Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 08:45 PM GMT

PDB ID	:	1LW4
Title	:	X-ray structure of L-Threonine Aldolase (low-specificity) in complex with L-allo-threonine
Authors	:	Kielkopf, C.L.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2002-05-30
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:

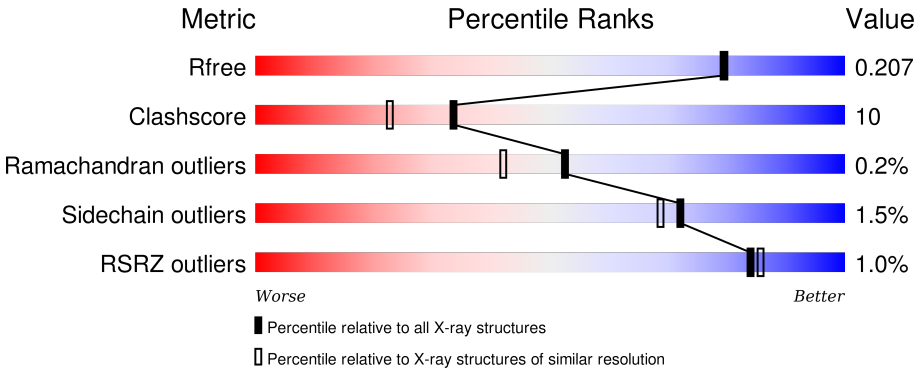
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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))
R_{free}	91344	4755 (1.90-1.90)
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	347	% 82% 16% ·
1	B	347	% 81% 17% ··
1	C	347	% 82% 16% ·
1	D	347	% 81% 17% ··

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11495 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 L-allo-threonine aldolase.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	P	S	Se	0	0	0
			2599	1626	463	493	1	3	13			
1	B	343	Total	C	N	O	S	Se		0	1	0
			2587	1621	461	489	3	13				
1	C	343	Total	C	N	O	S	Se		0	0	0
			2584	1618	463	487	3	13				
1	D	344	Total	C	N	O	S	Se		0	0	0
			2600	1627	463	493	3	14				

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	CLONING ARTIFACT	UNP Q9X266
A	-2	PRO	-	CLONING ARTIFACT	UNP Q9X266
A	-1	HIS	-	CLONING ARTIFACT	UNP Q9X266
A	0	MSE	-	CLONING ARTIFACT	UNP Q9X266
B	-3	GLY	-	CLONING ARTIFACT	UNP Q9X266
B	-2	PRO	-	CLONING ARTIFACT	UNP Q9X266
B	-1	HIS	-	CLONING ARTIFACT	UNP Q9X266
B	0	MSE	-	CLONING ARTIFACT	UNP Q9X266
C	-3	GLY	-	CLONING ARTIFACT	UNP Q9X266
C	-2	PRO	-	CLONING ARTIFACT	UNP Q9X266
C	-1	HIS	-	CLONING ARTIFACT	UNP Q9X266
D	-3	GLY	-	CLONING ARTIFACT	UNP Q9X266
D	-2	PRO	-	CLONING ARTIFACT	UNP Q9X266
D	-1	HIS	-	CLONING ARTIFACT	UNP Q9X266

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Ca	0	0
			3	3		

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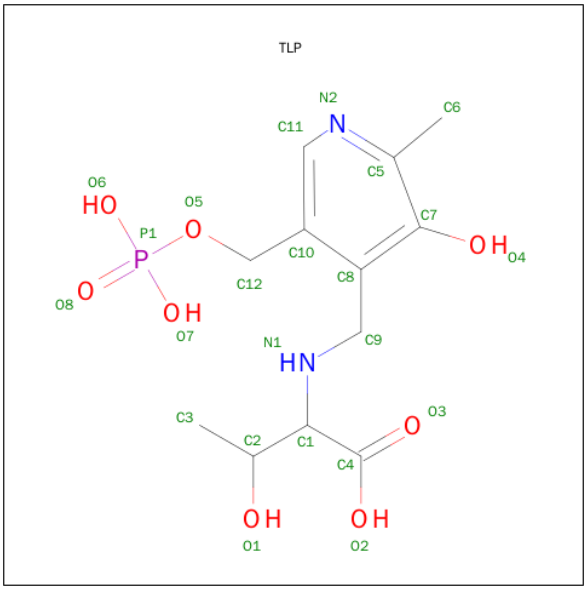
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	D	2	Total Ca 2 2	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is 3-HYDROXY-2-[(3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YLMETHYL)-AMINO]-BUTYRIC ACID (three-letter code: TLP) (formula: $C_{12}H_{19}N_2O_8P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O P 23 12 2 8 1	0	1
4	C	1	Total C N O P 23 12 2 8 1	0	0

