1	0.88	0.07	61,61,61,61	0
4	PO4	C	1001	5/5	0.92	0.25	79,79,79,79	0
2	MG	C	203	1/1	0.93	0.12	71,71,71,71	0
3	TYD	A	160	25/25	0.94	0.14	48,50,52,53	0
3	TYD	B	161	25/25	0.94	0.14	54,57,60,61	0
3	TYD	F	165	25/25	0.95	0.19	60,68,70,70	0
3	TYD	D	163	25/25	0.95	0.15	49,52,54,55	0
3	TYD	E	164	25/25	0.95	0.16	55,57,58,58	0
3	TYD	C	162	25/25	0.96	0.15	44,49,51,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.