wwPDB X-ray Structure Validation Summary Report (i)

Oct 11, 2016 – 02:27 PM EDT

PDB ID	:	5F8V
Title	:	Crystal structure of PLP bound phosphoserine aminotransferase (PSAT) from Trichomonas vaginalis
Authors	:	Singh, R.K.; Gourinath, S.
Deposited on	:	2015-12-09
Resolution	:	2.14 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

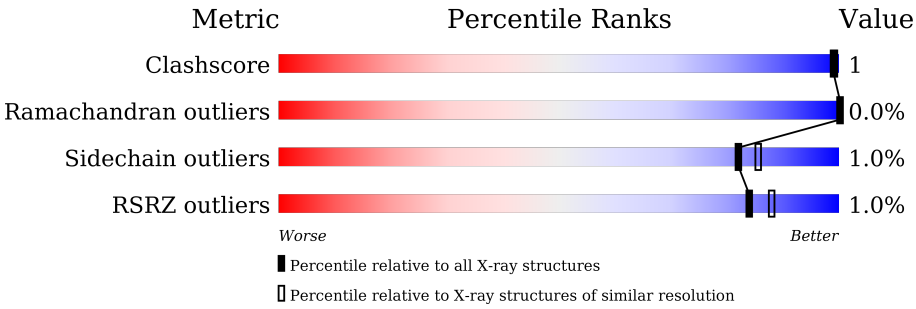
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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	1824 (2.16-2.12)
Ramachandran outliers	100387	1798 (2.16-2.12)
Sidechain outliers	100360	1798 (2.16-2.12)
RSRZ outliers	91569	1699 (2.16-2.12)

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	379	94%
1	B	379	2% 95%
1	C	379	92%
1	D	379	% 93%
1	E	379	2% 94%
1	F	379	% 88% 9%
1	G	379	94%

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Mol	Chain	Length	Quality of chain
1	H	379	2% 94%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 23601 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 Aminotransferase, class V family protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	367	2933	1878	499	531	1	24	0	0	0
1	E	364	2898	1852	495	526	1	24	0	0	0
1	B	367	2895	1854	492	524	1	24	0	0	0
1	C	363	2830	1809	483	513	1	24	0	0	0
1	D	367	2886	1848	495	518	1	24	0	0	0
1	F	343	2680	1723	452	481	1	23	0	0	0
1	G	367	2887	1854	495	513	1	24	0	0	0
1	H	366	2843	1825	483	510	1	24	0	0	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	372	LEU	-	expression tag	UNP A2DW27
A	373	GLU	-	expression tag	UNP A2DW27
A	374	HIS	-	expression tag	UNP A2DW27
A	375	HIS	-	expression tag	UNP A2DW27
A	376	HIS	-	expression tag	UNP A2DW27
A	377	HIS	-	expression tag	UNP A2DW27
A	378	HIS	-	expression tag	UNP A2DW27
A	379	HIS	-	expression tag	UNP A2DW27
E	372	LEU	-	expression tag	UNP A2DW27
E	373	GLU	-	expression tag	UNP A2DW27
E	374	HIS	-	expression tag	UNP A2DW27
E	375	HIS	-	expression tag	UNP A2DW27
E	376	HIS	-	expression tag	UNP A2DW27

