Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:28 PM GMT

PDB ID	:	1AX4
Title	:	TRYPTOPHANASE FROM PROTEUS VULGARIS
Authors	:	Isupov, M.N.; Antson, A.A.; Dodson, E.J.; Dodson, G.G.; Dementieva, I.S.; Zakomirdina, L.N.; Wilson, K.S.; Dauter, Z.; Lebedev, A.A.; Harutyunyan, E.H.
Deposited on	:	1997-10-28
Resolution	:	2.10 Å(reported)

The following versions of software and data (see references (i)) 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 2.10 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.
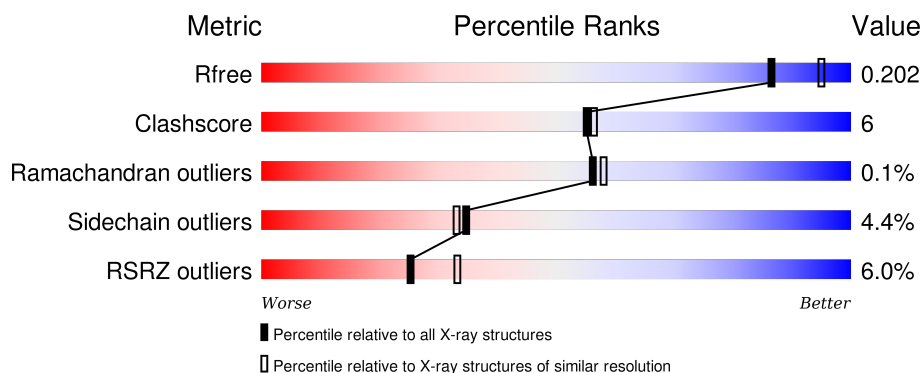
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	467	9% / 75% 22% •
1	B	467	5% / 84% 14% •
1	C	467	% / 85% 12% •
1	D	467	9% / 78% 20% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 15715 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 TRYPTOPHANASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	465	Total 3692	C 2356	N 627	O 690	P 1	S 18	0	0	0
1	B	465	Total 3693	C 2357	N 627	O 690	P 1	S 18	0	0	0
1	C	465	Total 3693	C 2357	N 627	O 690	P 1	S 18	0	0	0
1	D	465	Total 3693	C 2357	N 627	O 690	P 1	S 18	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	266	LLP	LYS	MODIFIED RESIDUE	UNP P28796
B	266	LLP	LYS	MODIFIED RESIDUE	UNP P28796
C	266	LLP	LYS	MODIFIED RESIDUE	UNP P28796
D	266	LLP	LYS	MODIFIED RESIDUE	UNP P28796

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	K 1	0	0
2	A	1	Total 1	K 1	0	0
2	D	1	Total 1	K 1	0	0
2	C	1	Total 1	K 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	225	Total 225	O 225	0	0
3	B	240	Total 240	O 240	0	0
3	C	261	Total 261	O 261	0	0
3	D	214	Total 214	O 214	0	0

3 Residue-property plots ⓘ

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: TRYPTOPHANASE
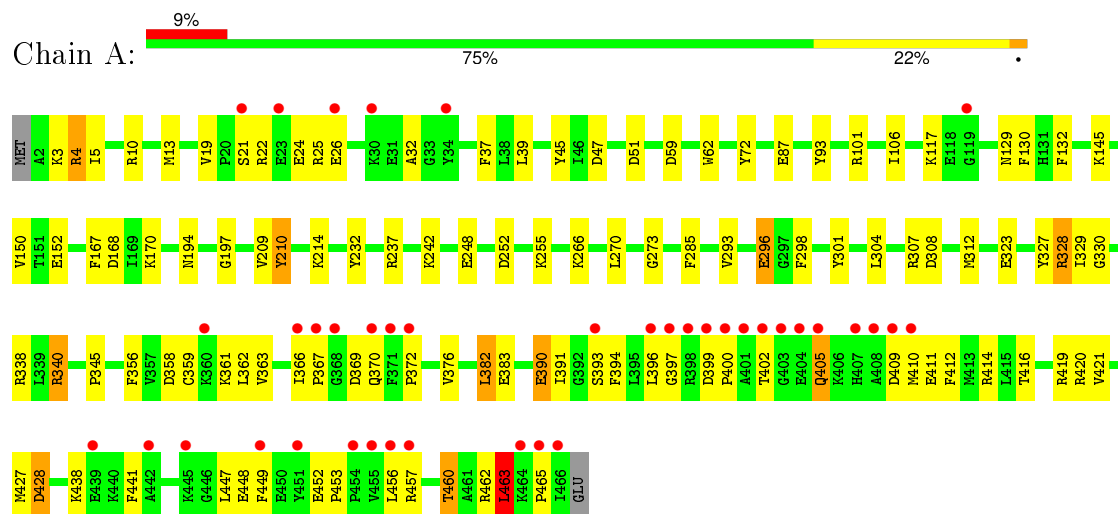
• Molecule 1: TRYPTOPHANASE

