



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 12:31 PM EDT

PDB ID : 5E0K
Title : X-ray crystal structure of tryptophan synthase complex from *Pyrococcus furiosus* at 2.76 Å
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

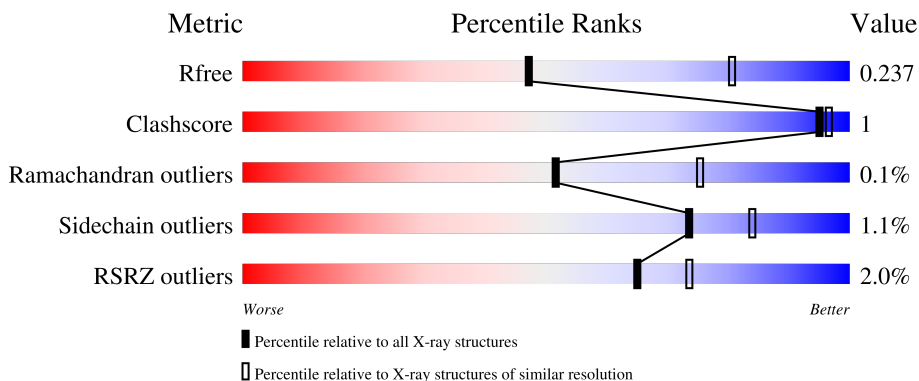
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 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}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	248	89% (8% outliers) .
1	C	248	94% (2% outliers) . .
1	E	248	91% (6% outliers) .
1	G	248	94% (2% outliers) . .
1	I	248	94% (2% outliers) . .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	248	 20% 94% . .
2	B	396	 2% 92% 5% . .
2	D	396	 % 93% . .
2	F	396	 % 93% . .
2	H	396	 % 94% . .
2	J	396	 % 93% 5% . .
2	L	396	 % 94% . .

2 Entry composition [i](#)

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

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

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

There are 48 discrepancies between the modelled and reference sequences:

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

Continued on next page...

Continued from previous page...

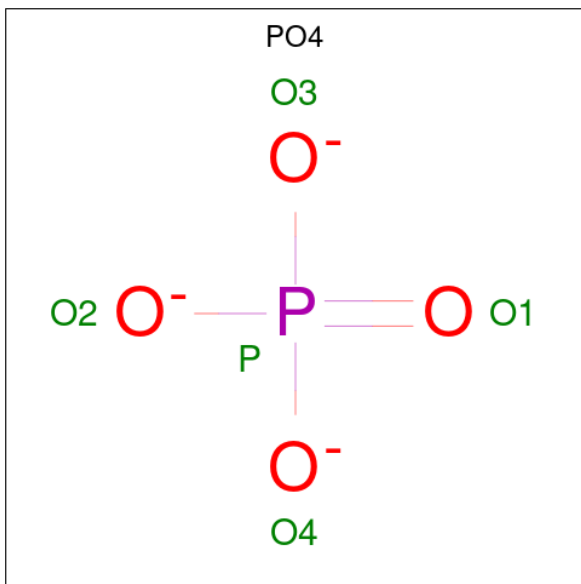
Chain	Residue	Modelled	Actual	Comment	Reference
B	390	GLU	-	expression tag	UNP Q8U093
B	391	HIS	-	expression tag	UNP Q8U093
B	392	HIS	-	expression tag	UNP Q8U093
B	393	HIS	-	expression tag	UNP Q8U093
B	394	HIS	-	expression tag	UNP Q8U093
B	395	HIS	-	expression tag	UNP Q8U093
B	396	HIS	-	expression tag	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

Continued on next page...

Continued from previous page...

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: O₄P).



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

- Molecule 4 is water.

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

Continued on next page...

Continued from previous page...