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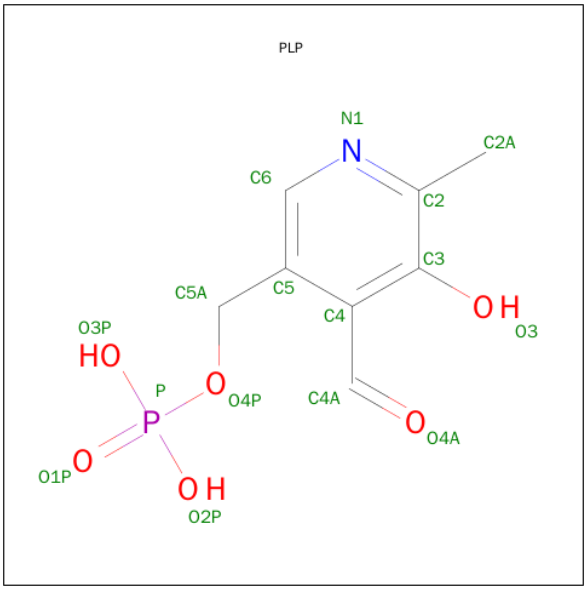
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	P	0	0
			23	12	2	8	1		

- 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	1
			15	8	1	5	1		

- Molecule 6 is water.

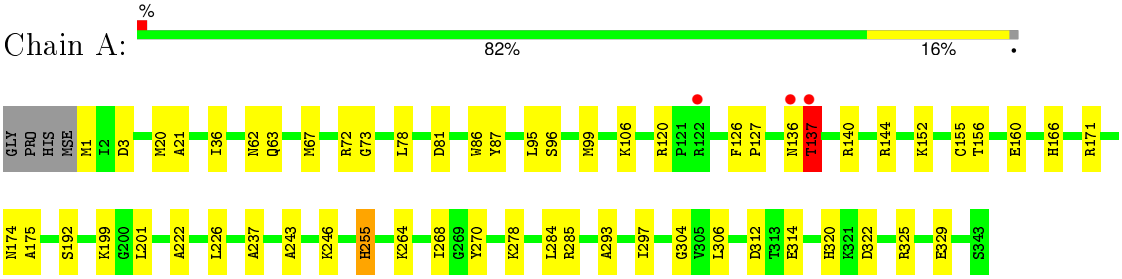
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	255	Total	O	0	0
			255	255		
6	B	234	Total	O	0	0
			234	234		
6	C	266	Total	O	0	0
			266	266		
6	D	274	Total	O	0	0
			274	274		

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.

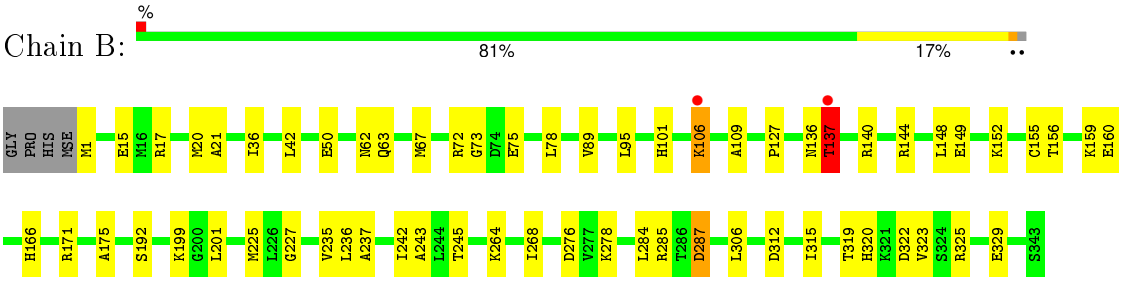
- Molecule 1: L-allo-threonine aldolase

Chain A:



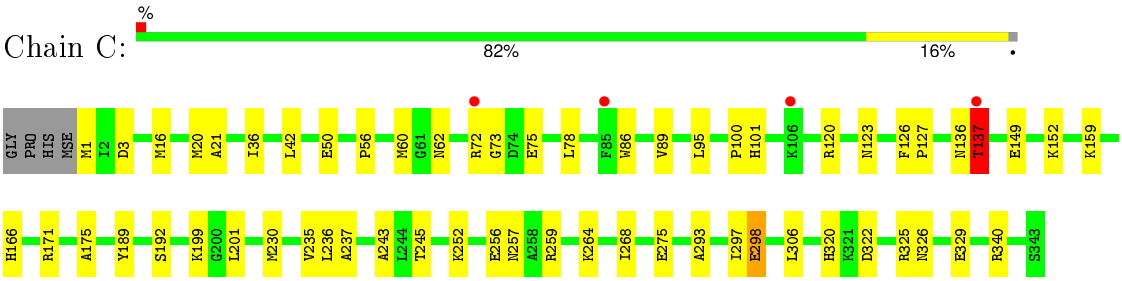
- Molecule 1: L-allo-threonine aldolase

Chain B:



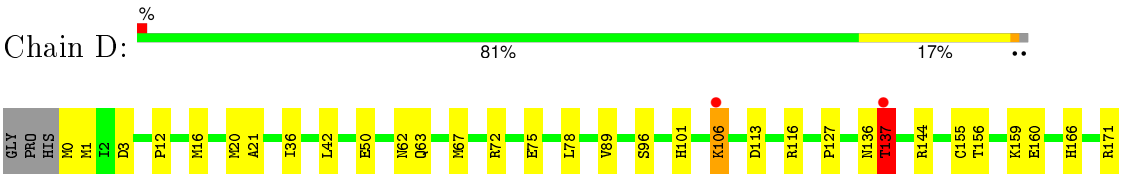
- Molecule 1: L-allo-threonine aldolase

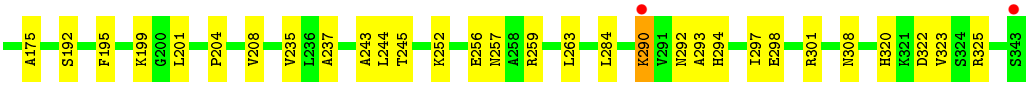
Chain C:



- Molecule 1: L-allo-threonine aldolase

Chain D:




A175
S192
F195
K199
G200
L201
P204
V208
V235
L236
A237
A243
L244
T245
K252
E256
N257
A258
R259
L263
L284
K290
V291
N292
A293
H294
I297
E298
R301
N308
H320
K321
D322
V323
S324
R325
S343

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	95.90Å 100.50Å 150.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 29.86 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.90) 99.8 (29.86-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.44 (at 1.91Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.183 , 0.206 0.184 , 0.207	Depositor DCC
R_{free} test set	7902 reflections (6.91%)	DCC
Wilson B-factor (Å^2)	19.8	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 57.7	EDS
Estimated twinning fraction	0.006 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 114556 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11495	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.31% 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: LLP, CA, TLP, PLP, CL

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	0.31	0/2603	0.63	1/3500 (0.0%)
1	B	0.30	0/2597	0.64	1/3493 (0.0%)
1	C	0.39	1/2603 (0.0%)	0.67	4/3500 (0.1%)
1	D	0.40	2/2618 (0.1%)	0.74	4/3517 (0.1%)
All	All	0.35	3/10421 (0.0%)	0.67	10/14010 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	301	ARG	CZ-NH1	10.15	1.46	1.33
1	C	298	GLU	CB-CG	10.13	1.71	1.52
1	D	301	ARG	CG-CD	6.41	1.68	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	301	ARG	NE-CZ-NH1	19.79	130.20	120.30
1	B	137	THR	N-CA-C	-10.13	83.65	111.00
1	A	137	THR	N-CA-C	-9.29	85.93	111.00
1	D	137	THR	N-CA-C	-9.26	86.00	111.00
1	C	137	THR	N-CA-C	-8.72	87.44	111.00
1	D	301	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	C	298	GLU	CA-CB-CG	6.16	126.94	113.40
1	D	301	ARG	NH1-CZ-NH2	-5.94	112.87	119.40
1	C	298	GLU	CG-CD-OE1	-5.82	106.66	118.30
1	C	298	GLU	N-CA-CB	-5.77	100.21	110.60

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	2599	0	2578	53	0
1	B	2587	0	2566	64	0
1	C	2584	0	2571	57	0
1	D	2600	0	2586	59	0
2	A	1	0	0	0	0
2	B	3	0	0	0	0
2	D	2	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	B	23	0	15	4	0
4	C	23	0	15	1	0
4	D	23	0	15	2	0
5	B	15	0	6	4	0
6	A	255	0	0	7	0
6	B	234	0	0	6	0
6	C	266	0	0	9	1
6	D	274	0	0	13	1
All	All	11495	0	10352	212	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 10.