• Molecule 1: TRYPTOPHANASE

• Molecule 1: TRYPTOPHANASE

Chain D:
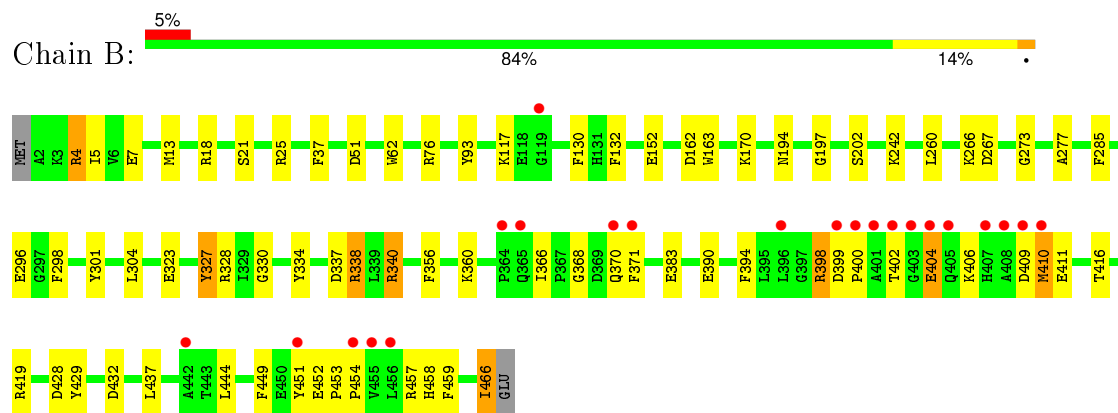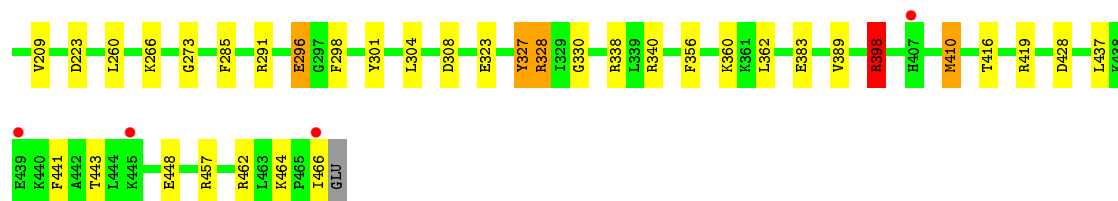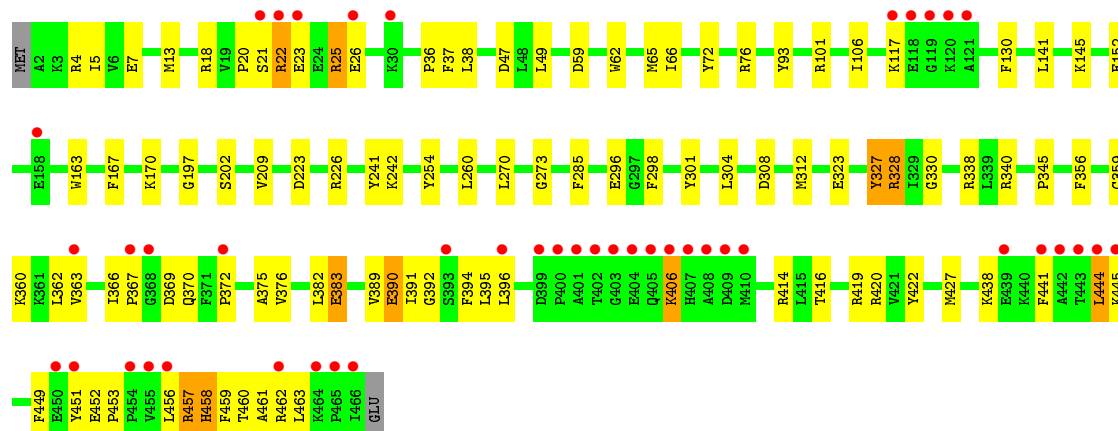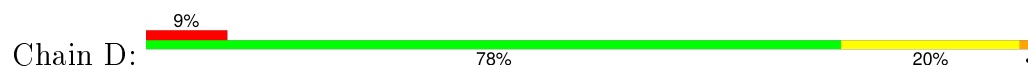
4 Data and refinement statistics (i)

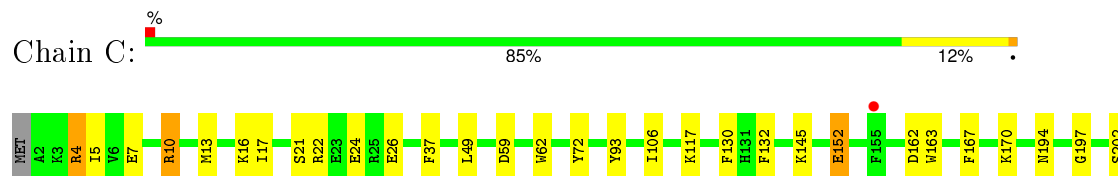| Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	114.99Å 118.23Å 153.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.00 – 2.10 17.95 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.6 (18.00-2.10) 97.0 (17.95-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	4.28 (at 2.11Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.187 , 0.227 0.168 , 0.202	Depositor DCC
R_{free} test set	2364 reflections (2.05%)	DCC
Wilson B-factor (Å^2)	17.7	Xtriage
Anisotropy	0.544	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 62.8	EDS
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Outliers	0 of 117863 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15715	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: K, 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	0.63	0/3747	1.32	34/5060 (0.7%)
1	B	0.62	0/3747	1.24	17/5060 (0.3%)
1	C	0.60	0/3747	1.20	15/5060 (0.3%)
1	D	0.61	0/3747	1.32	27/5060 (0.5%)
All	All	0.62	0/14988	1.27	93/20240 (0.5%)

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	C	0	1

There are no bond length outliers.

