Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:35 PM GMT

PDB ID	:	1UBS
Title	:	TRYPTOPHAN SYNTHASE (E.C.4.2.1.20) WITH A MUTATION OF LYS 87->THR IN THE B SUBUNIT AND IN THE PRESENCE OF LIGAND L-SERINE
Authors	:	Rhee, S.; Parris, K.; Ahmed, S.A.; Miles, E.W.; Davies, D.R.
Deposited on	:	1995-12-14
Resolution	:	1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

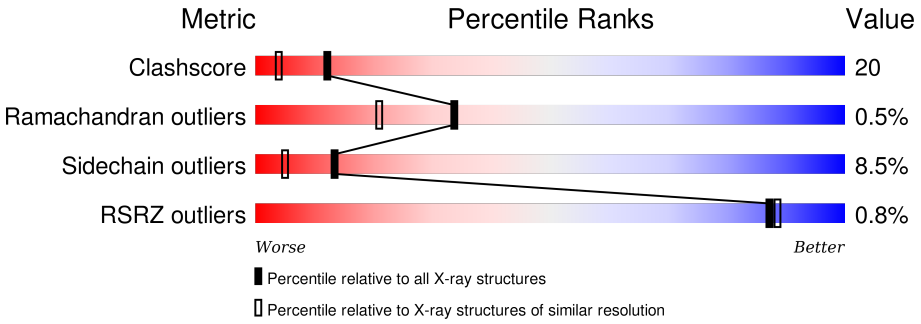
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	268	2% 57% 32% 7%
2	B	397	65% 27% 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5184 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	1	0
			1945	1235	338	364	8			

- Molecule 2 is a protein called TRYPTOPHAN SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	389	Total	C	N	O	S	0	4	0
			2962	1863	520	560	19			

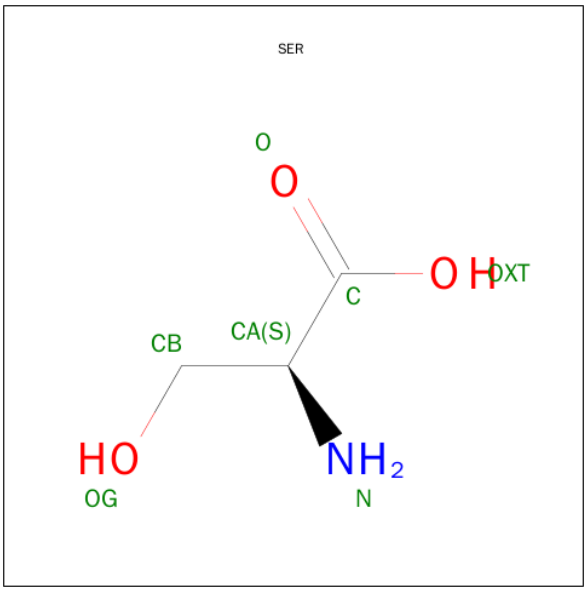
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	87	THR	LYS	ENGINEERED	UNP P00933
B	396	LEU	GLU	CONFLICT	UNP P00933

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

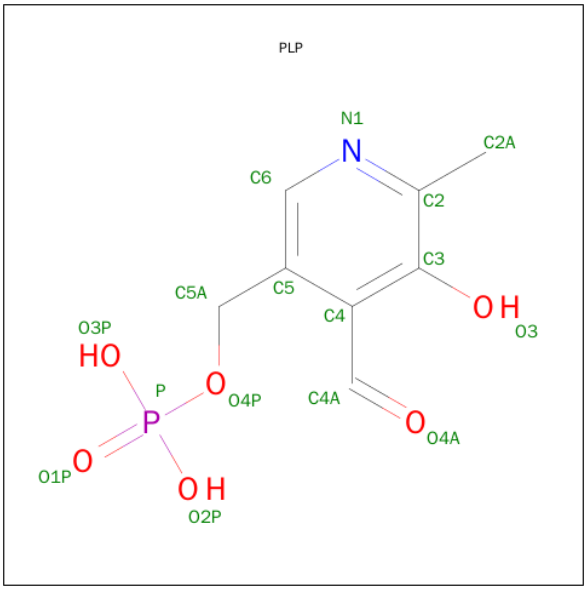
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		

- Molecule 4 is SERINE (three-letter code: SER) (formula: $C_3H_7NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			7	3	1	3		

- Molecule 5 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 6 is water.