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Chain	Residue	Modelled	Actual	Comment	Reference
E	377	HIS	-	expression tag	UNP A2DW27
E	378	HIS	-	expression tag	UNP A2DW27
E	379	HIS	-	expression tag	UNP A2DW27
B	372	LEU	-	expression tag	UNP A2DW27
B	373	GLU	-	expression tag	UNP A2DW27
B	374	HIS	-	expression tag	UNP A2DW27
B	375	HIS	-	expression tag	UNP A2DW27
B	376	HIS	-	expression tag	UNP A2DW27
B	377	HIS	-	expression tag	UNP A2DW27
B	378	HIS	-	expression tag	UNP A2DW27
B	379	HIS	-	expression tag	UNP A2DW27
C	372	LEU	-	expression tag	UNP A2DW27
C	373	GLU	-	expression tag	UNP A2DW27
C	374	HIS	-	expression tag	UNP A2DW27
C	375	HIS	-	expression tag	UNP A2DW27
C	376	HIS	-	expression tag	UNP A2DW27
C	377	HIS	-	expression tag	UNP A2DW27
C	378	HIS	-	expression tag	UNP A2DW27
C	379	HIS	-	expression tag	UNP A2DW27
D	372	LEU	-	expression tag	UNP A2DW27
D	373	GLU	-	expression tag	UNP A2DW27
D	374	HIS	-	expression tag	UNP A2DW27
D	375	HIS	-	expression tag	UNP A2DW27
D	376	HIS	-	expression tag	UNP A2DW27
D	377	HIS	-	expression tag	UNP A2DW27
D	378	HIS	-	expression tag	UNP A2DW27
D	379	HIS	-	expression tag	UNP A2DW27
F	372	LEU	-	expression tag	UNP A2DW27
F	373	GLU	-	expression tag	UNP A2DW27
F	374	HIS	-	expression tag	UNP A2DW27
F	375	HIS	-	expression tag	UNP A2DW27
F	376	HIS	-	expression tag	UNP A2DW27
F	377	HIS	-	expression tag	UNP A2DW27
F	378	HIS	-	expression tag	UNP A2DW27
F	379	HIS	-	expression tag	UNP A2DW27
G	372	LEU	-	expression tag	UNP A2DW27
G	373	GLU	-	expression tag	UNP A2DW27
G	374	HIS	-	expression tag	UNP A2DW27
G	375	HIS	-	expression tag	UNP A2DW27
G	376	HIS	-	expression tag	UNP A2DW27
G	377	HIS	-	expression tag	UNP A2DW27
G	378	HIS	-	expression tag	UNP A2DW27

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Chain	Residue	Modelled	Actual	Comment	Reference
G	379	HIS	-	expression tag	UNP A2DW27
H	372	LEU	-	expression tag	UNP A2DW27
H	373	GLU	-	expression tag	UNP A2DW27
H	374	HIS	-	expression tag	UNP A2DW27
H	375	HIS	-	expression tag	UNP A2DW27
H	376	HIS	-	expression tag	UNP A2DW27
H	377	HIS	-	expression tag	UNP A2DW27
H	378	HIS	-	expression tag	UNP A2DW27
H	379	HIS	-	expression tag	UNP A2DW27

- Molecule 2 is water.

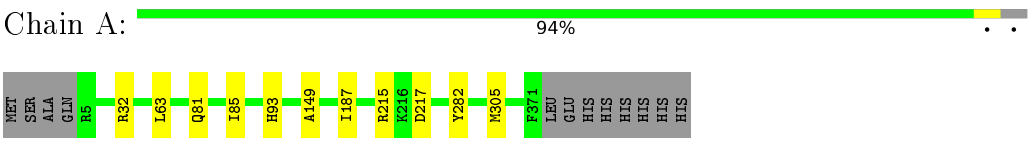
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	122	122	122	0	0
			Total	O		
2	E	50	50	50	0	0
			Total	O		
2	B	98	98	98	0	0
			Total	O		
2	C	41	41	41	0	0
			Total	O		
2	D	126	126	126	0	0
			Total	O		
2	F	77	77	77	0	0
			Total	O		
2	G	147	147	147	0	0
			Total	O		
2	H	88	88	88	0	0

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.

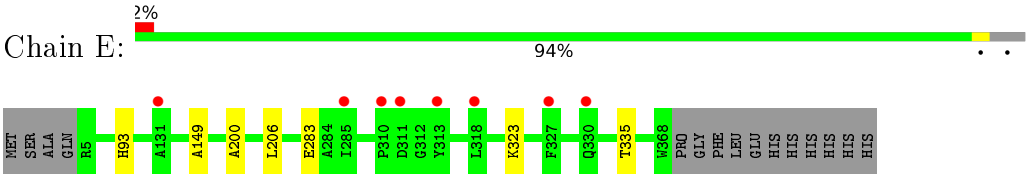
- Molecule 1: Aminotransferase, class V family protein

Chain A:



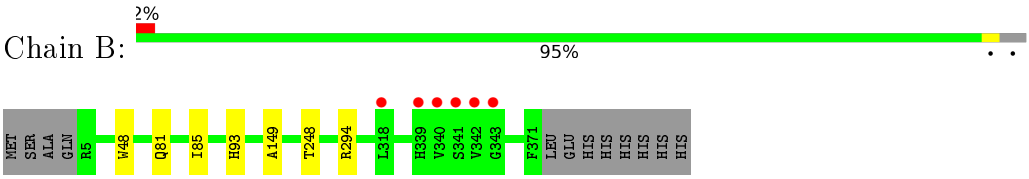
- Molecule 1: Aminotransferase, class V family protein

Chain E:



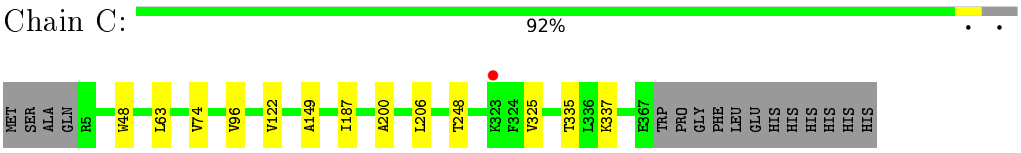
- Molecule 1: Aminotransferase, class V family protein

Chain B:



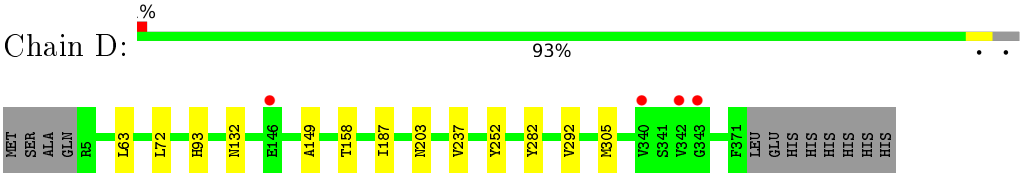
- Molecule 1: Aminotransferase, class V family protein

Chain C:



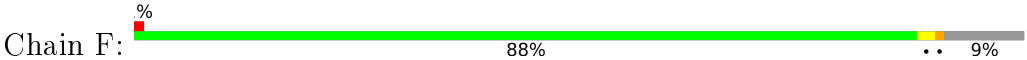
- Molecule 1: Aminotransferase, class V family protein

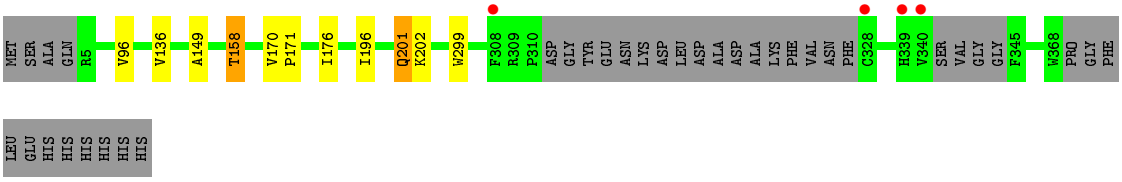
Chain D:



- Molecule 1: Aminotransferase, class V family protein

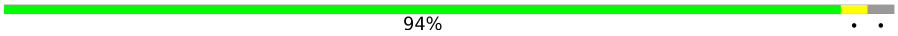
Chain F:

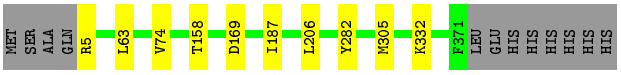




- Molecule 1: Aminotransferase, class V family protein

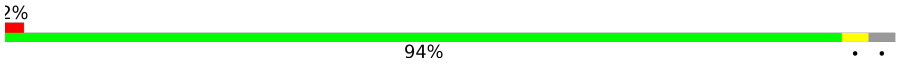
Chain G:

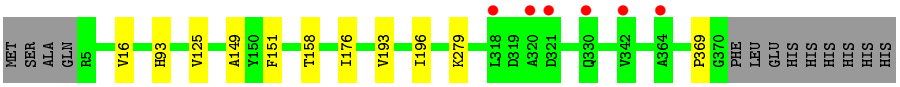




- Molecule 1: Aminotransferase, class V family protein

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	51.97Å 235.43Å 134.52Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	37.42 – 2.14 37.42 – 2.14	Depositor EDS
% Data completeness (in resolution range)	99.4 (37.42-2.14) 99.4 (37.42-2.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	2.99 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.209 , 0.239 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å^2)	21.8	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 10.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.288 for h,-k,-l	Xtriage
Reported twinning fraction	0.759 for H, K, L 0.241 for -H, -K, L	Depositor
Outliers	2 of 177323 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	23601	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.65 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.7105e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.41	0/2988	0.63	0/4049
1	B	0.40	0/2948	0.62	0/3998
1	C	0.39	0/2879	0.57	0/3907
1	D	0.42	0/2939	0.64	0/3986
1	E	0.39	0/2949	0.58	0/3995
1	F	0.39	0/2727	0.60	1/3705 (0.0%)
1	G	0.41	0/2942	0.65	0/3993
1	H	0.39	0/2895	0.60	0/3931
All	All	0.40	0/23267	0.61	1/31564 (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	F	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	201	GLN	N-CA-C	7.29	130.68	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	201	GLN	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	2933	0	2857	5	0
1	B	2895	0	2794	3	0
1	C	2830	0	2722	5	0
1	D	2886	0	2784	4	0
1	E	2898	0	2826	2	0
1	F	2680	0	2562	6	0
1	G	2887	0	2795	2	0
1	H	2843	0	2724	5	0
2	A	122	0	0	0	0
2	B	98	0	0	0	0
2	C	41	0	0	0	0
2	D	126	0	0	0	0
2	E	50	0	0	0	0
2	F	77	0	0	0	0
2	G	147	0	0	0	0
2	H	88	0	0	0	0
All	All	23601	0	22064	32	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 1.

The worst 5 of 32 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:215:ARG:HD2	1:A:217:ASP:OD1	1.99	0.61
1:B:93:HIS:HB2	1:B:149:ALA:HB2	1.86	0.57
1:F:136:VAL:HG22	1:F:299:TRP:CZ2	2.47	0.49
1:F:176:ILE:HD12	1:F:196:ILE:HD11	1.95	0.49
1:D:63:LEU:HD22	1:D:187:ILE:HD12	1.96	0.48

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	364/379 (96%)	356 (98%)	8 (2%)	0	100	100
1	B	364/379 (96%)	353 (97%)	11 (3%)	0	100	100
1	C	360/379 (95%)	353 (98%)	7 (2%)	0	100	100
1	D	364/379 (96%)	351 (96%)	13 (4%)	0	100	100
1	E	361/379 (95%)	357 (99%)	4 (1%)	0	100	100
1	F	336/379 (89%)	328 (98%)	8 (2%)	0	100	100
1	G	364/379 (96%)	357 (98%)	7 (2%)	0	100	100
1	H	363/379 (96%)	351 (97%)	11 (3%)	1 (0%)	46	41
All	All	2876/3032 (95%)	2806 (98%)	69 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	369	PRO

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	309/320 (97%)	308 (100%)	1 (0%)	94	97
1	B	299/320 (93%)	298 (100%)	1 (0%)	94	97
1	C	290/320 (91%)	287 (99%)	3 (1%)	82	85
1	D	296/320 (92%)	291 (98%)	5 (2%)	68	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	305/320 (95%)	302 (99%)	3 (1%)	82	85
1	F	273/320 (85%)	272 (100%)	1 (0%)	93	96
1	G	297/320 (93%)	291 (98%)	6 (2%)	63	66
1	H	286/320 (89%)	283 (99%)	3 (1%)	82	85
All	All	2355/2560 (92%)	2332 (99%)	23 (1%)	82	85

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	203	ASN
1	D	292	VAL
1	H	158	THR
1	D	252	TYR
1	F	158	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	30	ASN
1	G	240	ASN
1	H	70	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)