All (212) 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:B:199[A]:LLP:NZ	4:B:1050[A]:TLP:H13	1.37	1.37
1:A:99:MSE:HE3	1:C:100:PRO:HG3	1.29	1.08
1:C:340:ARG:HG2	6:C:1320:HOH:O	1.53	1.05
1:B:199[A]:LLP:NZ	4:B:1050[A]:TLP:C9	2.20	1.04
1:D:136:ASN:O	1:D:137:THR:HG23	1.58	1.04
1:D:12:PRO:HG3	1:D:204:PRO:HG3	1.46	0.98
1:B:1:MSE:HE3	1:B:306:LEU:HD21	1.49	0.94
1:D:72:ARG:HB3	6:D:1271:HOH:O	1.67	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:326:ASN:ND2	6:C:1316:HOH:O	2.05	0.90
1:D:137:THR:HG22	1:D:175:ALA:HB2	1.57	0.87
1:A:174:ASN:HD22	1:A:255:HIS:HE1	1.24	0.86
1:D:137:THR:HG21	1:D:171:ARG:O	1.78	0.83
1:C:137:THR:HG23	1:C:175:ALA:HB2	1.60	0.81
1:C:136:ASN:O	1:C:137:THR:OG1	1.99	0.81
1:C:1:MSE:HE3	1:C:306:LEU:HD21	1.61	0.81
1:B:21:ALA:HB2	1:C:21:ALA:HB2	1.61	0.81
1:B:199[B]:LLP:NZ	5:B:1053[B]:PLP:C4A	2.45	0.79
1:D:294:HIS:CD2	6:D:1280:HOH:O	2.35	0.79
1:B:106:LYS:O	1:B:106:LYS:HD2	1.84	0.78
1:A:1:MSE:HE3	1:A:306:LEU:HD21	1.67	0.77
1:A:21:ALA:HB2	1:D:21:ALA:HB2	1.67	0.76
1:B:136:ASN:O	1:B:137:THR:HG23	1.90	0.72
1:D:137:THR:HA	1:D:144:ARG:O	1.90	0.71
1:A:155:CYS:SG	6:A:1289:HOH:O	2.48	0.71
1:D:113:ASP:HB3	6:D:1270:HOH:O	1.91	0.70
1:D:259:ARG:CZ	6:D:1263:HOH:O	2.39	0.70
1:B:73:GLY:O	1:B:127:PRO:HB3	1.90	0.70
1:B:42:LEU:HD21	1:B:245:THR:CG2	2.21	0.70
1:B:15:GLU:HG2	1:B:242:ILE:HD13	1.72	0.70
1:C:72:ARG:NH2	6:C:1171:HOH:O	2.24	0.70
1:C:42:LEU:HD21	1:C:245:THR:CG2	2.21	0.69
1:B:199[A]:LLP:NZ	4:B:1050[A]:TLP:C8	2.55	0.69
1:B:199[B]:LLP:CE	5:B:1053[B]:PLP:C4A	2.71	0.69
1:A:137:THR:CG2	1:A:175:ALA:HB2	2.23	0.69
1:C:325:ARG:NH1	6:C:1254:HOH:O	2.26	0.69
1:A:137:THR:HA	1:A:144:ARG:O	1.94	0.68
1:B:137:THR:HA	1:B:144:ARG:O	1.94	0.68
1:A:156:THR:O	1:A:160:GLU:HG3	1.93	0.68
1:D:259:ARG:NE	6:D:1263:HOH:O	2.25	0.68
1:C:36:ILE:HD13	1:C:237:ALA:HB2	1.75	0.68
1:D:75:GLU:HG3	1:D:127:PRO:HG2	1.77	0.67
1:B:278:LYS:HB2	6:B:1251:HOH:O	1.93	0.67
1:D:259:ARG:NH2	6:D:1263:HOH:O	2.27	0.67
1:D:156:THR:O	1:D:160:GLU:HG3	1.95	0.67
1:D:257:ASN:ND2	1:D:325:ARG:HE	1.93	0.66
1:C:73:GLY:O	1:C:127:PRO:HB3	1.96	0.66
1:B:149:GLU:OE1	6:B:1266:HOH:O	2.14	0.65
1:D:290:LYS:HA	1:D:290:LYS:HE3	1.79	0.64
1:C:75:GLU:OE2	1:C:101:HIS:HD2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ASP:O	1:A:140:ARG:HD3	1.98	0.64
1:B:137:THR:HG22	1:B:175:ALA:HB2	1.80	0.64