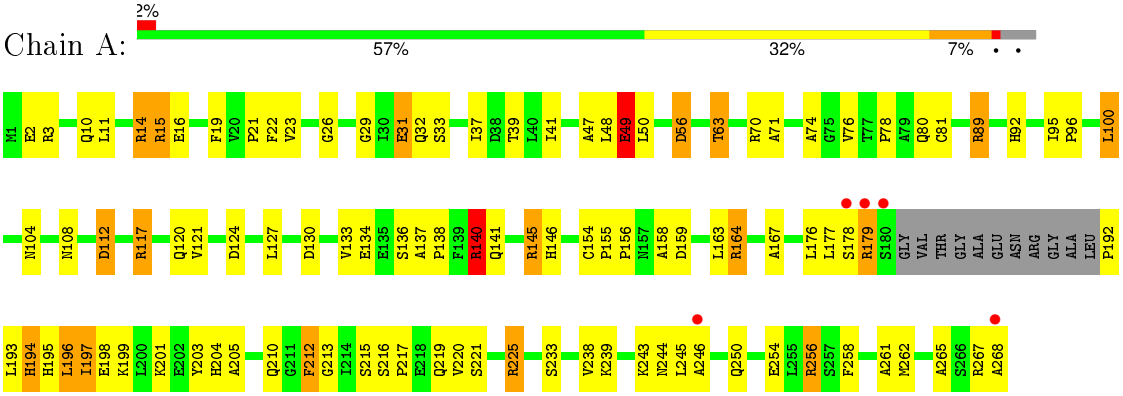
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	83	Total O 83 83	0	0
6	B	171	Total O 171 171	0	0

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.

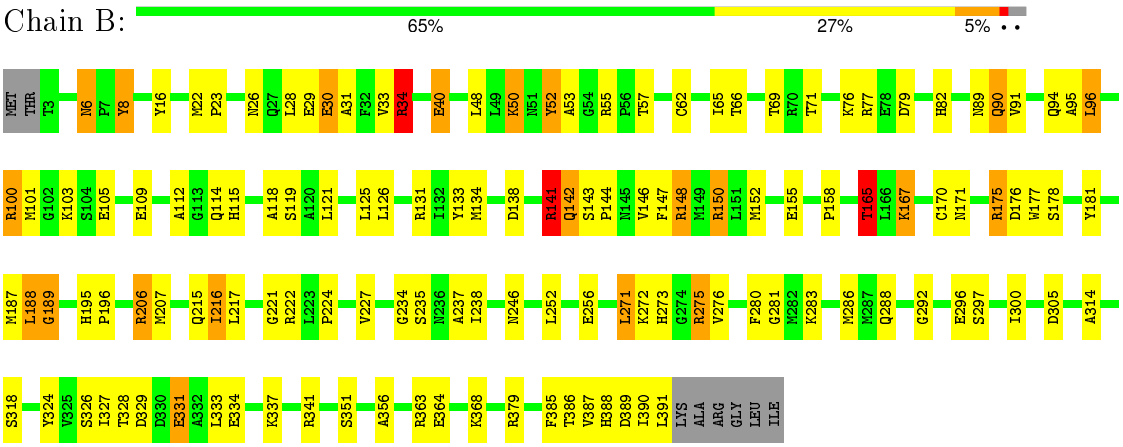
- Molecule 1: TRYPTOPHAN SYNTHASE

Chain A:



- Molecule 2: TRYPTOPHAN SYNTHASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	184.20Å 61.80Å 67.80Å 90.00° 94.80° 90.00°	Depositor
Resolution (Å)	8.00 – 1.90 67.56 – 1.86	Depositor EDS
% Data completeness (in resolution range)	84.9 (8.00-1.90) 87.7 (67.56-1.86)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 1.86Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.186 , (Not available) 0.176 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	23.6	Xtriage
Anisotropy	0.498	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 97.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 56520 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5184	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.88% 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: NA, PLP

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	0.72	0/1988	1.60	24/2698 (0.9%)
2	B	0.90	0/3043	1.73	52/4112 (1.3%)
All	All	0.83	0/5031	1.68	76/6810 (1.1%)

There are no bond length outliers.