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	327	TYR	CB-CG-CD2	14.96	129.97	121.00
1	A	338	ARG	CD-NE-CZ	14.30	143.61	123.60
1	A	338	ARG	NE-CZ-NH1	11.60	126.10	120.30
1	D	328	ARG	NE-CZ-NH1	11.20	125.90	120.30
1	D	420	ARG	NE-CZ-NH2	-11.01	114.80	120.30
1	A	4	ARG	NE-CZ-NH1	10.66	125.63	120.30
1	B	338	ARG	NE-CZ-NH1	10.62	125.61	120.30
1	D	327	TYR	CB-CG-CD1	-10.42	114.75	121.00
1	A	25	ARG	NE-CZ-NH1	10.23	125.41	120.30
1	D	101	ARG	NE-CZ-NH2	-10.12	115.24	120.30
1	B	419	ARG	NE-CZ-NH1	9.52	125.06	120.30
1	B	340	ARG	NE-CZ-NH1	9.09	124.85	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	327	TYR	CB-CG-CD1	-8.98	115.61	121.00
1	C	419	ARG	NE-CZ-NH1	8.92	124.76	120.30
1	A	338	ARG	NE-CZ-NH2	-8.42	116.09	120.30
1	A	463	LEU	CA-CB-CG	8.35	134.50	115.30
1	B	51	ASP	CB-CG-OD2	8.14	125.63	118.30
1	B	432	ASP	CB-CG-OD1	7.99	125.49	118.30
1	C	296	GLU	OE1-CD-OE2	-7.93	113.79	123.30
1	D	328	ARG	NE-CZ-NH2	-7.91	116.35	120.30
1	D	419	ARG	NE-CZ-NH1	7.91	124.25	120.30
1	C	398	ARG	CD-NE-CZ	7.85	134.59	123.60
1	A	59	ASP	CB-CG-OD1	7.61	125.14	118.30
1	C	10	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	A	296	GLU	OE1-CD-OE2	-7.51	114.29	123.30
1	D	226	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	C	10	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	A	4	ARG	CD-NE-CZ	7.37	133.92	123.60
1	D	422	TYR	CB-CG-CD2	-7.36	116.58	121.00
1	D	427	MET	CA-CB-CG	7.34	125.77	113.30
1	B	338	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	C	59	ASP	CB-CG-OD1	7.30	124.87	118.30
1	A	51	ASP	CB-CG-OD2	7.27	124.84	118.30
1	B	398	ARG	CD-NE-CZ	7.20	133.68	123.60
1	A	328	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	B	340	ARG	NE-CZ-NH2	-7.03	116.78	120.30
1	A	248	GLU	OE1-CD-OE2	-7.02	114.87	123.30
1	A	72	TYR	CB-CG-CD1	-6.99	116.81	121.00
1	D	59	ASP	CB-CG-OD1	6.98	124.58	118.30
1	D	328	ARG	CD-NE-CZ	6.90	133.26	123.60
1	C	72	TYR	CB-CG-CD1	-6.84	116.90	121.00
1	B	419	ARG	NE-CZ-NH2	-6.83	116.88	120.30
1	A	419	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	C	328	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	A	420	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	A	59	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	D	4	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	D	25	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	D	308	ASP	CB-CG-OD1	-6.41	112.53	118.30
1	D	422	TYR	CB-CG-CD1	6.39	124.83	121.00
1	A	10	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	D	47	ASP	CB-CG-OD1	6.30	123.97	118.30
1	A	414	ARG	NE-CZ-NH1	-6.30	117.15	120.30
1	A	428	ASP	CB-CG-OD1	6.28	123.95	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	308	ASP	CB-CG-OD1	-6.25	112.68	118.30
1	A	427	MET	CA-CB-CG	6.18	123.81	113.30
1	B	337	ASP	CB-CG-OD1	-6.17	112.75	118.30
1	B	267	ASP	CB-CG-OD1	6.14	123.83	118.30
1	D	338	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	A	101	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	A	237	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	A	248	GLU	CG-CD-OE1	6.03	130.36	118.30
1	D	72	TYR	CB-CG-CD1	-5.86	117.48	121.00
1	C	327	TYR	CB-CG-CD2	5.75	124.45	121.00
1	B	296	GLU	OE1-CD-OE2	-5.73	116.43	123.30
1	D	226	ARG	NH1-CZ-NH2	-5.59	113.25	119.40
1	D	65	MET	CG-SD-CE	5.55	109.09	100.20
1	B	162	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	A	420	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	C	291	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	C	328	ARG	CD-NE-CZ	5.49	131.29	123.60
1	A	4	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	340	ARG	NE-CZ-NH1	-5.45	117.58	120.30
1	B	334	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	D	254	TYR	CA-CB-CG	-5.38	103.17	113.40
1	B	429	TYR	CB-CG-CD2	-5.37	117.78	121.00
1	D	414	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	D	457	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	A	210	TYR	CB-CG-CD1	-5.30	117.82	121.00
1	D	241	TYR	CB-CG-CD2	5.27	124.16	121.00
1	D	76	ARG	CA-CB-CG	5.23	124.91	113.40
1	A	51	ASP	CB-CG-OD1	-5.21	113.61	118.30
1	C	462	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	4	ARG	CD-NE-CZ	5.21	130.90	123.60
1	A	307	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	A	327	TYR	CB-CG-CD2	5.21	124.12	121.00
1	D	223	ASP	CB-CG-OD2	5.16	122.95	118.30
1	A	327	TYR	CB-CG-CD1	-5.15	117.91	121.00
1	A	308	ASP	CB-CG-OD1	-5.15	113.66	118.30
1	C	4	ARG	CD-NE-CZ	5.14	130.80	123.60
1	A	168	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	B	327	TYR	CB-CG-CD2	5.06	124.04	121.00
1	A	47	ASP	CB-CG-OD1	5.02	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	162	ASP	Mainchain