1:A:36:ILE:HD13	1:A:237:ALA:HB2	1.80	0.64
1:A:325:ARG:O	1:A:329:GLU:HG3	1.98	0.63
1:D:199:LLP:CE	4:D:1052:TLP:H13	2.29	0.63
1:B:137:THR:HG21	1:B:171:ARG:O	2.00	0.62
1:B:199[A]:LLP:CE	4:B:1050[A]:TLP:H13	2.26	0.62
1:C:252:LYS:O	1:C:256:GLU:HG3	1.99	0.62
1:D:75:GLU:HG3	1:D:127:PRO:CG	2.30	0.61
1:B:225:MSE:HA	1:C:89:VAL:HG11	1.82	0.61
1:A:73:GLY:O	1:A:127:PRO:HB3	2.01	0.61
1:D:259:ARG:HG3	6:D:1249:HOH:O	1.98	0.61
1:B:225:MSE:HA	1:C:89:VAL:CG1	2.31	0.61
1:A:320:HIS:HD2	1:A:322:ASP:H	1.48	0.61
1:B:325:ARG:O	1:B:329:GLU:HG3	1.99	0.61
1:A:136:ASN:O	1:A:137:THR:HG23	2.01	0.60
6:C:1074:HOH:O	1:D:72:ARG:NH1	2.35	0.60
1:A:87:TYR:CD1	1:C:126:PHE:HE1	2.20	0.60
1:B:320:HIS:HD2	1:B:322:ASP:H	1.50	0.59
1:A:137:THR:OG1	1:A:171:ARG:HB2	2.03	0.59
1:A:21:ALA:HB2	1:D:21:ALA:CB	2.31	0.59
1:D:298:GLU:OE1	6:D:1295:HOH:O	2.17	0.59
1:A:72:ARG:NH1	6:A:1092:HOH:O	2.35	0.59
1:B:1:MSE:CE	1:B:306:LEU:HD21	2.28	0.58
1:B:42:LEU:HD21	1:B:245:THR:HG23	1.86	0.58
1:A:137:THR:HG22	1:A:175:ALA:HB2	1.86	0.58
1:C:275:GLU:CD	1:C:275:GLU:H	2.07	0.58
1:B:225:MSE:CA	1:C:89:VAL:HG11	2.33	0.57
1:C:264:LYS:O	1:C:268:ILE:HG13	2.04	0.57
6:A:1281:HOH:O	1:B:72:ARG:NH1	2.36	0.57
1:C:62:ASN:ND2	1:C:166:HIS:HE1	2.02	0.57
1:B:106:LYS:HE3	1:B:109:ALA:HB3	1.87	0.57
1:C:256:GLU:OE2	6:C:1271:HOH:O	2.17	0.57
1:A:285:ARG:HD2	1:A:314:GLU:HG2	1.87	0.57
1:A:137:THR:HG21	1:A:171:ARG:O	2.03	0.57
1:D:257:ASN:HD22	1:D:325:ARG:HE	1.53	0.57
1:C:1:MSE:CE	1:C:306:LEU:HD21	2.33	0.56
1:C:62:ASN:HD22	1:C:166:HIS:HE1	1.53	0.56
1:D:166:HIS:HD2	1:D:192:SER:OG	1.88	0.56
1:D:137:THR:CG2	1:D:171:ARG:O	2.52	0.56
1:D:292:ASN:ND2	6:D:1280:HOH:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:HIS:H	1:B:323:VAL:CG2	2.19	0.56
1:A:293:ALA:O	1:A:297:ILE:HG12	2.06	0.56
1:D:259:ARG:NH1	1:D:263:LEU:HD11	2.21	0.56
1:A:199:LLP:OP2	6:A:1266:HOH:O	2.18	0.55
1:B:137:THR:CG2	1:B:175:ALA:HB2	2.35	0.55
1:B:50:GLU:HG2	6:B:1083:HOH:O	2.07	0.55
1:D:42:LEU:HD21	1:D:245:THR:CG2	2.37	0.55
1:A:87:TYR:HD1	1:C:126:PHE:HE1	1.55	0.54
1:A:62:ASN:ND2	1:A:166:HIS:HE1	2.05	0.54
1:D:201:LEU:HB3	1:D:243:ALA:HB1	1.89	0.54
1:B:225:MSE:HG3	1:C:89:VAL:HG13	1.89	0.54
1:C:320:HIS:HD2	1:C:322:ASP:H	1.56	0.54
1:D:320:HIS:HD2	1:D:322:ASP:H	1.55	0.54
1:C:42:LEU:HD21	1:C:245:THR:HG23	1.90	0.54
1:D:36:ILE:HD13	1:D:237:ALA:HB2	1.90	0.54