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	140	ARG	NE-CZ-NH1	-15.13	112.73	120.30
2	B	206	ARG	NE-CZ-NH1	14.43	127.52	120.30
1	A	140	ARG	NE-CZ-NH2	13.50	127.05	120.30
2	B	100	ARG	NE-CZ-NH1	-12.94	113.83	120.30
2	B	131	ARG	NE-CZ-NH1	12.93	126.76	120.30
1	A	3	ARG	CD-NE-CZ	12.68	141.36	123.60
2	B	34	ARG	CD-NE-CZ	12.68	141.35	123.60
2	B	175	ARG	CD-NE-CZ	10.98	138.97	123.60
2	B	275	ARG	NE-CZ-NH1	-10.81	114.89	120.30
1	A	225	ARG	NE-CZ-NH1	10.44	125.52	120.30
2	B	206	ARG	CD-NE-CZ	10.40	138.16	123.60
1	A	3	ARG	NE-CZ-NH1	9.36	124.98	120.30
1	A	140	ARG	CD-NE-CZ	-8.93	111.10	123.60
1	A	164	ARG	CD-NE-CZ	8.54	135.55	123.60
2	B	206	ARG	NE-CZ-NH2	-8.35	116.13	120.30
2	B	222	ARG	NE-CZ-NH1	7.83	124.22	120.30
2	B	175	ARG	NE-CZ-NH1	7.75	124.17	120.30
2	B	100	ARG	CD-NE-CZ	-7.62	112.94	123.60
2	B	234	GLY	N-CA-C	7.47	131.78	113.10
2	B	148	ARG	NE-CZ-NH1	-7.46	116.57	120.30
2	B	100	ARG	NE-CZ-NH2	7.30	123.95	120.30
2	B	341	ARG	CD-NE-CZ	7.25	133.76	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	305	ASP	CB-CG-OD1	7.14	124.73	118.30
2	B	305	ASP	CB-CG-OD2	-7.12	111.89	118.30
2	B	147[A]	PHE	CA-CB-CG	7.11	130.96	113.90
2	B	147[B]	PHE	CA-CB-CG	7.11	130.96	113.90
1	A	159	ASP	CB-CG-OD1	7.08	124.67	118.30
2	B	34	ARG	NE-CZ-NH1	6.94	123.77	120.30
2	B	77	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	A	89	ARG	NE-CZ-NH1	-6.72	116.94	120.30
1	A	140	ARG	CA-CB-CG	6.58	127.87	113.40
2	B	275	ARG	CD-NE-CZ	-6.53	114.46	123.60
2	B	331	GLU	CG-CD-OE2	6.47	131.24	118.30
1	A	179	ARG	NE-CZ-NH1	6.41	123.51	120.30
2	B	141	ARG	NE-CZ-NH1	-6.33	117.14	120.30
1	A	56	ASP	CB-CG-OD1	6.32	123.99	118.30
2	B	363	ARG	NE-CZ-NH1	-6.32	117.14	120.30
1	A	145	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	A	49	GLU	CG-CD-OE1	-6.11	106.08	118.30
2	B	8	TYR	CG-CD2-CE2	-6.04	116.47	121.30
2	B	40	GLU	CA-CB-CG	6.01	126.63	113.40
1	A	145	ARG	NE-CZ-NH1	5.93	123.26	120.30
2	B	30	GLU	CA-CB-CG	5.78	126.12	113.40
2	B	77	ARG	NE-CZ-NH2	-5.75	117.42	120.30
2	B	105	GLU	OE1-CD-OE2	5.72	130.16	123.30
2	B	188	LEU	CA-CB-CG	5.69	128.38	115.30
2	B	222	ARG	CD-NE-CZ	5.68	131.56	123.60
2	B	119	SER	O-C-N	5.66	131.76	122.70
1	A	204	HIS	CA-CB-CG	-5.65	103.99	113.60
2	B	363	ARG	NE-CZ-NH2	5.64	123.12	120.30
2	B	275	ARG	NE-CZ-NH2	5.63	123.11	120.30
2	B	368	LYS	O-C-N	5.62	131.70	122.70
1	A	63	THR	N-CA-CB	5.52	120.79	110.30
2	B	34	ARG	NH1-CZ-NH2	-5.52	113.33	119.40
1	A	63	THR	O-C-N	5.51	131.52	122.70
1	A	19	PHE	CB-CG-CD1	-5.46	116.98	120.80
2	B	237	ALA	CB-CA-C	5.46	118.28	110.10
1	A	124	ASP	CB-CG-OD1	-5.42	113.42	118.30
2	B	167	LYS	CA-CB-CG	5.42	125.32	113.40
1	A	100	LEU	CB-CA-C	5.41	120.48	110.20
2	B	324	TYR	CG-CD1-CE1	5.37	125.59	121.30
2	B	314	ALA	CB-CA-C	5.36	118.14	110.10
2	B	189	GLY	N-CA-C	5.36	126.49	113.10
2	B	79	ASP	CB-CG-OD2	-5.33	113.50	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	273	HIS	CA-CB-CG	-5.27	104.64	113.60
1	A	136	SER	O-C-N	5.23	131.07	122.70
2	B	34	ARG	NE-CZ-NH2	5.19	122.90	120.30
2	B	275	ARG	CB-CA-C	-5.15	100.09	110.40
2	B	286	MET	O-C-N	5.13	130.90	122.70
1	A	134	GLU	CG-CD-OE1	5.12	128.54	118.30
2	B	331	GLU	CG-CD-OE1	-5.11	108.08	118.30
2	B	52	TYR	CB-CG-CD2	5.10	124.06	121.00
1	A	233	SER	C-N-CA	5.03	132.87	122.30
2	B	165	THR	N-CA-CB	-5.03	100.74	110.30
2	B	237	ALA	N-CA-CB	-5.02	103.07	110.10
2	B	379	ARG	CA-CB-CG	5.01	124.43	113.40