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

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Tryptophan synthase alpha chain

Chain A:  89% 8%

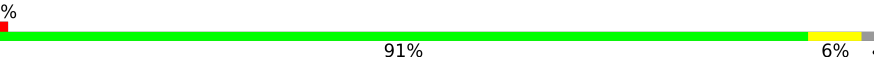


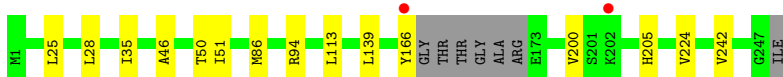
- Molecule 1: Tryptophan synthase alpha chain

Chain C:  94%



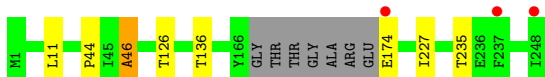
- Molecule 1: Tryptophan synthase alpha chain

Chain E:  91% 6%



- Molecule 1: Tryptophan synthase alpha chain

Chain G:  94%

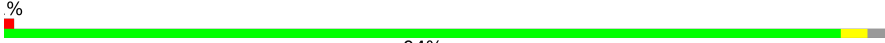


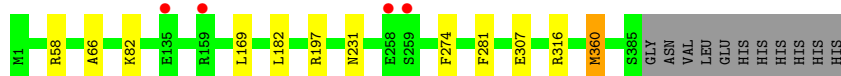
- Molecule 1: Tryptophan synthase alpha chain

Chain I:  94%



- Molecule 1: Tryptophan synthase alpha chain

Chain L:  %
94%



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.77Å)	Xtrriage
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 (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	66.3	Xtrriage
Anisotropy	0.206	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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.*

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: 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(°)	Ideal(°)
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

Continued on next page...

Continued from previous page...

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:A:25:LEU:HD22	1:A:35:ILE:HG21	1.90	0.53
1:E:86:MET:HE3	1:E:113:LEU:HD23	1.88	0.53
2:B:169:LEU:O	2:B:173:VAL:HG23	2.08	0.53
1:E:86:MET:HE2	1:E:113:LEU:HD23	1.90	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:25:LEU:HD22	1:C:35:ILE:HG21	1.93	0.51
1:C:28:LEU:HD22	1:C:242:VAL:HG21	1.92	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:C:10:TYR:CE1	1:C:51:ILE:HD12	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:101:LEU:HD13	1:K:129:ALA:HA	1.96	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:44:PRO:O	2:H:166:ASN:ND2	2.49	0.45
1:G:46:ALA:HB2	2:H:12:PRO:HG3	1.99	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
1:A:200:VAL:HG13	1:A:205:HIS:HB2	2.02	0.42
2:D:46:TRP:CD2	2:D:120:LEU:HD22	2.54	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:A:5:GLY:HA2	1:A:210:LEU:HD22	2.02	0.41
1:I:126:THR:HG22	1:I:136:THR:HG21	2.01	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%)	41	60
2	D	382/396 (96%)	371 (97%)	10 (3%)	1 (0%)	41	60
2	F	382/396 (96%)	375 (98%)	7 (2%)	0	100	100
2	H	382/396 (96%)	374 (98%)	7 (2%)	1 (0%)	41	60
2	J	382/396 (96%)	371 (97%)	10 (3%)	1 (0%)	41	60
2	L	382/396 (96%)	369 (97%)	13 (3%)	0	100	100
All	All	3715/3864 (96%)	3623 (98%)	88 (2%)	4 (0%)	51	75

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%)	88	92
1	C	192/205 (94%)	192 (100%)	0	100	100
1	E	186/205 (91%)	184 (99%)	2 (1%)	73	84
1	G	188/205 (92%)	187 (100%)	1 (0%)	88	92
1	I	192/205 (94%)	190 (99%)	2 (1%)	76	85
1	K	171/205 (83%)	171 (100%)	0	100	100
2	B	297/315 (94%)	294 (99%)	3 (1%)	76	85
2	D	300/315 (95%)	294 (98%)	6 (2%)	55	72
2	F	299/315 (95%)	295 (99%)	4 (1%)	69	81
2	H	302/315 (96%)	298 (99%)	4 (1%)	69	81
2	J	300/315 (95%)	297 (99%)	3 (1%)	76	85
2	L	299/315 (95%)	294 (98%)	5 (2%)	60	76
All	All	2910/3120 (93%)	2879 (99%)	31 (1%)	73	84

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

Continued on next page...