1:A:63:GLN:O	1:A:67:MSE:HG3	2.07	0.54
1:D:0:MSE:HG3	1:D:1:MSE:H	1.74	0.53
1:A:1:MSE:CE	1:A:306:LEU:HD21	2.38	0.53
1:D:50:GLU:HG3	6:D:1080:HOH:O	2.09	0.53
1:B:323:VAL:O	1:B:323:VAL:HG23	2.10	0.52
1:D:136:ASN:C	1:D:137:THR:HG23	2.28	0.52
1:A:120:ARG:HH22	1:C:86:TRP:HA	1.75	0.52
1:B:36:ILE:HD13	1:B:237:ALA:HB2	1.92	0.52
1:C:166:HIS:HD2	1:C:192:SER:OG	1.93	0.51
1:D:3:ASP:O	1:D:320:HIS:HE1	1.94	0.51
1:C:259:ARG:NE	6:C:1180:HOH:O	2.43	0.51
1:D:252:LYS:O	1:D:256:GLU:HG3	2.10	0.51
1:A:137:THR:HG23	1:A:175:ALA:HB2	1.93	0.50
1:B:20:MSE:SE	1:C:235:VAL:HG11	2.60	0.50
1:D:116:ARG:NH2	6:D:1270:HOH:O	2.43	0.50
1:D:63:GLN:O	1:D:67:MSE:HG3	2.12	0.50
1:C:89:VAL:HG22	1:C:89:VAL:O	2.11	0.50
1:B:63:GLN:O	1:B:67:MSE:HG3	2.12	0.49
1:B:285:ARG:HB3	1:B:287:ASP:OD1	2.12	0.49
1:B:137:THR:CA	1:B:144:ARG:O	2.60	0.49
1:A:246:LYS:HB3	1:A:246:LYS:NZ	2.27	0.49
1:A:137:THR:OG1	1:A:137:THR:O	2.29	0.49
1:D:42:LEU:HD21	1:D:245:THR:HG23	1.94	0.49
1:B:166:HIS:HD2	1:B:192:SER:OG	1.95	0.49
1:A:174:ASN:HD22	1:A:255:HIS:CE1	2.16	0.48
1:B:75:GLU:OE1	1:B:101:HIS:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:HIS:HD2	1:A:192:SER:OG	1.96	0.48
1:B:62:ASN:ND2	1:B:166:HIS:HE1	2.12	0.48
1:D:195:PHE:CE1	1:D:208:VAL:HB	2.48	0.48
1:D:106:LYS:HD3	1:D:106:LYS:N	2.29	0.48
1:D:293:ALA:O	1:D:297:ILE:HG12	2.13	0.48
1:B:171:ARG:NH1	5:B:1053[B]:PLP:O3	2.45	0.48
1:C:56:PRO:HG3	1:C:230:MSE:HE2	1.96	0.48
1:A:285:ARG:CD	1:A:314:GLU:HG2	2.44	0.48
1:A:137:THR:CA	1:A:144:ARG:O	2.61	0.47
1:D:199:LLP:HE3	4:D:1052:TLP:H13	1.96	0.47
1:A:20:MSE:SE	1:D:235:VAL:HG11	2.63	0.47
1:C:257:ASN:ND2	1:C:325:ARG:HE	2.11	0.47
1:B:148:LEU:O	1:B:152:LYS:HG3	2.14	0.47
1:D:75:GLU:OE2	1:D:101:HIS:HD2	1.98	0.47
1:C:329:GLU:OE2	6:C:1316:HOH:O	2.20	0.47
1:B:201:LEU:HB3	1:B:243:ALA:HB1	1.97	0.47
1:C:3:ASP:O	1:C:320:HIS:HE1	1.98	0.46
1:B:264:LYS:O	1:B:268:ILE:HG13	2.16	0.46
1:B:140:ARG:HD3	6:B:1220:HOH:O	2.14	0.46
1:D:284:LEU:C	1:D:284:LEU:HD23	2.35	0.46
1:D:320:HIS:H	1:D:323:VAL:CG2	2.29	0.46
1:D:136:ASN:O	1:D:137:THR:CG2	2.48	0.46
1:B:17:ARG:HA	1:B:20:MSE:HE3	1.97	0.46
1:D:101:HIS:HE1	6:D:1158:HOH:O	1.98	0.46
1:C:149:GLU:OE1	1:C:152:LYS:HE2	2.15	0.46
1:A:201:LEU:HB3	1:A:243:ALA:HB1	1.97	0.45
1:B:95:LEU:HD22	1:C:95:LEU:HD22	1.98	0.45
1:D:0:MSE:HE3	1:D:1:MSE:HG2	1.98	0.45
1:B:225:MSE:CB	1:C:89:VAL:HG11	2.47	0.45