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	1945	0	1954	82	0
2	B	2962	0	2934	118	0
3	B	1	0	0	0	0
4	B	7	0	4	0	0
5	B	15	0	6	0	0
6	A	83	0	0	4	0
6	B	171	0	0	8	1
All	All	5184	0	4898	195	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 20.

All (195) 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:B:50:LYS:HB2	2:B:50:LYS:NZ	1.54	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:GLN:HE22	2:B:94:GLN:HE21	1.10	1.00
2:B:50:LYS:HB2	2:B:50:LYS:HZ2	1.05	0.99
1:A:63:THR:HG22	1:A:238:VAL:HG12	1.44	0.99
2:B:6:ASN:HD22	2:B:8:TYR:H	1.13	0.96
2:B:6:ASN:ND2	2:B:8:TYR:H	1.64	0.96
1:A:220:VAL:HG21	1:A:262:MET:HE3	1.47	0.95
2:B:271:LEU:O	2:B:271:LEU:HD12	1.68	0.92
1:A:22:PHE:HD2	1:A:49:GLU:HG2	1.33	0.91
2:B:31:ALA:HA	2:B:34:ARG:CD	2.03	0.89
2:B:65[B]:ILE:HD13	2:B:66:THR:HG23	1.55	0.88
2:B:50:LYS:NZ	2:B:50:LYS:CB	2.34	0.85
1:A:23:VAL:HG12	1:A:50:LEU:HD23	1.59	0.84
2:B:138:ASP:O	2:B:142:GLN:HB2	1.77	0.84
2:B:69:THR:HG22	2:B:71:THR:H	1.43	0.81
2:B:34:ARG:HG2	2:B:100:ARG:HH21	1.45	0.81
2:B:31:ALA:HA	2:B:34:ARG:HD3	1.64	0.80
2:B:69:THR:CG2	2:B:71:THR:H	1.97	0.78
2:B:62:CYS:HB3	2:B:65[B]:ILE:HD11	1.66	0.77
1:A:63:THR:HG22	1:A:238:VAL:CG1	2.16	0.75
2:B:50:LYS:HZ3	2:B:50:LYS:HB2	1.51	0.75
1:A:250:GLN:NE2	1:A:254:GLU:OE1	2.19	0.75
2:B:55:ARG:HH11	2:B:89:ASN:HD21	1.33	0.75
2:B:62:CYS:CB	2:B:65[B]:ILE:HD11	2.16	0.75
1:A:41:ILE:HD11	1:A:48:LEU:HD11	1.68	0.74
2:B:143:SER:HB2	2:B:144:PRO:HD3	1.68	0.74
1:A:194:HIS:O	1:A:198:GLU:HB2	1.87	0.74
2:B:65[B]:ILE:CD1	2:B:66:THR:HG23	2.17	0.73
1:A:163:LEU:HD21	1:A:196:LEU:HD11	1.68	0.73
1:A:220:VAL:CG2	1:A:262:MET:HE3	2.18	0.72
2:B:103:LYS:NZ	2:B:181:TYR:O	2.23	0.71
2:B:57:THR:OG1	2:B:76:LYS:HE3	1.90	0.71
1:A:22:PHE:CD2	1:A:49:GLU:HG2	2.24	0.70
1:A:63:THR:CG2	1:A:238:VAL:HG12	2.22	0.69
2:B:175:ARG:O	2:B:178:SER:HB2	1.94	0.68
2:B:29:GLU:OE2	2:B:195:HIS:HE1	1.76	0.68
2:B:31:ALA:HA	2:B:34:ARG:HD2	1.75	0.68
2:B:62:CYS:HB3	2:B:65[B]:ILE:CD1	2.24	0.68
2:B:142:GLN:O	2:B:146:VAL:HG23	1.94	0.67
1:A:31:GLU:H	1:A:31:GLU:CD	1.95	0.67
2:B:165:THR:CG2	6:B:442:HOH:O	2.42	0.66
1:A:23:VAL:HG12	1:A:50:LEU:CD2	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:ARG:CG	2:B:100:ARG:HH21	2.08	0.66