Continued from previous page...

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

Sometimes 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	J	82	2	23,24,25	2.79	5 (21%)	25,32,34	1.37	3 (12%)
2	LLP	H	82	2	23,24,25	2.68	5 (21%)	25,32,34	1.59	4 (16%)
2	LLP	D	82	2	23,24,25	2.68	5 (21%)	25,32,34	1.37	4 (16%)
2	LLP	F	82	2	23,24,25	2.74	5 (21%)	25,32,34	1.41	4 (16%)
2	LLP	B	82	2	23,24,25	2.73	5 (21%)	25,32,34	1.57	3 (12%)
2	LLP	L	82	2	23,24,25	2.74	5 (21%)	25,32,34	1.65	4 (16%)

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	J	82	2	-	7/16/17/19	0/1/1/1
2	LLP	H	82	2	-	3/16/17/19	0/1/1/1
2	LLP	D	82	2	-	5/16/17/19	0/1/1/1
2	LLP	F	82	2	-	2/16/17/19	0/1/1/1
2	LLP	B	82	2	-	6/16/17/19	0/1/1/1
2	LLP	L	82	2	-	6/16/17/19	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	82	LLP	C3-C2	8.03	1.48	1.40
2	B	82	LLP	C3-C2	7.89	1.48	1.40
2	H	82	LLP	C3-C2	7.82	1.48	1.40
2	L	82	LLP	C3-C2	7.73	1.48	1.40
2	J	82	LLP	C3-C2	7.53	1.48	1.40
2	D	82	LLP	C3-C2	7.53	1.48	1.40
2	J	82	LLP	C4-C5	6.55	1.50	1.42
2	L	82	LLP	C4-C5	6.33	1.49	1.42
2	B	82	LLP	C4-C5	6.12	1.49	1.42
2	D	82	LLP	C4-C5	5.94	1.49	1.42
2	F	82	LLP	C4-C5	5.92	1.49	1.42
2	J	82	LLP	C4-C3	5.78	1.49	1.40
2	H	82	LLP	C4-C5	5.77	1.49	1.42
2	J	82	LLP	C4'-NZ	5.55	1.45	1.27
2	D	82	LLP	C4-C3	5.52	1.49	1.40
2	L	82	LLP	C4'-NZ	5.49	1.45	1.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	82	LLP	C4'-NZ	5.47	1.45	1.27
2	F	82	LLP	C4-C3	5.47	1.49	1.40
2	F	82	LLP	C4'-NZ	5.46	1.45	1.27
2	L	82	LLP	C4-C3	5.44	1.49	1.40
2	D	82	LLP	C4'-NZ	5.40	1.45	1.27
2	H	82	LLP	C4'-NZ	5.40	1.45	1.27
2	H	82	LLP	C4-C3	5.21	1.48	1.40
2	B	82	LLP	C4-C3	5.20	1.48	1.40
2	H	82	LLP	C4-C4'	2.96	1.52	1.46
2	J	82	LLP	C4-C4'	2.89	1.52	1.46
2	L	82	LLP	C4-C4'	2.85	1.52	1.46
2	F	82	LLP	C4-C4'	2.75	1.51	1.46
2	D	82	LLP	C4-C4'	2.70	1.51	1.46
2	B	82	LLP	C4-C4'	2.69	1.51	1.46