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	3692	0	3659	66	0
1	B	3693	0	3661	37	0
1	C	3693	0	3662	43	0
1	D	3693	0	3661	56	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	225	0	0	4	0
3	B	240	0	0	3	0
3	C	261	0	0	4	0
3	D	214	0	0	4	0
All	All	15715	0	14643	184	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (184) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ARG:HH21	1:C:4:ARG:NH2	1.11	1.48
1:A:4:ARG:NH2	1:C:4:ARG:NH2	1.67	1.41
1:A:4:ARG:NH2	1:C:4:ARG:HH21	1.16	1.36
1:A:266:LLP:C4	1:A:266:LLP:NZ	2.34	0.90
1:A:26:GLU:HG3	1:A:382:LEU:HD21	1.52	0.89
1:C:383:GLU:HG2	1:C:437:LEU:HD21	1.56	0.85
1:A:4:ARG:NH2	1:C:4:ARG:CZ	2.43	0.81
1:B:453:PRO:HG2	1:B:457:ARG:HA	1.64	0.78
1:D:145:LYS:HE3	3:D:615:HOH:O	1.85	0.77
1:D:141:LEU:HG	3:D:692:HOH:O	1.85	0.76
1:C:266:LLP:H4'1	3:C:589:HOH:O	1.84	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ARG:CZ	1:C:4:ARG:NH2	2.49	0.75
1:A:399:ASP:HB3	1:A:402:THR:OG1	1.94	0.68
1:A:453:PRO:HG2	1:A:460:THR:HB	1.74	0.68
1:B:383:GLU:HG3	1:B:437:LEU:HD21	1.74	0.67
1:A:410:MET:HB2	3:A:723:HOH:O	1.94	0.67
1:D:453:PRO:HG2	1:D:457:ARG:HA	1.76	0.67
1:D:375:ALA:HB1	1:D:444:LEU:HD22	1.76	0.65
1:A:197:GLY:HA2	1:A:356:PHE:CE1	2.32	0.65
1:B:197:GLY:HA2	1:B:356:PHE:CE1	2.32	0.64
1:D:367:PRO:HG2	1:D:370:GLN:HG3	1.80	0.63
1:D:390:GLU:O	1:D:391:ILE:HD13	1.98	0.63
1:C:145:LYS:HE3	3:C:698:HOH:O	1.99	0.62
1:A:87:GLU:HB2	3:A:643:HOH:O	2.00	0.62
1:D:197:GLY:HA2	1:D:356:PHE:CE1	2.35	0.62
1:D:366:ILE:HD11	1:D:444:LEU:HB3	1.83	0.61
1:B:383:GLU:HG2	3:B:668:HOH:O	2.00	0.61
1:D:445:LYS:HD2	1:D:445:LYS:H	1.65	0.61
1:C:197:GLY:HA2	1:C:356:PHE:CE1	2.37	0.60
1:A:399:ASP:OD1	1:A:400:PRO:HD2	2.02	0.60
1:D:20:PRO:HG2	1:D:25:ARG:HG2	1.82	0.60
1:B:402:THR:HB	1:B:404:GLU:HG2	1.84	0.59
1:A:359:CYS:HA	1:A:362:LEU:HG	1.84	0.59
1:D:458:HIS:H	1:D:458:HIS:CD2	2.20	0.59
1:C:448:GLU:HG3	1:C:466:ILE:HG13	1.84	0.59
1:B:410:MET:SD	3:B:705:HOH:O	2.57	0.59
1:B:370:GLN:NE2	1:B:466:ILE:HD13	2.18	0.58
1:D:21:SER:O	1:D:25:ARG:HG3	2.04	0.58
1:A:4:ARG:CZ	1:C:4:ARG:CZ	2.82	0.57
1:C:152:GLU:HG2	3:C:646:HOH:O	2.05	0.56
1:A:32:ALA:HB2	1:A:39:LEU:HD23	1.88	0.56
1:D:26:GLU:HG2	1:D:382:LEU:HD22	1.89	0.55
1:A:394:PHE:CZ	1:A:463:LEU:HD21	2.42	0.55
1:A:21:SER:OG	1:A:24:GLU:HG3	2.07	0.55
1:D:396:LEU:HD23	1:D:406:LYS:HB3	1.89	0.54
1:D:438:LYS:HA	1:D:441:PHE:CD2	2.42	0.54
1:C:340:ARG:HD3	3:C:645:HOH:O	2.06	0.53
1:D:345:PRO:HD2	1:D:362:LEU:HD21	1.90	0.53
1:A:4:ARG:HH21	1:C:4:ARG:HH21	0.75	0.53
1:A:4:ARG:NH1	1:A:428:ASP:OD2	2.41	0.53
1:C:22:ARG:O	1:C:26:GLU:HG3	2.09	0.53
1:D:451:TYR:HB3	1:D:462:ARG:HG3	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:TYR:HB3	1:D:285:PHE:CD1	2.44	0.53
1:D:362:LEU:O	1:D:441:PHE:HB3	2.09	0.52
1:A:5:ILE:HD12	1:A:330:GLY:HA3	1.91	0.52
1:A:438:LYS:HA	1:A:441:PHE:CD2	2.43	0.52
1:C:448:GLU:HG3	1:C:466:ILE:CG1	2.39	0.52
1:D:340:ARG:HD3	3:D:676:HOH:O	2.10	0.52
1:A:397:GLY:HA2	1:A:457:ARG:HH11	1.74	0.52
1:A:390:GLU:O	1:A:391:ILE:HD13	2.09	0.52
1:D:5:ILE:HD12	1:D:330:GLY:HA3	1.92	0.51
1:A:456:LEU:HD23	1:A:460:THR:OG1	2.10	0.51
1:A:323:GLU:H	1:A:323:GLU:CD	2.14	0.51
1:A:145:LYS:HE3	3:A:671:HOH:O	2.11	0.51
1:A:447:LEU:HD23	1:A:465:PRO:HA	1.93	0.50
1:C:398:ARG:HG2	1:C:398:ARG:HH11	1.76	0.50
1:D:38:LEU:HD21	1:D:460:THR:HA	1.93	0.50
1:B:13:MET:HE2	1:D:62:TRP:CG	2.47	0.49
1:C:410:MET:HE2	1:C:410:MET:HA	1.94	0.49
1:B:7:GLU:HG3	1:B:327:TYR:CZ	2.47	0.49
1:A:366:ILE:HG22	1:A:372:PRO:HD3	1.94	0.49
1:B:398:ARG:HH11	1:B:398:ARG:HG2	1.77	0.49
1:A:359:CYS:HB3	1:A:376:VAL:HG21	1.94	0.49
1:A:449:PHE:CD1	1:A:463:LEU:HD22	2.46	0.49
1:A:22:ARG:HH21	1:A:382:LEU:HD22	1.77	0.49
1:D:395:LEU:HG	1:D:395:LEU:O	2.12	0.49
1:C:93:TYR:HB3	1:C:285:PHE:CD1	2.47	0.49
1:B:93:TYR:HB3	1:B:285:PHE:CD1	2.48	0.49
1:B:21:SER:O	1:B:25:ARG:HG3	2.13	0.49
1:B:197:GLY:HA2	1:B:356:PHE:CZ	2.48	0.48
1:B:323:GLU:CD	1:B:323:GLU:H	2.16	0.48
1:C:7:GLU:HG3	1:C:327:TYR:CZ	2.49	0.48
1:B:451:TYR:OH	1:B:453:PRO:HB3	2.13	0.48