2:B:364:GLU:OE1	6:B:474:HOH:O	2.14	0.65
2:B:385:PHE:O	2:B:388:HIS:HB3	1.97	0.65
2:B:288:GLN:HE21	2:B:292:GLY:HA2	1.60	0.65
2:B:28:LEU:HA	2:B:101:MET:HE2	1.78	0.65
2:B:90:GLN:NE2	2:B:94:GLN:HE21	1.91	0.65
1:A:70:ARG:NH2	6:A:431:HOH:O	2.29	0.65
2:B:31:ALA:CB	2:B:34:ARG:HH11	2.10	0.64
1:A:178:SER:HB2	1:A:212:PHE:CB	2.27	0.64
1:A:199:LYS:HD2	1:A:203:TYR:CE2	2.33	0.64
1:A:220:VAL:HG21	1:A:262:MET:CE	2.27	0.64
1:A:156:PRO:HG3	1:A:179:ARG:H	1.63	0.63
1:A:220:VAL:CG2	1:A:262:MET:CE	2.76	0.63
1:A:154:CYS:HB3	1:A:176:LEU:HD12	1.79	0.63
2:B:386:THR:O	2:B:390:ILE:HG12	1.98	0.62
2:B:170:CYS:HB3	2:B:280:PHE:CE1	2.34	0.62
1:A:26:GLY:HA3	1:A:76:VAL:HG21	1.81	0.62
1:A:39:THR:HG23	1:A:256:ARG:HH11	1.67	0.60
2:B:165:THR:HG22	6:B:442:HOH:O	2.02	0.60
2:B:76:LYS:NZ	2:B:215:GLN:HE22	1.99	0.60
1:A:156:PRO:HG3	1:A:179:ARG:N	2.17	0.59
2:B:216:ILE:HG21	2:B:224:PRO:HD3	1.83	0.59
1:A:265:ALA:O	1:A:268:ALA:OXT	2.22	0.58
2:B:133:TYR:OH	2:B:176:ASP:OD2	2.11	0.58
2:B:387:VAL:O	2:B:391:LEU:HG	2.04	0.58
2:B:333:LEU:O	2:B:337:LYS:HG3	2.03	0.57
1:A:70:ARG:HD3	1:A:245:LEU:HD21	1.85	0.57
1:A:22:PHE:HD2	1:A:49:GLU:CG	2.13	0.57
1:A:56:ASP:OD2	2:B:167:LYS:HG2	2.05	0.57
2:B:66:THR:O	2:B:69:THR:HB	2.05	0.56
1:A:137:ALA:HB3	1:A:138:PRO:CD	2.35	0.56
2:B:288:GLN:NE2	2:B:292:GLY:HA2	2.20	0.56
2:B:167:LYS:HB2	6:B:442:HOH:O	2.06	0.56
1:A:163:LEU:HD21	1:A:196:LEU:CD1	2.33	0.56
1:A:192:PRO:O	1:A:195:HIS:HB3	2.05	0.56
1:A:216:SER:N	1:A:219:GLN:OE1	2.38	0.56
2:B:271:LEU:C	2:B:271:LEU:HD12	2.27	0.55
1:A:117:ARG:HG3	1:A:117:ARG:O	2.07	0.55
2:B:272:LYS:HE3	6:B:410:HOH:O	2.06	0.54
2:B:69:THR:CG2	2:B:71:THR:HB	2.37	0.54
2:B:31:ALA:HB3	2:B:101:MET:HE2	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ARG:NH1	1:A:92:HIS:O	2.39	0.54
2:B:177:TRP:O	2:B:181:TYR:HB3	2.08	0.54
2:B:121:LEU:HB3	2:B:152:MET:CE	2.38	0.54
1:A:117:ARG:HD2	6:A:590:HOH:O	2.08	0.53
2:B:121:LEU:HB3	2:B:152:MET:HE1	1.89	0.53
2:B:6:ASN:C	2:B:6:ASN:HD22	2.12	0.53
1:A:104:ASN:HD21	2:B:288:GLN:NE2	2.07	0.53
1:A:14:ARG:O	1:A:15:ARG:C	2.47	0.53
2:B:334:GLU:HB2	6:B:515:HOH:O	2.08	0.53
2:B:69:THR:HG21	2:B:71:THR:HB	1.91	0.53
