Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:57 PM GMT

PDB ID	:	5E0K
Title	:	X-ray crystal structure of tryptophan synthase complex from Pyrococcus furiosus at 2.76 A
Authors	:	Buller, A.R.; Murciano-Calles, J.; Arnold, F.H.
Deposited on	:	2015-09-29
Resolution	:	2.76 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 ①) were used in the production of this report:

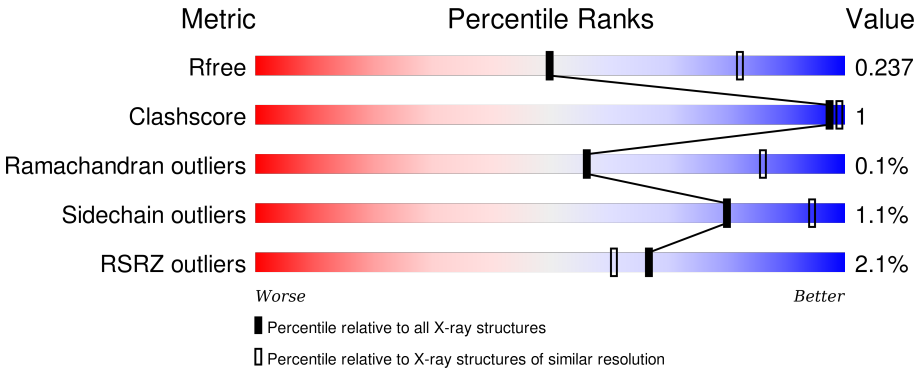
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.76 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	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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 <=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	248	89% 8%
1	C	248	94%
1	E	248	% 91% 6%
1	G	248	% 94%
1	I	248	94%

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Mol	Chain	Length	Quality of chain
1	K	248	21% 94%
2	B	396	2% 93%
2	D	396	93%
2	F	396	% 93%
2	H	396	% 94%
2	J	396	93%
2	L	396	% 94%

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	PO4	L	401	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28872 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 Tryptophan synthase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	0	0
			1821	1177	301	339	4			
1	C	241	Total	C	N	O	S	0	0	0
			1850	1196	308	342	4			
1	E	241	Total	C	N	O	S	0	0	0
			1826	1179	304	339	4			
1	G	241	Total	C	N	O	S	0	0	0
			1838	1184	308	342	4			
1	I	242	Total	C	N	O	S	0	0	0
			1860	1202	310	344	4			
1	K	240	Total	C	N	O	S	0	0	0
			1756	1132	290	331	3			

- Molecule 2 is a protein called Tryptophan synthase beta chain 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	385	Total	C	N	O	P	S	0	0	0
			2958	1889	506	550	1	12			
2	D	385	Total	C	N	O	P	S	0	0	0
			2972	1897	510	552	1	12			
2	F	385	Total	C	N	O	P	S	0	0	0
			2968	1894	509	552	1	12			
2	H	385	Total	C	N	O	P	S	0	0	0
			2980	1901	510	556	1	12			
2	J	385	Total	C	N	O	P	S	0	0	0
			2972	1897	510	552	1	12			
2	L	385	Total	C	N	O	P	S	0	0	0
			2968	1893	508	554	1	12			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	389	LEU	-	expression tag	UNP Q8U093

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Chain	Residue	Modelled	Actual	Comment	Reference
B	390	GLU	-	expression tag	UNP Q8U093
B	391	HIS	-	expression tag	UNP Q8U093
B	392	HIS	-	expression tag	UNP Q8U093
B	393	HIS	-	expression tag	UNP Q8U093
B	394	HIS	-	expression tag	UNP Q8U093
B	395	HIS	-	expression tag	UNP Q8U093
B	396	HIS	-	expression tag	UNP Q8U093
D	389	LEU	-	expression tag	UNP Q8U093
D	390	GLU	-	expression tag	UNP Q8U093
D	391	HIS	-	expression tag	UNP Q8U093
D	392	HIS	-	expression tag	UNP Q8U093
D	393	HIS	-	expression tag	UNP Q8U093
D	394	HIS	-	expression tag	UNP Q8U093
D	395	HIS	-	expression tag	UNP Q8U093
D	396	HIS	-	expression tag	UNP Q8U093
F	389	LEU	-	expression tag	UNP Q8U093
F	390	GLU	-	expression tag	UNP Q8U093
F	391	HIS	-	expression tag	UNP Q8U093
F	392	HIS	-	expression tag	UNP Q8U093
F	393	HIS	-	expression tag	UNP Q8U093
F	394	HIS	-	expression tag	UNP Q8U093
F	395	HIS	-	expression tag	UNP Q8U093
F	396	HIS	-	expression tag	UNP Q8U093
H	389	LEU	-	expression tag	UNP Q8U093
H	390	GLU	-	expression tag	UNP Q8U093
H	391	HIS	-	expression tag	UNP Q8U093
H	392	HIS	-	expression tag	UNP Q8U093
H	393	HIS	-	expression tag	UNP Q8U093
H	394	HIS	-	expression tag	UNP Q8U093
H	395	HIS	-	expression tag	UNP Q8U093
H	396	HIS	-	expression tag	UNP Q8U093
J	389	LEU	-	expression tag	UNP Q8U093
J	390	GLU	-	expression tag	UNP Q8U093
J	391	HIS	-	expression tag	UNP Q8U093
J	392	HIS	-	expression tag	UNP Q8U093
J	393	HIS	-	expression tag	UNP Q8U093
J	394	HIS	-	expression tag	UNP Q8U093
J	395	HIS	-	expression tag	UNP Q8U093
J	396	HIS	-	expression tag	UNP Q8U093
L	389	LEU	-	expression tag	UNP Q8U093
L	390	GLU	-	expression tag	UNP Q8U093
L	391	HIS	-	expression tag	UNP Q8U093