1:A:345:PRO:HD2	1:A:362:LEU:HD21	1.95	0.48
1:C:5:ILE:HD12	1:C:330:GLY:HA3	1.95	0.48
1:D:7:GLU:HG3	1:D:327:TYR:CZ	2.48	0.48
1:D:106:ILE:HD11	1:D:296:GLU:HG3	1.96	0.48
1:A:369:ASP:HA	1:A:405:GLN:HE21	1.78	0.48
1:A:453:PRO:CG	1:A:460:THR:HB	2.43	0.48
1:D:21:SER:HG	1:D:23:GLU:HG2	1.79	0.48
1:D:451:TYR:HB3	1:D:462:ARG:HB2	1.96	0.48
1:B:5:ILE:HD12	1:B:330:GLY:HA3	1.95	0.47
1:A:210:TYR:CE1	1:A:214:LYS:HE3	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:390:GLU:OE1	1:D:392:GLY:N	2.45	0.47
1:A:62:TRP:CG	1:C:13:MET:HE2	2.49	0.47
1:B:360:LYS:HD2	1:B:411:GLU:HG2	1.97	0.47
1:D:449:PHE:CD1	1:D:452:GLU:HB2	2.49	0.47
1:B:163:TRP:CD2	1:B:202:SER:HB3	2.49	0.47
1:A:421:VAL:CG1	1:C:10:ARG:HD2	2.44	0.47
1:A:62:TRP:CD1	1:C:13:MET:HE2	2.50	0.47
1:C:106:ILE:HD11	1:C:296:GLU:HG3	1.96	0.46
1:B:260:LEU:HG	1:B:277:ALA:HB3	1.96	0.46
1:B:266:LLP:H4'1	3:B:583:HOH:O	2.15	0.46
1:D:22:ARG:HH21	1:D:382:LEU:HD13	1.81	0.46
1:D:167:PHE:CD1	1:D:209:VAL:HG21	2.50	0.46
1:C:383:GLU:HG2	1:C:437:LEU:CD2	2.38	0.46
1:A:19:VAL:HG22	1:A:45:TYR:CD2	2.50	0.46
1:C:16:LYS:HG2	1:C:17:ILE:N	2.30	0.46
1:A:273:GLY:HA2	1:A:304:LEU:HD21	1.97	0.46
1:D:359:CYS:HB3	1:D:376:VAL:HG21	1.97	0.45
1:A:197:GLY:HA2	1:A:356:PHE:CZ	2.52	0.45
1:D:163:TRP:CD2	1:D:202:SER:HB3	2.50	0.45
1:D:36:PRO:HB2	3:D:610:HOH:O	2.16	0.45
1:B:371:PHE:CE1	1:B:394:PHE:HA	2.51	0.45
1:A:106:ILE:HD11	1:A:296:GLU:HG3	1.98	0.45
1:A:132:PHE:HD1	1:A:194:ASN:HD22	1.65	0.45
1:B:62:TRP:CG	1:D:13:MET:HE2	2.52	0.45
1:C:21:SER:OG	1:C:24:GLU:HG3	2.17	0.45
1:A:167:PHE:CD1	1:A:209:VAL:HG21	2.52	0.44
1:D:394:PHE:CZ	1:D:463:LEU:HD21	2.52	0.44
1:B:366:ILE:HD11	1:B:444:LEU:O	2.16	0.44
1:D:21:SER:OG	1:D:23:GLU:HG2	2.18	0.44
1:B:4:ARG:NH1	1:B:428:ASP:OD2	2.49	0.44
1:A:372:PRO:HG3	1:A:411:GLU:HG3	1.99	0.44
1:A:448:GLU:O	1:A:463:LEU:HB3	2.18	0.44
1:A:396:LEU:HA	1:A:396:LEU:HD12	1.83	0.44
1:B:399:ASP:OD1	1:B:400:PRO:HD2	2.18	0.44
1:C:197:GLY:HA2	1:C:356:PHE:CZ	2.52	0.44
1:B:13:MET:HE2	1:D:62:TRP:CD1	2.52	0.44
1:C:163:TRP:CD2	1:C:202:SER:HB3	2.53	0.44
1:C:49:LEU:HD12	1:C:389:VAL:HB	1.99	0.44
1:D:372:PRO:O	1:D:376:VAL:HG23	2.18	0.43
1:C:323:GLU:CD	1:C:323:GLU:H	2.22	0.43
1:D:273:GLY:HA2	1:D:304:LEU:HD21	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:VAL:HG11	1:B:459:PHE:CE2	2.54	0.43
1:D:323:GLU:H	1:D:323:GLU:CD	2.21	0.43
1:A:358:ASP:O	1:A:362:LEU:HG	2.19	0.43
1:B:132:PHE:HD1	1:B:194:ASN:HD22	1.65	0.43
1:A:13:MET:HE2	1:C:62:TRP:CG	2.54	0.43
1:B:449:PHE:CZ	1:B:457:ARG:NH1	2.87	0.42
1:B:449:PHE:CZ	1:B:457:ARG:HD2	2.54	0.42
1:D:22:ARG:NH2	1:D:382:LEU:HB3	2.34	0.42
1:A:298:PHE:HB3	1:A:301:TYR:CE2	2.54	0.42
1:A:13:MET:HE2	1:C:62:TRP:CD1	2.54	0.42
1:B:273:GLY:HA2	1:B:304:LEU:HD21	2.01	0.42
1:D:457:ARG:O	1:D:461:ALA:N	2.39	0.42
1:D:340:ARG:HD3	1:D:340:ARG:HH11	1.64	0.42
1:C:273:GLY:HA2	1:C:304:LEU:HD21	2.00	0.42
1:A:93:TYR:HB3	1:A:285:PHE:CD1	2.54	0.42
1:D:456:LEU:HD22	1:D:459:PHE:HD2	1.84	0.42
1:A:232:TYR:CD2	1:A:329:ILE:HD13	2.54	0.42
1:C:298:PHE:HB3	1:C:301:TYR:CE2	2.54	0.42
1:B:449:PHE:CD1	1:B:452:GLU:HB2	2.54	0.42
1:A:397:GLY:HA2	1:A:457:ARG:NH1	2.34	0.42
1:A:393:SER:HB2	1:A:405:GLN:HE22	1.85	0.42
1:A:449:PHE:CD1	1:A:452:GLU:HB2	2.55	0.42
1:D:22:ARG:NH1	1:D:383:GLU:OE2	2.49	0.41
1:D:49:LEU:HD12	1:D:389:VAL:HB	2.02	0.41
1:D:298:PHE:HB3	1:D:301:TYR:CE2	2.55	0.41
1:A:367:PRO:O	1:A:372:PRO:HD3	2.21	0.41
1:A:252:ASP:O	1:A:255:LYS:HB2	2.21	0.41
1:A:369:ASP:HA	1:A:405:GLN:NE2	2.35	0.41
1:B:453:PRO:HA	1:B:454:PRO:HD3	1.88	0.41
1:B:260:LEU:C	1:B:260:LEU:HD12	2.41	0.41
1:D:260:LEU:HD12	1:D:260:LEU:C	2.41	0.41
1:A:367:PRO:HG2	1:A:370:GLN:HG3	2.02	0.41
1:C:132:PHE:HD1	1:C:194:ASN:HD22	1.69	0.41
1:C:4:ARG:NH1	1:C:428:ASP:OD2	2.53	0.41
1:C:223:ASP:OD1	1:C:266:LLP:H2'2	2.21	0.41
1:D:396:LEU:HA	1:D:396:LEU:HD12	1.96	0.41
1:D:394:PHE:CE1	1:D:463:LEU:HD21	2.56	0.41
1:B:298:PHE:HB3	1:B:301:TYR:CE1	2.56	0.41
1:C:62:TRP:CZ3	1:D:66:ILE:HD13	2.56	0.41
1:C:167:PHE:CD1	1:C:209:VAL:HG21	2.56	0.41
1:A:129:ASN:O	1:A:150:VAL:HB	2.22	0.40