1:B:137:THR:OG1	1:B:171:ARG:HB2	2.15	0.45
1:D:137:THR:CA	1:D:144:ARG:O	2.61	0.45
1:A:67:MSE:HG2	1:A:96:SER:OG	2.17	0.45
1:A:278:LYS:HG3	6:A:1126:HOH:O	2.15	0.45
1:D:155:CYS:O	1:D:159:LYS:HG3	2.17	0.45
1:C:16:MSE:O	1:C:20:MSE:HG3	2.17	0.45
1:B:155:CYS:O	1:B:159:LYS:HG2	2.17	0.45
1:B:236:LEU:HD11	1:C:236:LEU:HD11	1.99	0.45
1:A:222:ALA:O	1:A:226:LEU:HG	2.17	0.44
1:B:319:THR:HA	1:B:323:VAL:HG21	2.00	0.44
1:A:106:LYS:HB2	1:A:106:LYS:NZ	2.33	0.44
1:C:201:LEU:HB3	1:C:243:ALA:HB1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ASP:O	1:A:320:HIS:HE1	2.01	0.43
1:A:86:TRP:HA	1:C:120:ARG:HH22	1.82	0.43
1:B:235:VAL:HG11	1:C:20:MSE:SE	2.68	0.43
1:B:284:LEU:C	1:B:284:LEU:HD23	2.38	0.43
1:A:95:LEU:HD12	1:A:95:LEU:N	2.33	0.43
1:B:227:GLY:HA3	1:C:60:MSE:HB2	2.00	0.43
1:B:276:ASP:OD1	6:B:1233:HOH:O	2.22	0.43
1:D:320:HIS:CD2	1:D:322:ASP:H	2.34	0.43
1:D:67:MSE:HB3	1:D:67:MSE:HE2	1.89	0.43
1:A:1:MSE:HE3	1:A:306:LEU:CD2	2.44	0.42
1:A:99:MSE:CE	1:C:100:PRO:HG3	2.22	0.42
1:B:320:HIS:H	1:B:323:VAL:HG22	1.84	0.42
1:D:166:HIS:CD2	1:D:192:SER:OG	2.71	0.42
1:D:67:MSE:HG2	1:D:96:SER:OG	2.19	0.42
1:D:16:MSE:O	1:D:20:MSE:HG3	2.20	0.42
1:B:156:THR:O	1:B:160:GLU:HG3	2.20	0.42
1:A:320:HIS:CD2	1:A:322:ASP:H	2.33	0.42
1:A:152:LYS:HD2	6:A:1192:HOH:O	2.20	0.42
1:A:171:ARG:NH1	1:A:199:LLP:O3	2.52	0.42
1:A:126:PHE:HA	1:A:127:PRO:HD3	1.92	0.42
1:C:50:GLU:HG3	6:C:1092:HOH:O	2.19	0.42
1:C:137:THR:OG1	1:C:171:ARG:HB2	2.20	0.42
1:D:62:ASN:OD1	1:D:166:HIS:HE1	2.02	0.41
1:C:293:ALA:O	1:C:297:ILE:HG12	2.19	0.41
1:C:199:LLP:CE	4:C:1051:TLP:H13	2.50	0.41
1:A:270:TYR:HB3	1:A:284:LEU:CD1	2.50	0.41
1:A:1:MSE:SE	1:A:304:GLY:HA2	2.70	0.41
1:C:152:LYS:HG3	1:C:189:TYR:CE1	2.56	0.41
1:B:137:THR:OG1	1:B:137:THR:O	2.38	0.41
1:B:101:HIS:HE1	6:B:1153:HOH:O	2.03	0.41
1:B:225:MSE:HB2	1:C:89:VAL:HG11	2.03	0.41
1:B:284:LEU:HB3	1:B:315:ILE:CG1	2.50	0.41
1:D:308:ASN:HB2	6:D:1099:HOH:O	2.19	0.41
1:A:264:LYS:O	1:A:268:ILE:HG13	2.20	0.41
6:A:1079:HOH:O	1:C:89:VAL:HG22	2.21	0.41
1:C:123:ASN:HB3	1:C:126:PHE:CD2	2.56	0.41
1:C:78:LEU:HD12	1:C:78:LEU:O	2.21	0.41
1:B:199[B]:LLP:HE3	5:B:1053[B]:PLP:C4A	2.49	0.41
1:C:159:LYS:HB3	1:C:159:LYS:HE2	1.85	0.41
1:B:285:ARG:HG3	1:B:285:ARG:HH11	1.86	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)
6:C:1316:HOH:O	6:D:1270:HOH:O[2_665]	2.15	0.05