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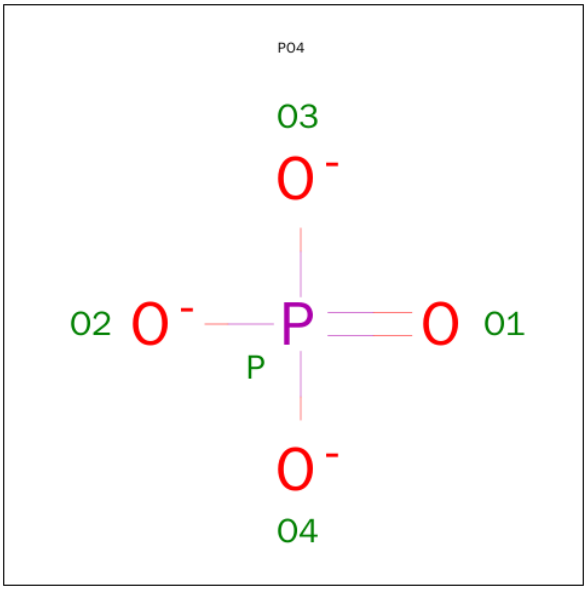
Chain	Residue	Modelled	Actual	Comment	Reference
L	392	HIS	-	expression tag	UNP Q8U093
L	393	HIS	-	expression tag	UNP Q8U093
L	394	HIS	-	expression tag	UNP Q8U093
L	395	HIS	-	expression tag	UNP Q8U093
L	396	HIS	-	expression tag	UNP Q8U093

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0
3	F	1	Total O P 5 4 1	0	0
3	H	1	Total O P 5 4 1	0	0
3	J	1	Total O P 5 4 1	0	0
3	L	1	Total O P 5 4 1	0	0

- Molecule 4 is water.

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

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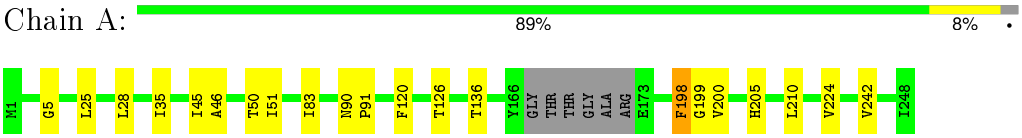
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	10	Total O 10 10	0	0
4	C	11	Total O 11 11	0	0
4	D	11	Total O 11 11	0	0
4	E	1	Total O 1 1	0	0
4	F	4	Total O 4 4	0	0
4	G	3	Total O 3 3	0	0
4	H	12	Total O 12 12	0	0
4	I	2	Total O 2 2	0	0
4	J	8	Total O 8 8	0	0
4	K	1	Total O 1 1	0	0
4	L	8	Total O 8 8	0	0

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.

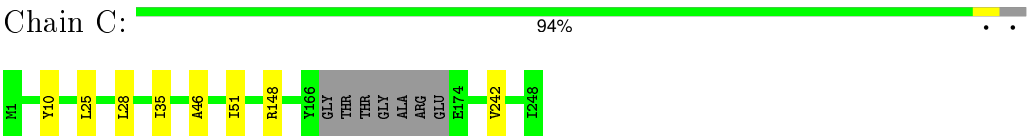
- Molecule 1: Tryptophan synthase alpha chain

Chain A:



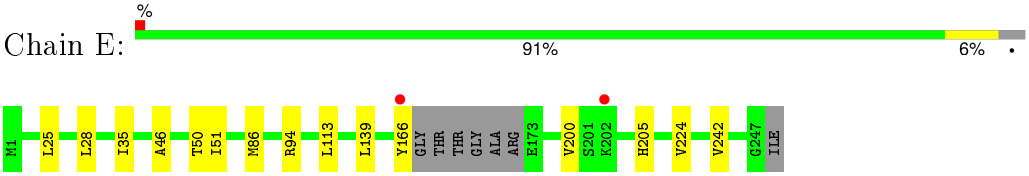
- Molecule 1: Tryptophan synthase alpha chain

Chain C:



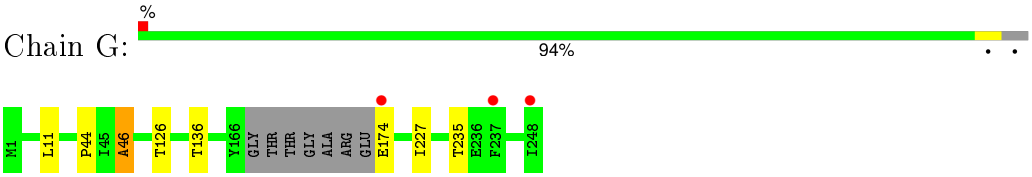
- Molecule 1: Tryptophan synthase alpha chain

Chain E:



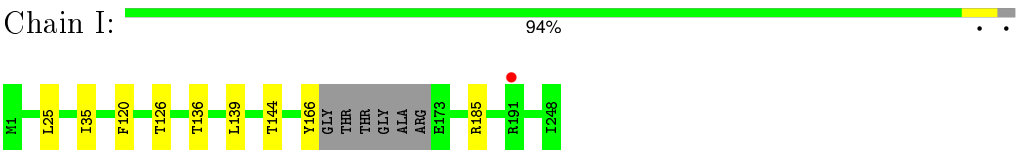
- Molecule 1: Tryptophan synthase alpha chain

Chain G:



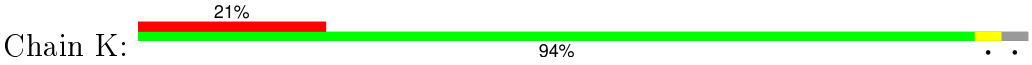
- Molecule 1: Tryptophan synthase alpha chain

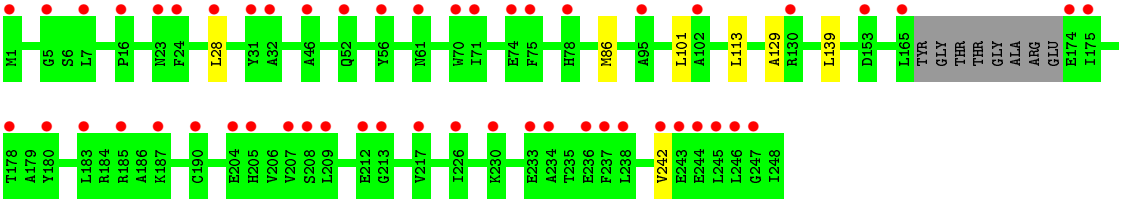
Chain I:



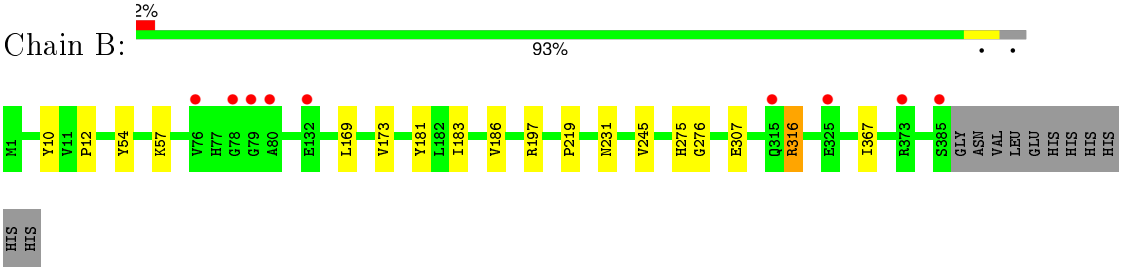
- Molecule 1: Tryptophan synthase alpha chain

Chain K:

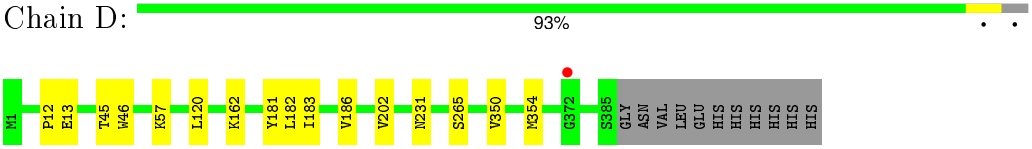




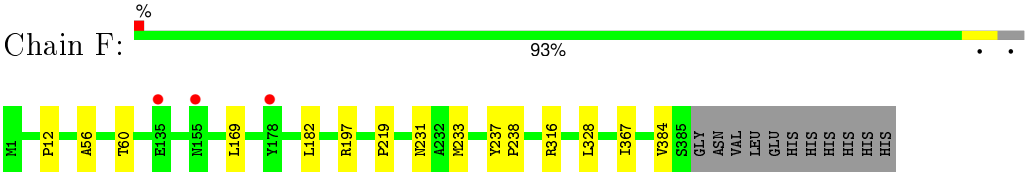
• Molecule 2: Tryptophan synthase beta chain 1