Continued on next page...

Full wwPDB X-ray Structure Validation Report

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:LEU:HD11	1:A:312:MET:HA	2.02	0.40
1:D:270:LEU:HD11	1:D:312:MET:HA	2.03	0.40
1:B:62:TRP:CD1	1:D:13:MET:HE2	2.55	0.40
1:A:340:ARG:HD3	1:A:340:ARG:HH11	1.68	0.40
1:A:3:LYS:CE	3:A:651:HOH:O	2.69	0.40
1:B:76:ARG:HH11	1:B:76:ARG:HG3	1.85	0.40
1:C:362:LEU:HD13	1:C:441:PHE:CZ	2.57	0.40
1:D:367:PRO:HG2	1:D:369:ASP:OD1	2.22	0.40
1:C:260:LEU:HD12	1:C:260:LEU:C	2.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	462/467 (99%)	440 (95%)	22 (5%)	0	100	100
1	B	462/467 (99%)	439 (95%)	21 (4%)	2 (0%)	39	37
1	C	462/467 (99%)	446 (96%)	16 (4%)	0	100	100
1	D	462/467 (99%)	442 (96%)	20 (4%)	0	100	100
All	All	1848/1868 (99%)	1767 (96%)	79 (4%)	2 (0%)	56	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	409	ASP
1	B	368	GLY

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	383/385 (100%)	364 (95%)	19 (5%)	30	27
1	B	383/385 (100%)	366 (96%)	17 (4%)	35	33
1	C	383/385 (100%)	369 (96%)	14 (4%)	41	41
1	D	383/385 (100%)	366 (96%)	17 (4%)	35	33
All	All	1532/1540 (100%)	1465 (96%)	67 (4%)	35	33