2:B:134:MET:O	2:B:158:PRO:HA	2.09	0.52
1:A:32:GLN:HB2	6:A:568:HOH:O	2.09	0.52
2:B:95:ALA:HB2	2:B:187:MET:HE1	1.91	0.51
1:A:11:LEU:HD22	1:A:16:GLU:HG3	1.93	0.51
1:A:197:ILE:O	1:A:201:LYS:HG3	2.11	0.51
2:B:55:ARG:HD2	2:B:89:ASN:ND2	2.25	0.51
2:B:50:LYS:HZ3	2:B:50:LYS:CB	2.15	0.51
2:B:48:LEU:O	2:B:52:TYR:HB3	2.10	0.51
1:A:11:LEU:HD23	1:A:14:ARG:HH11	1.76	0.51
2:B:388:HIS:HD2	2:B:389:ASP:OD1	1.93	0.50
1:A:156:PRO:HG3	1:A:179:ARG:CB	2.41	0.50
1:A:71:ALA:O	1:A:74:ALA:HB3	2.10	0.50
2:B:141:ARG:O	2:B:141:ARG:HG2	2.11	0.50
2:B:146:VAL:O	2:B:150[A]:ARG:HG3	2.11	0.50
2:B:195:HIS:HD2	6:B:408:HOH:O	1.94	0.50
1:A:29:GLY:O	1:A:33:SER:HB2	2.11	0.50
2:B:50:LYS:HZ2	2:B:50:LYS:CB	1.95	0.50
2:B:143:SER:N	2:B:144:PRO:CD	2.75	0.50
1:A:239:LYS:O	1:A:243:LYS:HG3	2.11	0.49
2:B:112:ALA:O	2:B:142:GLN:CG	2.60	0.49
1:A:258:PHE:O	1:A:262:MET:HG2	2.12	0.49
2:B:34:ARG:HG2	2:B:100:ARG:NH2	2.21	0.49
1:A:258:PHE:O	1:A:261:ALA:HB3	2.13	0.49
1:A:78:PRO:O	1:A:81:CYS:HB2	2.13	0.49
2:B:109:GLU:O	2:B:115:HIS:HD2	1.96	0.49
2:B:22:MET:N	2:B:23:PRO:CD	2.76	0.49
1:A:267:ARG:HG3	1:A:267:ARG:HH11	1.78	0.48
2:B:76:LYS:HZ2	2:B:215:GLN:HE22	1.60	0.48
1:A:112:ASP:OD1	1:A:146:HIS:HE1	1.97	0.48
1:A:221:SER:OG	1:A:225:ARG:NH1	2.47	0.47
2:B:29:GLU:O	2:B:33:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:300:ILE:HB	2:B:329:ASP:CG	2.35	0.47
1:A:250:GLN:O	1:A:250:GLN:NE2	2.47	0.47
2:B:171:ASN:O	2:B:175:ARG:HG3	2.14	0.47
2:B:275:ARG:HD2	2:B:275:ARG:HH11	1.42	0.47
1:A:137:ALA:O	1:A:141:GLN:HG3	2.15	0.46
1:A:155:PRO:HD2	1:A:158:ALA:HB2	1.96	0.46
2:B:16:TYR:O	2:B:281:GLY:HA2	2.16	0.46
1:A:22:PHE:CE2	1:A:100:LEU:HD23	2.51	0.46
2:B:150[B]:ARG:HH21	2:B:155:GLU:HA	1.81	0.45
1:A:196:LEU:HD13	1:A:196:LEU:HA	1.69	0.45
2:B:91:VAL:HG11	2:B:118:ALA:O	2.16	0.45
2:B:115:HIS:CE1	2:B:189:GLY:HA2	2.52	0.45
2:B:26:ASN:O	2:B:30:GLU:HG3	2.16	0.45
1:A:216:SER:HA	1:A:217:PRO:HD3	1.82	0.44
2:B:28:LEU:HA	2:B:101:MET:CE	2.45	0.44
2:B:96:LEU:HD13	2:B:126:LEU:HD11	1.99	0.44
1:A:56:ASP:CG	2:B:167:LYS:HZ3	2.19	0.44
2:B:69:THR:HG22	2:B:71:THR:N	2.23	0.44
1:A:267:ARG:HG3	1:A:267:ARG:NH1	2.32	0.44
2:B:53:ALA:HA	2:B:82:HIS:HB3	2.00	0.43
2:B:333:LEU:CD1	2:B:390:ILE:HG21	2.48	0.43