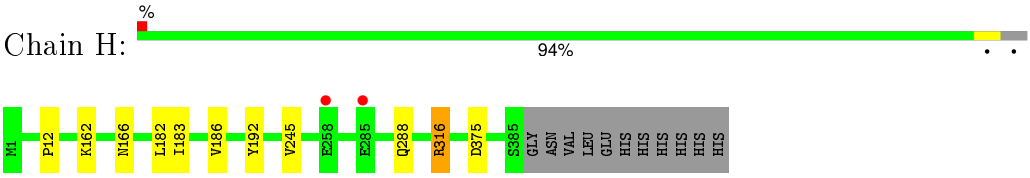
• Molecule 2: Tryptophan synthase beta chain 1



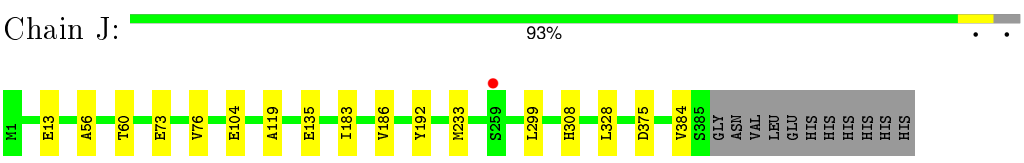
• Molecule 2: Tryptophan synthase beta chain 1



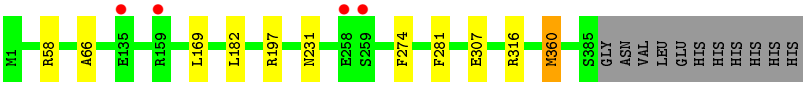
• Molecule 2: Tryptophan synthase beta chain 1



• Molecule 2: Tryptophan synthase beta chain 1



• Molecule 2: Tryptophan synthase beta chain 1


M1
R58
A66
E135
R159
L169
L182
R197
N231
E258
S259
F274
F281
E307
R316
M360
S385
GLY
ASN
VAL
LEU
GLU
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	87.86Å 225.01Å 296.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.91 – 2.76 39.69 – 2.76	Depositor EDS
% Data completeness (in resolution range)	98.5 (39.91-2.76) 98.6 (39.69-2.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, R_{free}	0.204 , 0.238 0.207 , 0.237	Depositor DCC
R_{free} test set	7314 reflections (5.15%)	DCC
Wilson B-factor (Å^2)	66.3	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 34.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 149458 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	28872	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 2.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, LLP

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	0.30	0/1856	0.61	0/2521
1	C	0.30	0/1885	0.61	0/2551
1	E	0.31	0/1861	0.58	0/2526
1	G	0.30	0/1873	0.60	0/2541
1	I	0.31	0/1896	0.61	0/2568
1	K	0.32	0/1789	0.56	0/2443
2	B	0.29	0/2994	0.58	0/4047
2	D	0.29	0/3008	0.61	0/4063
2	F	0.29	0/3004	0.58	0/4059
2	H	0.30	0/3016	0.60	1/4073 (0.0%)
2	J	0.29	0/3008	0.60	0/4063
2	L	0.29	0/3004	0.59	0/4060
All	All	0.30	0/29194	0.59	1/39515 (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	A	0	1
1	G	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	316	ARG	NE-CZ-NH1	5.19	122.89	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	198	PHE	Peptide
1	G	46	ALA	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	1821	0	1793	13	0
1	C	1850	0	1865	6	0
1	E	1826	0	1808	10	0
1	G	1838	0	1821	6	1
1	I	1860	0	1863	4	0
1	K	1756	0	1676	4	0
2	B	2958	0	2938	11	0
2	D	2972	0	2964	9	0
2	F	2968	0	2953	6	0
2	H	2980	0	2972	6	0
2	J	2972	0	2964	7	1
2	L	2968	0	2947	4	0
3	B	5	0	0	0	0
3	D	5	0	0	0	0
3	F	5	0	0	0	0
3	H	5	0	0	0	0
3	J	5	0	0	0	0
3	L	5	0	0	0	0
4	A	2	0	0	0	0
4	B	10	0	0	0	0
4	C	11	0	0	0	0
4	D	11	0	0	0	0
4	E	1	0	0	0	0
4	F	4	0	0	0	0
4	G	3	0	0	0	0
4	H	12	0	0	0	0
4	I	2	0	0	0	0
4	J	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	1	0	0	0	0
4	L	8	0	0	0	0
All	All	28872	0	28564	71	1

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 1.