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	82	LLP	C4-C3-C2	-5.49	116.79	120.19
2	B	82	LLP	C4-C3-C2	-4.49	117.41	120.19
2	F	82	LLP	C4-C3-C2	-4.00	117.72	120.19
2	H	82	LLP	C4-C3-C2	-3.94	117.75	120.19
2	J	82	LLP	C4-C3-C2	-3.70	117.89	120.19
2	H	82	LLP	C3-C4-C5	-3.64	115.47	118.26
2	D	82	LLP	C4-C3-C2	-3.57	117.98	120.19
2	B	82	LLP	C4-C4'-NZ	-3.12	109.97	124.31
2	L	82	LLP	C4-C4'-NZ	-2.88	111.07	124.31
2	D	82	LLP	C4-C4'-NZ	-2.86	111.19	124.31
2	J	82	LLP	C4-C4'-NZ	-2.68	111.99	124.31
2	H	82	LLP	C4-C4'-NZ	-2.65	112.15	124.31
2	F	82	LLP	C4-C4'-NZ	-2.55	112.58	124.31
2	J	82	LLP	C6-N1-C2	2.46	123.72	119.17
2	F	82	LLP	C6-N1-C2	2.42	123.66	119.17
2	B	82	LLP	C6-N1-C2	2.26	123.36	119.17
2	L	82	LLP	C6-N1-C2	2.25	123.34	119.17
2	D	82	LLP	C6-N1-C2	2.21	123.27	119.17
2	D	82	LLP	C3-C4-C5	-2.11	116.64	118.26
2	L	82	LLP	C3-C4-C5	-2.06	116.68	118.26
2	H	82	LLP	OP4-C5'-C5	-2.03	105.48	109.35
2	F	82	LLP	C3-C4-C5	-2.03	116.70	118.26

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	82	LLP	C4-C4'-NZ-CE
2	B	82	LLP	C5'-OP4-P-OP2
2	B	82	LLP	C5'-OP4-P-OP3
2	D	82	LLP	C4-C4'-NZ-CE
2	D	82	LLP	O-C-CA-CB
2	D	82	LLP	CG-CD-CE-NZ
2	F	82	LLP	C4-C4'-NZ-CE
2	H	82	LLP	C4-C4'-NZ-CE
2	J	82	LLP	C4-C4'-NZ-CE
2	J	82	LLP	C5'-OP4-P-OP1
2	J	82	LLP	O-C-CA-CB
2	L	82	LLP	C4-C4'-NZ-CE
2	L	82	LLP	C5'-OP4-P-OP2
2	L	82	LLP	C5'-OP4-P-OP3
2	F	82	LLP	CG-CD-CE-NZ
2	B	82	LLP	CA-CB-CG-CD
2	L	82	LLP	C5'-OP4-P-OP1
2	H	82	LLP	CG-CD-CE-NZ
2	J	82	LLP	CG-CD-CE-NZ
2	J	82	LLP	C5'-OP4-P-OP3
2	L	82	LLP	CD-CE-NZ-C4'
2	B	82	LLP	CD-CE-NZ-C4'
2	B	82	LLP	C3-C4-C4'-NZ
2	L	82	LLP	C3-C4-C4'-NZ
2	D	82	LLP	CD-CE-NZ-C4'
2	J	82	LLP	CD-CE-NZ-C4'
2	D	82	LLP	C3-C4-C4'-NZ
2	H	82	LLP	C3-C4-C4'-NZ
2	J	82	LLP	C3-C4-C4'-NZ