2:B:28:LEU:CD1	2:B:101:MET:HE1	2.48	0.43
2:B:328:THR:OG1	2:B:331:GLU:HG3	2.18	0.43
1:A:104:ASN:HD21	2:B:288:GLN:HE22	1.65	0.43
2:B:246:ASN:HB2	6:B:544:HOH:O	2.18	0.43
1:A:220:VAL:HG23	1:A:262:MET:HE1	2.00	0.43
2:B:31:ALA:CB	2:B:101:MET:HE2	2.48	0.43
2:B:31:ALA:HB2	2:B:34:ARG:HH11	1.80	0.43
2:B:55:ARG:NH1	2:B:89:ASN:HD21	2.07	0.43
1:A:37:ILE:O	1:A:41:ILE:HG13	2.18	0.43
2:B:91:VAL:O	2:B:187:MET:HE2	2.18	0.43
1:A:89:ARG:HA	1:A:89:ARG:HD3	1.76	0.43
1:A:140:ARG:HD2	1:A:140:ARG:HH11	1.18	0.43
2:B:6:ASN:HD22	2:B:8:TYR:N	1.96	0.43
2:B:227:VAL:HG22	2:B:252:LEU:HD23	2.01	0.43
2:B:327:ILE:HG21	2:B:356:ALA:HB3	2.01	0.43
2:B:141:ARG:HD2	2:B:141:ARG:HH11	1.60	0.42
1:A:11:LEU:HD23	1:A:14:ARG:NH1	2.33	0.42
2:B:31:ALA:CB	2:B:101:MET:CE	2.97	0.42
2:B:31:ALA:HB3	2:B:101:MET:CE	2.48	0.42
1:A:244:ASN:C	1:A:246:ALA:N	2.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:LEU:HG	1:A:178:SER:H	1.85	0.42
2:B:333:LEU:HD11	2:B:390:ILE:HG21	2.01	0.42
2:B:143:SER:CB	2:B:144:PRO:HD3	2.41	0.42
1:A:22:PHE:CD1	1:A:22:PHE:C	2.93	0.42
2:B:28:LEU:HD12	2:B:101:MET:HE1	2.01	0.42
1:A:117:ARG:NH1	6:A:590:HOH:O	2.51	0.42
2:B:217:LEU:O	2:B:221:GLY:HA2	2.19	0.42
1:A:167:ALA:CB	1:A:205:ALA:HB2	2.50	0.42
1:A:56:ASP:OD2	2:B:167:LYS:NZ	2.47	0.41
1:A:163:LEU:HD23	1:A:163:LEU:HA	1.84	0.41
1:A:21:PRO:HD2	1:A:47:ALA:O	2.20	0.41
1:A:195:HIS:O	1:A:198:GLU:HB3	2.20	0.41
2:B:6:ASN:ND2	2:B:8:TYR:N	2.48	0.41
1:A:112:ASP:OD2	1:A:145:ARG:NH2	2.38	0.41
2:B:90:GLN:HE22	2:B:94:GLN:NE2	1.94	0.41
1:A:244:ASN:O	1:A:245:LEU:C	2.59	0.41
1:A:137:ALA:HB3	1:A:138:PRO:HD3	2.02	0.41
1:A:213:GLY:O	1:A:219:GLN:NE2	2.54	0.41
2:B:235:SER:HA	2:B:238:ILE:HG22	2.03	0.41
2:B:148:ARG:HE	2:B:148:ARG:HB2	1.47	0.41
2:B:125:LEU:HG	2:B:125:LEU:O	2.21	0.41
2:B:256:GLU:O	2:B:326:SER:HA	2.21	0.41
2:B:333:LEU:HA	2:B:333:LEU:HD23	1.91	0.40
2:B:31:ALA:O	2:B:34:ARG:HD3	2.22	0.40
1:A:95:ILE:HA	1:A:96:PRO:HD3	1.81	0.40
2:B:31:ALA:CA	2:B:34:ARG:HD3	2.42	0.40
2:B:195:HIS:CD2	2:B:196:PRO:HA	2.57	0.40
1:A:130:ASP:N	1:A:130:ASP:OD1	2.55	0.40
1:A:220:VAL:CG2	1:A:262:MET:HE1	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:488:HOH:O	6:B:488:HOH:O[2_655]	2.14	0.06