All (71) 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)
2:J:328:LEU:HD21	2:J:384:VAL:HG21	1.71	0.73
1:E:86:MET:CE	1:E:113:LEU:HD23	2.23	0.67
1:E:113:LEU:HD21	1:E:139:LEU:HD23	1.78	0.65
1:A:50:THR:HG22	1:A:224:VAL:HG23	1.80	0.62
1:K:86:MET:CE	1:K:113:LEU:HD23	2.29	0.62
2:F:328:LEU:HD21	2:F:384:VAL:HG21	1.81	0.61
2:B:245:VAL:O	2:B:316:ARG:NH2	2.35	0.60
1:E:51:ILE:HD13	1:E:224:VAL:HG21	1.84	0.58
1:E:50:THR:HG22	1:E:224:VAL:HG23	1.86	0.57
1:G:46:ALA:HB2	2:H:12:PRO:CG	2.35	0.56
1:A:45:ILE:HD11	2:B:275:HIS:HA	1.88	0.55
1:K:113:LEU:HD21	1:K:139:LEU:HD23	1.89	0.54
1:E:86:MET:HE3	1:E:113:LEU:HD23	1.88	0.53
1:A:25:LEU:HD22	1:A:35:ILE:HG21	1.90	0.53
1:E:86:MET:HE2	1:E:113:LEU:HD23	1.90	0.53
2:B:169:LEU:O	2:B:173:VAL:HG23	2.08	0.53
1:I:25:LEU:HD22	1:I:35:ILE:HG21	1.91	0.53
1:A:46:ALA:HB2	2:B:12:PRO:HG3	1.93	0.51
2:B:54:TYR:HA	2:D:45:THR:HG23	1.92	0.51
1:C:28:LEU:HD22	1:C:242:VAL:HG21	1.92	0.51
1:C:25:LEU:HD22	1:C:35:ILE:HG21	1.93	0.51
1:A:46:ALA:HB2	2:B:12:PRO:CG	2.42	0.50
2:D:181:TYR:CE2	2:D:183:ILE:HD11	2.47	0.49
2:H:245:VAL:O	2:H:316:ARG:NH2	2.38	0.49
1:A:28:LEU:HD22	1:A:242:VAL:HG21	1.95	0.49
2:J:119:ALA:O	2:L:58:ARG:NH1	2.45	0.49
2:J:233:MET:HE2	2:J:308:HIS:CE1	2.48	0.49
1:K:28:LEU:HD22	1:K:242:VAL:HG21	1.95	0.48
1:A:126:THR:HG22	1:A:136:THR:HG21	1.94	0.48
1:I:144:THR:O	1:I:185:ARG:NH2	2.45	0.48
1:K:101:LEU:HD13	1:K:129:ALA:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:TYR:CE1	1:C:51:ILE:HD12	2.49	0.48
1:A:51:ILE:HD13	1:A:224:VAL:HG21	1.96	0.48
1:G:46:ALA:HB2	2:H:12:PRO:HG2	1.94	0.47
1:C:46:ALA:HB2	2:D:12:PRO:CG	2.45	0.47
1:A:198:PHE:N	1:A:199:GLY:HA2	2.30	0.47
1:E:46:ALA:HB2	2:F:12:PRO:CG	2.45	0.47
2:F:197:ARG:HG3	2:F:233:MET:HG3	1.97	0.47
2:B:181:TYR:CE2	2:B:183:ILE:HD11	2.50	0.47
2:L:274:PHE:HB2	2:L:281:PHE:CZ	2.50	0.46
1:G:46:ALA:HB2	2:H:12:PRO:HG3	1.99	0.45
1:G:44:PRO:O	2:H:166:ASN:ND2	2.49	0.45
1:E:200:VAL:HG13	1:E:205:HIS:HB2	1.99	0.45
2:J:56:ALA:O	2:J:60:THR:HG23	2.16	0.45
1:G:126:THR:HG22	1:G:136:THR:HG21	1.98	0.44
2:B:197:ARG:HD3	2:B:307:GLU:OE1	2.18	0.44
1:E:25:LEU:HD22	1:E:35:ILE:HG21	1.99	0.44
2:F:219:PRO:HG3	2:F:367:ILE:HD12	2.00	0.44
1:I:139:LEU:HD12	2:J:13:GLU:HB3	2.00	0.43
2:L:197:ARG:HD3	2:L:307:GLU:OE1	2.19	0.43
2:L:66:ALA:HB2	2:L:360:MET:HB2	2.01	0.43
1:C:148:ARG:NE	2:D:13:GLU:OE1	2.47	0.43
2:D:350:VAL:O	2:D:354:MET:HG3	2.19	0.42
2:D:46:TRP:CE3	2:D:120:LEU:HD22	2.54	0.42
2:D:46:TRP:CD2	2:D:120:LEU:HD22	2.54	0.42
1:A:200:VAL:HG13	1:A:205:HIS:HB2	2.02	0.42
2:H:183:ILE:HD12	2:H:192:TYR:CG	2.54	0.42
1:C:46:ALA:HB2	2:D:12:PRO:HG3	2.01	0.42
2:J:73:GLU:O	2:J:76:VAL:HG22	2.19	0.42
1:E:28:LEU:HD22	1:E:242:VAL:HG21	2.03	0.41
1:I:126:THR:HG22	1:I:136:THR:HG21	2.01	0.41
1:A:5:GLY:HA2	1:A:210:LEU:HD22	2.02	0.41
2:B:219:PRO:HG3	2:B:367:ILE:HD12	2.02	0.41
2:F:56:ALA:O	2:F:60:THR:HG23	2.20	0.41
1:G:11:LEU:HD22	1:G:227:ILE:CD1	2.51	0.41
2:B:54:TYR:HD1	2:D:45:THR:HG22	1.85	0.41
1:A:90:ASN:HB3	1:A:91:PRO:HD3	2.03	0.41
1:A:35:ILE:HB	1:A:83:ILE:HD13	2.02	0.40
2:B:10:TYR:O	2:B:276:GLY:HA2	2.20	0.40
2:F:237:TYR:HB3	2:F:238:PRO:HD3	2.03	0.40
2:J:183:ILE:HD12	2:J:192:TYR:CD2	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:235:THR:OG1	2:J:135:GLU:OE2[2_555]	2.07	0.13