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	PHE
1	A	117	LYS
1	A	130	PHE
1	A	152	GLU
1	A	170	LYS
1	A	242	LYS
1	A	328	ARG
1	A	361	LYS
1	A	363	VAL
1	A	382	LEU
1	A	383	GLU
1	A	390	GLU
1	A	405	GLN
1	A	409	ASP
1	A	412	PHE
1	A	416	THR
1	A	460	THR
1	A	462	ARG
1	A	463	LEU
1	B	18	ARG
1	B	37	PHE
1	B	117	LYS
1	B	130	PHE
1	B	152	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	170	LYS
1	B	242	LYS
1	B	328	ARG
1	B	338	ARG
1	B	340	ARG
1	B	390	GLU
1	B	404	GLU
1	B	406	LYS
1	B	410	MET
1	B	416	THR
1	B	458	HIS
1	B	466	ILE
1	C	37	PHE
1	C	117	LYS
1	C	130	PHE
1	C	152	GLU
1	C	170	LYS
1	C	328	ARG
1	C	338	ARG
1	C	360	LYS
1	C	398	ARG
1	C	410	MET
1	C	416	THR
1	C	443	THR
1	C	457	ARG
1	C	464	LYS
1	D	18	ARG
1	D	22	ARG
1	D	37	PHE
1	D	117	LYS
1	D	130	PHE
1	D	152	GLU
1	D	170	LYS
1	D	242	LYS
1	D	328	ARG
1	D	360	LYS
1	D	363	VAL
1	D	383	GLU
1	D	390	GLU
1	D	406	LYS
1	D	416	THR
1	D	444	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	458	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	194	ASN
1	A	374	GLN
1	A	378	ASN
1	B	194	ASN
1	C	194	ASN
1	D	194	ASN
1	D	458	HIS

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

4 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	$\#|Z| > 2$
1	LLP	A	266	1	20,22,25	1.71	5 (25%)	23,28,34	1.80	6 (26%)
1	LLP	B	266	1	23,24,25	1.37	3 (13%)	28,32,34	1.81	9 (32%)
1	LLP	C	266	1	23,24,25	1.44	4 (17%)	28,32,34	1.92	6 (21%)
1	LLP	D	266	1	23,24,25	1.38	4 (17%)	28,32,34	1.69	8 (28%)

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
1	LLP	A	266	1	-	0/11/13/19	0/1/1/1
1	LLP	B	266	1	-	0/15/17/19	0/1/1/1
1	LLP	C	266	1	-	0/15/17/19	0/1/1/1
1	LLP	D	266	1	-	0/15/17/19	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	266	LLP	O3-C3	-4.09	1.27	1.37
1	B	266	LLP	O3-C3	-3.51	1.28	1.37
1	A	266	LLP	O3-C3	-3.02	1.30	1.36
1	D	266	LLP	O3-C3	-2.76	1.30	1.37
1	A	266	LLP	P-OP3	-2.33	1.46	1.54
1	B	266	LLP	P-OP3	-2.01	1.47	1.54
1	D	266	LLP	P-OP3	-2.00	1.47	1.54
1	D	266	LLP	C2-N1	2.01	1.38	1.34
1	C	266	LLP	C2'-C2	2.15	1.54	1.50
1	A	266	LLP	C4-C5	2.25	1.43	1.39
1	C	266	LLP	C2-N1	2.28	1.38	1.34
1	D	266	LLP	C2'-C2	2.33	1.55	1.50
1	C	266	LLP	C4-C3	2.47	1.43	1.40
1	A	266	LLP	C2'-C2	2.64	1.55	1.50
1	B	266	LLP	C2'-C2	3.22	1.56	1.50
1	A	266	LLP	C4-C3	3.87	1.44	1.38