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	254/268 (95%)	239 (94%)	12 (5%)	3 (1%)	16 5
2	B	391/397 (98%)	381 (97%)	10 (3%)	0	100 100
All	All	645/665 (97%)	620 (96%)	22 (3%)	3 (0%)	34 21

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	PHE
1	A	15	ARG
1	A	108	ASN

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	202/208 (97%)	180 (89%)	22 (11%)	8 2
2	B	309/311 (99%)	285 (92%)	24 (8%)	16 6
All	All	511/519 (98%)	465 (91%)	46 (9%)	13 4

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	10[A]	GLN
1	A	10[B]	GLN

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Mol	Chain	Res	Type
1	A	14	ARG
1	A	31	GLU
1	A	49	GLU
1	A	80	GLN
1	A	112	ASP
1	A	117	ARG
1	A	120	GLN
1	A	121	VAL
1	A	127	LEU
1	A	133	VAL
1	A	140	ARG
1	A	164	ARG
1	A	193	LEU
1	A	194	HIS
1	A	196	LEU
1	A	197	ILE
1	A	210	GLN
1	A	215	SER
1	A	256	ARG
2	B	6	ASN
2	B	34	ARG
2	B	40	GLU
2	B	50	LYS
2	B	90	GLN
2	B	96	LEU
2	B	114	GLN
2	B	141	ARG
2	B	142	GLN
2	B	150[A]	ARG
2	B	150[B]	ARG
2	B	165	THR
2	B	188	LEU
2	B	206	ARG
2	B	207	MET
2	B	216	ILE
2	B	271	LEU
2	B	276	VAL
2	B	283	LYS
2	B	296	GLU
2	B	297	SER
2	B	318[A]	SER
2	B	318[B]	SER

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Mol	Chain	Res	Type
2	B	351	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	80	GLN
1	A	120	GLN
1	A	244	ASN
1	A	250	GLN
2	B	6	ASN
2	B	27	GLN
2	B	89	ASN
2	B	90	GLN
2	B	115	HIS
2	B	145	ASN
2	B	160	HIS
2	B	195	HIS
2	B	215	GLN
2	B	260	HIS
2	B	288	GLN
2	B	317	ASN
2	B	365	GLN
2	B	370	GLN
2	B	388	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\#\|Z\| > 2$
4	SER	B	398	5	3,6,6	0.92	0	1,7,7	2.87	1 (100%)
5	PLP	B	401	4	15,15,16	1.88	6 (40%)	21,22,23	2.79	8 (38%)

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
4	SER	B	398	5	-	0/2/6/6	0/0/0/0
5	PLP	B	401	4	-	0/6/6/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	401	PLP	P-O4P	-3.52	1.48	1.60
5	B	401	PLP	C5-C4	-3.09	1.36	1.40
5	B	401	PLP	P-O1P	-2.86	1.41	1.51
5	B	401	PLP	P-O3P	-2.43	1.46	1.54
5	B	401	PLP	O3-C3	-2.36	1.31	1.37
5	B	401	PLP	P-O2P	2.23	1.62	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	401	PLP	C5-C6-N1	-3.06	118.55	123.86
5	B	401	PLP	C4A-C4-C5	-2.62	118.15	120.88
5	B	401	PLP	C3-C2-N1	-2.02	117.83	120.61
5	B	401	PLP	C3-C4-C5	2.09	121.06	118.78
5	B	401	PLP	C6-N1-C2	2.67	124.73	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	398	SER	OG-CB-CA	2.87	117.28	111.16
5	B	401	PLP	O4P-C5A-C5	4.75	116.85	108.99
5	B	401	PLP	O3-C3-C2	4.88	126.14	117.66
5	B	401	PLP	O3P-P-O4P	8.41	130.79	106.56

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	257/268 (95%)	-0.02	5 (1%) 70 73	18, 38, 72, 102	0
2	B	389/397 (97%)	-0.42	0 100 100	9, 23, 44, 70	0
All	All	646/665 (97%)	-0.26	5 (0%) 87 88	9, 28, 60, 102	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	180	SER	7.9
1	A	179	ARG	7.6
1	A	268	ALA	6.0
1	A	178	SER	3.1
1	A	246	ALA	2.2

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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
5	PLP	B	401	15/16	0.99	0.08	0.20	11,23,26,27	0
4	SER	B	398	7/7	0.98	0.08	-0.14	18,20,25,25	0
3	NA	B	400	1/1	0.99	0.05	-2.91	21,21,21,21	0

6.5 Other polymers (i)

There are no such residues in this entry.