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	238/248 (96%)	231 (97%)	7 (3%)	0	100	100
1	C	237/248 (96%)	233 (98%)	4 (2%)	0	100	100
1	E	237/248 (96%)	234 (99%)	3 (1%)	0	100	100
1	G	237/248 (96%)	230 (97%)	7 (3%)	0	100	100
1	I	238/248 (96%)	233 (98%)	5 (2%)	0	100	100
1	K	236/248 (95%)	229 (97%)	7 (3%)	0	100	100
2	B	382/396 (96%)	373 (98%)	8 (2%)	1 (0%)	46	77
2	D	382/396 (96%)	371 (97%)	10 (3%)	1 (0%)	46	77
2	F	382/396 (96%)	375 (98%)	7 (2%)	0	100	100
2	H	382/396 (96%)	374 (98%)	7 (2%)	1 (0%)	46	77
2	J	382/396 (96%)	371 (97%)	10 (3%)	1 (0%)	46	77
2	L	382/396 (96%)	369 (97%)	13 (3%)	0	100	100
All	All	3715/3864 (96%)	3623 (98%)	88 (2%)	4 (0%)	56	86

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	186	VAL
2	J	186	VAL
2	D	186	VAL
2	H	186	VAL

5.3.2 Protein sidechains (i)

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	184/205 (90%)	183 (100%)	1 (0%)	92 97
1	C	192/205 (94%)	192 (100%)	0	100 100
1	E	186/205 (91%)	184 (99%)	2 (1%)	80 94
1	G	188/205 (92%)	187 (100%)	1 (0%)	92 97
1	I	192/205 (94%)	190 (99%)	2 (1%)	82 95
1	K	171/205 (83%)	171 (100%)	0	100 100
2	B	297/315 (94%)	294 (99%)	3 (1%)	82 95
2	D	300/315 (95%)	294 (98%)	6 (2%)	63 89
2	F	299/315 (95%)	295 (99%)	4 (1%)	76 93
2	H	302/315 (96%)	298 (99%)	4 (1%)	76 93
2	J	300/315 (95%)	297 (99%)	3 (1%)	82 95
2	L	299/315 (95%)	294 (98%)	5 (2%)	68 90
All	All	2910/3120 (93%)	2879 (99%)	31 (1%)	80 94

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	PHE
2	B	57	LYS
2	B	231	ASN
2	B	316	ARG
2	D	57	LYS
2	D	162	LYS
2	D	182	LEU
2	D	202	VAL
2	D	231	ASN
2	D	265	SER
1	E	94	ARG
1	E	166	TYR
2	F	169	LEU
2	F	182	LEU

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Mol	Chain	Res	Type
2	F	231	ASN
2	F	316	ARG
1	G	174	GLU
2	H	162	LYS
2	H	182	LEU
2	H	288	GLN
2	H	375	ASP
1	I	120	PHE
1	I	166	TYR
2	J	104	GLU
2	J	299	LEU
2	J	375	ASP
2	L	169	LEU
2	L	182	LEU
2	L	231	ASN
2	L	316	ARG
2	L	360	MET

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	52	GLN
1	A	61	ASN
2	B	166	ASN
2	J	267	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)