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	D	401	-	4,4,4	0.89	0	6,6,6	0.46	0
3	PO4	F	401	-	4,4,4	0.91	0	6,6,6	0.45	0
3	PO4	J	401	-	4,4,4	0.87	0	6,6,6	0.52	0
3	PO4	H	401	-	4,4,4	0.89	0	6,6,6	0.47	0
3	PO4	L	401	-	4,4,4	0.90	0	6,6,6	0.45	0
3	PO4	B	401	-	4,4,4	0.87	0	6,6,6	0.55	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 [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 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	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%) 86 90	63, 75, 94, 118	0
1	G	241/248 (97%)	-0.07	3 (1%) 79 85	52, 65, 88, 111	0
1	I	242/248 (97%)	-0.07	1 (0%) 92 95	55, 69, 83, 101	0
1	K	240/248 (96%)	1.05	50 (20%) 1 1	92, 129, 151, 161	0
2	B	384/396 (96%)	0.08	8 (2%) 63 72	48, 67, 93, 114	0
2	D	384/396 (96%)	-0.13	1 (0%) 94 96	45, 54, 79, 101	0
2	F	384/396 (96%)	0.04	3 (0%) 86 90	55, 71, 90, 100	0
2	H	384/396 (96%)	-0.13	2 (0%) 91 94	52, 62, 77, 93	0
2	J	384/396 (96%)	-0.12	1 (0%) 94 96	48, 60, 79, 95	0
2	L	384/396 (96%)	-0.04	4 (1%) 82 87	48, 63, 91, 111	0
All	All	3751/3864 (97%)	0.02	75 (1%) 65 73	45, 66, 116, 161	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	245	LEU	5.2
1	K	7	LEU	4.6
1	K	78	HIS	4.4
1	K	46	ALA	4.4
1	K	209	LEU	4.1
1	K	247	GLY	4.0
2	L	258	GLU	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	28	LEU	3.2
1	K	180	TYR	3.2
1	K	237	PHE	3.2
1	K	204	GLU	3.1
1	E	166	TYR	3.1
1	K	1	MET	3.0
1	K	243	GLU	3.0
1	K	56	TYR	2.9
1	K	208	SER	2.9
1	K	238	LEU	2.9
1	K	130	ARG	2.9
1	K	213	GLY	2.8
1	K	74	GLU	2.8
1	K	52	GLN	2.7
1	K	75	PHE	2.7
2	J	259	SER	2.7
2	L	135	GLU	2.7
2	L	259	SER	2.6
1	G	248	ILE	2.6
1	G	237	PHE	2.6
1	K	187	LYS	2.6
2	B	132	GLU	2.6
1	K	5	GLY	2.6
2	B	76	VAL	2.5
1	K	185	ARG	2.5
2	B	325	GLU	2.5
1	K	102	ALA	2.5
1	K	205	HIS	2.5
2	L	159	ARG	2.4
1	K	23	ASN	2.4
1	K	95	ALA	2.4
1	K	24	PHE	2.4
1	K	70	TRP	2.4
2	F	135	GLU	2.3
1	K	183	LEU	2.3
2	F	178	TYR	2.3
2	H	285	GLU	2.3
1	K	16	PRO	2.3
2	H	258	GLU	2.3
1	K	242	VAL	2.3
2	B	79	GLY	2.3
1	K	178	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	165	LEU	2.3
1	K	175	ILE	2.3
1	K	246	LEU	2.2
1	K	236	GLU	2.2
1	K	230	LYS	2.2
2	B	80	ALA	2.2
1	K	61	ASN	2.2
1	I	191	ARG	2.2
1	K	174	GLU	2.1
2	B	315	GLN	2.1
1	K	32	ALA	2.1
1	K	190	CYS	2.1
2	F	155	ASN	2.1
1	K	217	VAL	2.1
1	K	234	ALA	2.1
2	B	373	ARG	2.1
1	G	174	GLU	2.1
1	K	244	GLU	2.1
2	D	372	GLY	2.1
1	K	31	TYR	2.1
1	E	202	LYS	2.0
1	K	71	ILE	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. 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(Å ²)	Q<0.9
2	LLP	B	82	24/25	0.97	0.26	52,59,60,61	0
2	LLP	J	82	24/25	0.97	0.17	49,53,54,54	0
2	LLP	L	82	24/25	0.97	0.25	53,57,58,58	0
2	LLP	H	82	24/25	0.98	0.21	52,52,52,53	0
2	LLP	D	82	24/25	0.98	0.21	46,47,48,48	0
2	LLP	F	82	24/25	0.98	0.22	56,58,60,61	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(Å ²)	Q<0.9
3	PO4	L	401	5/5	0.82	0.37	139,139,140,140	0
3	PO4	J	401	5/5	0.88	0.21	97,98,100,102	0
3	PO4	B	401	5/5	0.89	0.21	96,97,100,101	0
3	PO4	D	401	5/5	0.91	0.21	95,98,99,99	0
3	PO4	H	401	5/5	0.92	0.20	103,106,108,109	0
3	PO4	F	401	5/5	0.93	0.21	109,110,110,110	0

6.5 Other polymers [i](#)

There are no such residues in this entry.