8 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	202	1	22,24,25	3.29	5 (22%)	28,32,34	1.57	4 (14%)
1	LLP	B	202	1	22,24,25	3.52	5 (22%)	28,32,34	1.49	5 (17%)
1	LLP	C	202	1	22,24,25	3.69	5 (22%)	28,32,34	1.49	7 (25%)
1	LLP	D	202	1	22,24,25	3.42	5 (22%)	28,32,34	1.57	9 (32%)
1	LLP	E	202	1	22,24,25	3.53	5 (22%)	28,32,34	1.50	8 (28%)
1	LLP	F	202	1	22,24,25	3.56	5 (22%)	28,32,34	1.79	11 (39%)
1	LLP	G	202	1	22,24,25	3.32	5 (22%)	28,32,34	1.61	5 (17%)
1	LLP	H	202	1	22,24,25	3.44	5 (22%)	28,32,34	1.80	9 (32%)

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	202	1	-	1/15/17/19	0/1/1/1
1	LLP	B	202	1	-	1/15/17/19	0/1/1/1
1	LLP	C	202	1	-	1/15/17/19	0/1/1/1
1	LLP	D	202	1	-	0/15/17/19	0/1/1/1
1	LLP	E	202	1	-	0/15/17/19	0/1/1/1
1	LLP	F	202	1	-	0/15/17/19	0/1/1/1
1	LLP	G	202	1	-	1/15/17/19	0/1/1/1
1	LLP	H	202	1	-	0/15/17/19	0/1/1/1

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	202	LLP	C4-C4'	3.34	1.52	1.46
1	D	202	LLP	C4-C4'	3.53	1.52	1.46
1	H	202	LLP	C4-C4'	3.58	1.52	1.46
1	F	202	LLP	C4-C4'	3.61	1.52	1.46
1	A	202	LLP	C4-C4'	3.72	1.52	1.46

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	202	LLP	C3-C4-C5	-4.54	114.97	118.26
1	C	202	LLP	C3-C4-C5	-3.75	115.54	118.26
1	D	202	LLP	C3-C4-C5	-3.67	115.60	118.26
1	A	202	LLP	C3-C4-C5	-3.62	115.63	118.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	202	LLP	C3-C4-C5	-3.39	115.80	118.26

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	202	LLP	C4-C4'-NZ-CE
1	C	202	LLP	C4-C4'-NZ-CE
1	A	202	LLP	C4-C4'-NZ-CE
1	G	202	LLP	C4-C4'-NZ-CE

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	202	LLP	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	366/379 (96%)	-0.34	0 100 100	11, 18, 29, 39	0
1	B	366/379 (96%)	-0.21	6 (1%) 74 80	11, 19, 35, 57	0
1	C	362/379 (95%)	-0.04	1 (0%) 94 96	16, 31, 51, 61	0
1	D	366/379 (96%)	-0.23	4 (1%) 82 86	12, 18, 35, 44	0
1	E	363/379 (95%)	-0.02	8 (2%) 65 72	14, 29, 54, 69	0
1	F	342/379 (90%)	-0.10	4 (1%) 81 85	16, 28, 45, 55	0
1	G	366/379 (96%)	-0.33	0 100 100	12, 18, 28, 34	0
1	H	365/379 (96%)	-0.04	6 (1%) 74 80	14, 27, 48, 60	0
All	All	2896/3032 (95%)	-0.16	29 (1%) 84 88	11, 23, 45, 69	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	339	HIS	6.8
1	B	340	VAL	5.8
1	D	343	GLY	4.4
1	H	320	ALA	3.4
1	D	342	VAL	3.0

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	D	202	24/25	0.96	0.10	-	16,18,20,20	0
1	LLP	B	202	24/25	0.96	0.10	-	18,20,22,22	0
1	LLP	A	202	24/25	0.94	0.11	-	16,22,23,24	0
1	LLP	G	202	24/25	0.93	0.12	-	17,22,23,24	0
1	LLP	H	202	24/25	0.94	0.13	-	20,23,24,25	0
1	LLP	C	202	24/25	0.93	0.15	-	26,29,31,31	0
1	LLP	F	202	24/25	0.90	0.15	-	24,26,30,31	0
1	LLP	E	202	24/25	0.93	0.14	-	25,30,32,33	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.