6 non-standard protein/DNA/RNA residues 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	$\#\|Z\|>2$
2	LLP	B	82	2	22,24,25	3.39	5 (22%)	28,32,34	1.27	4 (14%)
2	LLP	D	82	2	22,24,25	3.32	5 (22%)	28,32,34	1.23	3 (10%)
2	LLP	F	82	2	22,24,25	3.42	5 (22%)	28,32,34	1.26	6 (21%)
2	LLP	H	82	2	22,24,25	3.34	5 (22%)	28,32,34	1.39	3 (10%)
2	LLP	J	82	2	22,24,25	3.42	5 (22%)	28,32,34	1.19	3 (10%)
2	LLP	L	82	2	22,24,25	3.39	5 (22%)	28,32,34	1.32	5 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LLP	B	82	2	-	0/15/17/19	0/1/1/1
2	LLP	D	82	2	-	0/15/17/19	0/1/1/1
2	LLP	F	82	2	-	0/15/17/19	0/1/1/1
2	LLP	H	82	2	-	0/15/17/19	0/1/1/1
2	LLP	J	82	2	-	0/15/17/19	0/1/1/1
2	LLP	L	82	2	-	0/15/17/19	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	82	LLP	C4-C4'	3.01	1.51	1.46
2	D	82	LLP	C4-C4'	3.02	1.51	1.46
2	F	82	LLP	C4-C4'	3.07	1.51	1.46
2	L	82	LLP	C4-C4'	3.19	1.52	1.46
2	J	82	LLP	C4-C4'	3.24	1.52	1.46
2	H	82	LLP	C4-C4'	3.31	1.52	1.46
2	H	82	LLP	C4-C5	5.48	1.49	1.42
2	F	82	LLP	C4-C5	5.63	1.49	1.42
2	D	82	LLP	C4-C5	5.65	1.49	1.42
2	B	82	LLP	C4-C5	5.82	1.49	1.42
2	B	82	LLP	C4-C3	5.98	1.48	1.40
2	H	82	LLP	C4-C3	5.99	1.48	1.40
2	L	82	LLP	C4-C5	6.02	1.49	1.42
2	H	82	LLP	C4'-NZ	6.08	1.45	1.27
2	D	82	LLP	C4'-NZ	6.08	1.45	1.27
2	F	82	LLP	C4'-NZ	6.15	1.45	1.27
2	B	82	LLP	C4'-NZ	6.16	1.45	1.27
2	L	82	LLP	C4'-NZ	6.18	1.45	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	82	LLP	C4-C5	6.23	1.50	1.42
2	J	82	LLP	C4'-NZ	6.25	1.45	1.27
2	L	82	LLP	C4-C3	6.26	1.49	1.40
2	F	82	LLP	C4-C3	6.29	1.49	1.40
2	D	82	LLP	C4-C3	6.35	1.49	1.40
2	J	82	LLP	C4-C3	6.65	1.49	1.40
2	D	82	LLP	C3-C2	10.81	1.48	1.40
2	J	82	LLP	C3-C2	10.81	1.48	1.40
2	L	82	LLP	C3-C2	11.09	1.48	1.40
2	H	82	LLP	C3-C2	11.22	1.48	1.40
2	B	82	LLP	C3-C2	11.32	1.48	1.40
2	F	82	LLP	C3-C2	11.51	1.48	1.40

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	82	LLP	C3-C4-C5	-3.86	115.47	118.26
2	B	82	LLP	C4-C4'-NZ	-2.73	109.97	125.14
2	L	82	LLP	C4-C4'-NZ	-2.53	111.07	125.14
2	D	82	LLP	C4-C4'-NZ	-2.51	111.19	125.14
2	D	82	LLP	O-C-CA	-2.38	119.33	125.72
2	J	82	LLP	C4-C4'-NZ	-2.36	111.99	125.14
2	H	82	LLP	C4-C4'-NZ	-2.34	112.15	125.14
2	F	82	LLP	C4-C4'-NZ	-2.26	112.58	125.14
2	H	82	LLP	O-C-CA	-2.25	119.69	125.72
2	F	82	LLP	OP4-P-OP1	-2.24	101.46	107.08
2	D	82	LLP	C3-C4-C5	-2.24	116.64	118.26
2	J	82	LLP	O-C-CA	-2.23	119.75	125.72
2	L	82	LLP	C3-C4-C5	-2.18	116.68	118.26
2	F	82	LLP	O-C-CA	-2.17	119.90	125.72
2	B	82	LLP	O-C-CA	-2.16	119.94	125.72
2	F	82	LLP	C3-C4-C5	-2.15	116.70	118.26
2	L	82	LLP	O-C-CA	-2.14	119.97	125.72
2	L	82	LLP	C6-N1-C2	2.03	123.34	119.26
2	B	82	LLP	C6-N1-C2	2.04	123.36	119.26
2	B	82	LLP	O3-C3-C2	2.18	120.72	117.53
2	F	82	LLP	C6-N1-C2	2.19	123.66	119.26
2	J	82	LLP	C6-N1-C2	2.22	123.72	119.26
2	F	82	LLP	O3-C3-C2	2.29	120.89	117.53
2	L	82	LLP	O3-C3-C2	2.32	120.93	117.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