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	266	LLP	C3-C4-C5	-5.31	114.13	118.11
1	A	266	LLP	C3-C4-C5	-4.55	115.31	120.83
1	B	266	LLP	O-C-CA	-3.57	116.20	125.49
1	C	266	LLP	O-C-CA	-3.51	116.34	125.49
1	B	266	LLP	C5-C6-N1	-3.35	118.04	123.86
1	D	266	LLP	C5-C6-N1	-3.08	118.52	123.86
1	D	266	LLP	O-C-CA	-2.74	118.35	125.49
1	D	266	LLP	C3-C2-N1	-2.56	117.07	120.61
1	D	266	LLP	OP3-P-OP1	-2.43	102.75	110.58
1	B	266	LLP	C3-C2-N1	-2.43	117.25	120.61
1	A	266	LLP	O-C-CA	-2.29	119.53	125.49
1	B	266	LLP	C4-C4'-NZ	-2.24	112.60	125.06
1	C	266	LLP	C3-C2-N1	-2.24	117.52	120.61
1	B	266	LLP	CD-CE-NZ	-2.11	107.53	110.98
1	A	266	LLP	C5-C6-N1	-2.02	120.36	123.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	266	LLP	OP2-P-OP4	-2.01	100.79	106.56
1	A	266	LLP	OP3-P-OP4	2.20	112.89	106.56
1	B	266	LLP	OP3-P-OP2	2.27	116.03	107.38
1	D	266	LLP	O3-C3-C2	2.33	121.71	117.66
1	D	266	LLP	OP3-P-OP2	2.51	116.93	107.38
1	C	266	LLP	C3-C4-C4'	2.55	123.46	120.16
1	D	266	LLP	C6-N1-C2	2.62	124.63	119.28
1	C	266	LLP	OP3-P-OP4	2.91	114.94	106.56
1	D	266	LLP	CE-NZ-C4'	2.96	127.51	118.97
1	A	266	LLP	OP3-P-OP2	3.04	118.96	107.38
1	B	266	LLP	C6-N1-C2	3.23	125.86	119.28
1	A	266	LLP	C4-C5-C6	4.01	120.94	116.57
1	B	266	LLP	CE-NZ-C4'	4.32	131.45	118.97
1	C	266	LLP	CE-NZ-C4'	5.02	133.47	118.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	266	LLP	1	0
1	B	266	LLP	1	0
1	C	266	LLP	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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(Å²)	Q<0.9
1	A	464/467 (99%)	0.04	40 (8%)	13	18	8, 21, 64, 89	0
1	B	464/467 (99%)	-0.35	22 (4%)	35	44	8, 21, 64, 89	0
1	C	464/467 (99%)	-0.47	5 (1%)	82	86	8, 21, 64, 88	0
1	D	464/467 (99%)	-0.10	44 (9%)	10	14	7, 22, 64, 89	0
All	All	1856/1868 (99%)	-0.22	111 (5%)	25	33	7, 21, 65, 89	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	401	ALA	11.3
1	A	400	PRO	9.6
1	A	401	ALA	8.1
1	D	456	LEU	7.9
1	B	403	GLY	7.8
1	D	407	HIS	7.7
1	A	399	ASP	6.9
1	D	400	PRO	6.6
1	A	456	LEU	6.4
1	B	407	HIS	6.1
1	D	402	THR	6.0
1	A	403	GLY	5.9
1	A	451	TYR	5.9
1	B	402	THR	5.9
1	B	401	ALA	5.7
1	A	404	GLU	5.6
1	A	407	HIS	5.5
1	D	405	GLN	5.4
1	D	404	GLU	5.4
1	D	442	ALA	5.2
1	A	402	THR	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	372	PRO	4.6
1	D	118	GLU	4.2
1	B	456	LEU	4.2
1	B	365	GLN	4.1
1	A	23	GLU	4.1
1	A	393	SER	4.1
1	A	455	VAL	4.1
1	A	445	LYS	4.0
1	B	404	GLU	4.0
1	A	396	LEU	3.9
1	A	398	ARG	3.9
1	A	405	GLN	3.8
1	A	466	ILE	3.8
1	A	439	GLU	3.8
1	A	366	ILE	3.8
1	D	454	PRO	3.7
1	B	399	ASP	3.7
1	D	399	ASP	3.7
1	B	396	LEU	3.6
1	B	119	GLY	3.6
1	A	454	PRO	3.6
1	D	23	GLU	3.5
1	C	445	LYS	3.5
1	D	121	ALA	3.5
1	D	465	PRO	3.4
1	A	408	ALA	3.4
1	A	397	GLY	3.4
1	B	410	MET	3.3
1	D	393	SER	3.3
1	A	34	TYR	3.3
1	A	30	LYS	3.3
1	D	451	TYR	3.2
1	D	410	MET	3.2
1	B	400	PRO	3.1
1	A	409	ASP	3.1
1	A	465	PRO	3.1
1	D	408	ALA	3.1
1	D	444	LEU	3.0
1	D	439	GLU	3.0
1	B	442	ALA	3.0
1	B	364	PRO	2.9
1	D	403	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	155	PHE	2.9
1	A	457	ARG	2.9
1	A	410	MET	2.9
1	D	372	PRO	2.9
1	A	26	GLU	2.8
1	D	120	LYS	2.8
1	B	451	TYR	2.8
1	A	449	PHE	2.8
1	C	407	HIS	2.7
1	D	396	LEU	2.7
1	A	464	LYS	2.7
1	D	450	GLU	2.7
1	D	26	GLU	2.6
1	D	22	ARG	2.6
1	A	442	ALA	2.6
1	A	370	GLN	2.6
1	D	409	ASP	2.6
1	D	367	PRO	2.6
1	D	466	ILE	2.5
1	D	455	VAL	2.5
1	D	368	GLY	2.5
1	D	464	LYS	2.5
1	D	21	SER	2.5
1	D	443	THR	2.4
1	D	445	LYS	2.4
1	D	406	LYS	2.4
1	D	117	LYS	2.4
1	A	21	SER	2.4
1	B	408	ALA	2.4
1	A	367	PRO	2.3
1	D	158	GLU	2.3
1	A	119	GLY	2.3
1	A	371	PHE	2.3
1	D	30	LYS	2.3
1	D	119	GLY	2.3
1	B	409	ASP	2.2
1	C	466	ILE	2.2
1	A	360	LYS	2.2
1	D	462	ARG	2.2
1	D	441	PHE	2.2
1	B	405	GLN	2.1
1	B	454	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	370	GLN	2.1
1	B	371	PHE	2.1
1	C	439	GLU	2.1
1	B	455	VAL	2.1
1	A	368	GLY	2.0
1	D	363	VAL	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
1	LLP	A	266	23/25	0.97	0.08	-	7,12,17,19	0
1	LLP	B	266	24/25	0.98	0.06	-	7,12,18,21	0
1	LLP	C	266	24/25	0.98	0.08	-	7,12,18,21	0
1	LLP	D	266	24/25	0.98	0.06	-	7,12,18,22	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
2	K	C	500	1/1	1.00	0.03	-1.96	10,10,10,10	0
2	K	B	500	1/1	1.00	0.02	-2.76	10,10,10,10	0
2	K	A	500	1/1	1.00	0.02	-3.83	12,12,12,12	0
2	K	D	500	1/1	1.00	0.03	-4.46	12,12,12,12	0

6.5 Other polymers (i)

There are no such residues in this entry.