6 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	PO4	B	401	-	4,4,4	0.64	0	6,6,6	0.24	0
3	PO4	D	401	-	4,4,4	0.65	0	6,6,6	0.23	0
3	PO4	F	401	-	4,4,4	0.67	0	6,6,6	0.23	0
3	PO4	H	401	-	4,4,4	0.66	0	6,6,6	0.23	0
3	PO4	J	401	-	4,4,4	0.64	0	6,6,6	0.24	0
3	PO4	L	401	-	4,4,4	0.67	0	6,6,6	0.23	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PO4	B	401	-	-	0/0/0/0	0/0/0/0
3	PO4	D	401	-	-	0/0/0/0	0/0/0/0
3	PO4	F	401	-	-	0/0/0/0	0/0/0/0
3	PO4	H	401	-	-	0/0/0/0	0/0/0/0
3	PO4	J	401	-	-	0/0/0/0	0/0/0/0
3	PO4	L	401	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	242/248 (97%)	-0.02	0 100 100	62, 76, 90, 117	0
1	C	241/248 (97%)	-0.20	0 100 100	54, 63, 78, 94	0
1	E	241/248 (97%)	0.03	2 (0%) 87 83	63, 75, 94, 118	0
1	G	241/248 (97%)	-0.07	3 (1%) 81 76	52, 65, 88, 111	0
1	I	242/248 (97%)	-0.07	1 (0%) 93 92	55, 69, 83, 101	0
1	K	240/248 (96%)	1.06	52 (21%) 1 1	92, 129, 151, 161	0
2	B	384/396 (96%)	0.08	9 (2%) 64 57	48, 67, 93, 114	0
2	D	384/396 (96%)	-0.13	1 (0%) 94 93	45, 54, 79, 101	0
2	F	384/396 (96%)	0.04	3 (0%) 87 83	55, 71, 90, 100	0
2	H	384/396 (96%)	-0.13	2 (0%) 91 90	52, 62, 77, 93	0
2	J	384/396 (96%)	-0.12	1 (0%) 94 93	48, 60, 79, 95	0
2	L	384/396 (96%)	-0.04	4 (1%) 84 80	48, 63, 91, 111	0
All	All	3751/3864 (97%)	0.02	78 (2%) 67 61	45, 66, 116, 161	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	245	LEU	5.3
1	K	7	LEU	4.7
1	K	46	ALA	4.4
1	K	78	HIS	4.3
1	K	209	LEU	4.2
2	L	258	GLU	3.9
1	K	247	GLY	3.9
1	K	233	GLU	3.7
1	K	207	VAL	3.5
1	K	226	ILE	3.5
2	B	78	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	K	180	TYR	3.3
1	K	28	LEU	3.3
1	K	237	PHE	3.2
1	K	204	GLU	3.2
1	K	208	SER	3.0
1	E	166	TYR	3.0
1	K	243	GLU	3.0
1	K	56	TYR	2.9
1	K	238	LEU	2.9
1	K	130	ARG	2.9
1	K	1	MET	2.9
1	K	74	GLU	2.9
1	K	213	GLY	2.8
1	K	75	PHE	2.7
1	K	52	GLN	2.7
2	J	259	SER	2.7
2	L	135	GLU	2.6
2	L	259	SER	2.6
1	G	248	ILE	2.6
2	B	132	GLU	2.6
1	G	237	PHE	2.6
1	K	5	GLY	2.6
2	B	76	VAL	2.6
1	K	187	LYS	2.6
2	B	325	GLU	2.5
1	K	205	HIS	2.5
1	K	102	ALA	2.5
1	K	185	ARG	2.5
2	L	159	ARG	2.4
1	K	23	ASN	2.4
1	K	95	ALA	2.4
2	F	135	GLU	2.4
1	K	24	PHE	2.3
1	K	70	TRP	2.3
1	K	183	LEU	2.3
2	F	178	TYR	2.3
1	K	242	VAL	2.3
2	H	258	GLU	2.3
1	K	178	THR	2.3
2	B	79	GLY	2.3
1	K	236	GLU	2.3
1	K	16	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	285	GLU	2.3
1	K	175	ILE	2.3
1	K	217	VAL	2.2
1	K	165	LEU	2.2
1	K	32	ALA	2.2
1	K	234	ALA	2.2
1	K	61	ASN	2.2
1	K	246	LEU	2.2
2	B	80	ALA	2.2
1	K	174	GLU	2.1
1	I	191	ARG	2.1
1	K	230	LYS	2.1
2	F	155	ASN	2.1
1	K	190	CYS	2.1
1	G	174	GLU	2.1
2	B	315	GLN	2.1
2	B	373	ARG	2.1
2	D	372	GLY	2.1
1	K	244	GLU	2.1
1	K	31	TYR	2.1
1	K	71	ILE	2.0
1	K	153	ASP	2.0
2	B	385	SER	2.0
1	K	212	GLU	2.0
1	E	202	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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
2	LLP	L	82	24/25	0.97	0.25	-	53,57,58,58	0
2	LLP	J	82	24/25	0.97	0.17	-	49,53,54,54	0
2	LLP	F	82	24/25	0.98	0.22	-	56,58,60,61	0
2	LLP	D	82	24/25	0.98	0.21	-	46,47,48,48	0
2	LLP	B	82	24/25	0.97	0.26	-	52,59,60,61	0
2	LLP	H	82	24/25	0.98	0.21	-	52,52,52,53	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	PO4	L	401	5/5	0.82	0.37	5.75	139,139,140,140	0
3	PO4	J	401	5/5	0.89	0.20	1.96	97,98,100,102	0
3	PO4	D	401	5/5	0.91	0.21	1.32	95,98,99,99	0
3	PO4	F	401	5/5	0.93	0.21	1.02	109,110,110,110	0
3	PO4	H	401	5/5	0.92	0.20	0.97	103,106,108,109	0
3	PO4	B	401	5/5	0.89	0.21	0.72	96,97,100,101	0

6.5 Other polymers (i)

There are no such residues in this entry.