5.3 Torsion angles

5.3.1 Protein backbone

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	340/347 (98%)	333 (98%)	6 (2%)	1 (0%)	46	35
1	B	340/347 (98%)	331 (97%)	8 (2%)	1 (0%)	46	35
1	C	340/347 (98%)	334 (98%)	5 (2%)	1 (0%)	46	35
1	D	341/347 (98%)	333 (98%)	8 (2%)	0	100	100
All	All	1361/1388 (98%)	1331 (98%)	27 (2%)	3 (0%)	52	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	137	THR
1	A	137	THR
1	B	137	THR

5.3.2 Protein sidechains

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	269/269 (100%)	266 (99%)	3 (1%)	80	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	268/269 (100%)	263 (98%)	5 (2%)	65 59
1	C	269/269 (100%)	267 (99%)	2 (1%)	88 88
1	D	272/269 (101%)	266 (98%)	6 (2%)	60 53
All	All	1078/1076 (100%)	1062 (98%)	16 (2%)	72 69

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	LEU
1	A	255	HIS
1	A	312	ASP
1	B	78	LEU
1	B	89	VAL
1	B	106	LYS
1	B	287	ASP
1	B	312	ASP
1	C	137	THR
1	C	298	GLU
1	D	78	LEU
1	D	89	VAL
1	D	106	LYS
1	D	137	THR
1	D	244	LEU
1	D	290	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	71	GLN
1	A	166	HIS
1	A	255	HIS
1	A	257	ASN
1	A	320	HIS
1	B	62	ASN
1	B	101	HIS
1	B	166	HIS
1	B	320	HIS
1	C	22	GLN
1	C	62	ASN

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Mol	Chain	Res	Type
1	C	63	GLN
1	C	101	HIS
1	C	107	ASN
1	C	150	ASN
1	C	166	HIS
1	C	257	ASN
1	C	320	HIS
1	C	326	ASN
1	D	101	HIS
1	D	107	ASN
1	D	125	HIS
1	D	161	HIS
1	D	166	HIS
1	D	257	ASN
1	D	308	ASN
1	D	320	HIS
1	D	333	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

5 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	199	1	23,24,25	3.81	7 (30%)	28,32,34	2.39	12 (42%)
1	LLP	B	199[A]	1	7,8,25	0.45	0	6,8,34	1.18	1 (16%)
1	LLP	B	199[B]	1	7,8,25	0.95	1 (14%)	6,8,34	1.12	0
1	LLP	C	199	1	7,8,25	0.48	0	6,8,34	0.93	1 (16%)
1	LLP	D	199	1	7,8,25	0.45	0	6,8,34	0.94	1 (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
1	LLP	A	199	1	-	0/15/17/19	0/1/1/1
1	LLP	B	199[A]	1	-	0/5/7/19	0/0/0/1
1	LLP	B	199[B]	1	-	0/5/7/19	0/0/0/1
1	LLP	C	199	1	-	0/5/7/19	0/0/0/1
1	LLP	D	199	1	-	0/5/7/19	0/0/0/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	199	LLP	P-OP3	-2.55	1.45	1.54
1	B	199[B]	LLP	CB-CA	-2.25	1.51	1.53
1	A	199	LLP	C4-C3	2.08	1.43	1.40
1	A	199	LLP	C6-N1	3.19	1.41	1.34
1	A	199	LLP	C2-N1	3.38	1.41	1.34
1	A	199	LLP	C4'-NZ	3.58	1.38	1.27
1	A	199	LLP	C4-C5	11.48	1.57	1.42
1	A	199	LLP	C3-C2	11.95	1.49	1.40

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	199	LLP	C3-C4-C4'	-3.66	115.43	120.16
1	A	199	LLP	C3-C2-N1	-3.16	116.25	120.61
1	A	199	LLP	C5-C6-N1	-2.79	119.02	123.86
1	A	199	LLP	C4-C4'-NZ	-2.78	109.60	125.06
1	A	199	LLP	O3-C3-C2	-2.37	113.53	117.66
1	A	199	LLP	O-C-CA	-2.34	119.38	125.49
1	B	199[A]	LLP	O-C-CA	-2.19	119.78	125.49
1	D	199	LLP	O-C-CA	-2.11	119.99	125.49
1	C	199	LLP	O-C-CA	-2.03	120.20	125.49
1	A	199	LLP	O3-C3-C4	2.19	125.38	119.96
1	A	199	LLP	OP4-C5'-C5	3.34	114.51	108.99
1	A	199	LLP	C5-C4-C4'	3.67	126.79	121.52
1	A	199	LLP	C6-N1-C2	3.67	126.78	119.28
1	A	199	LLP	CE-NZ-C4'	4.48	131.89	118.97
1	A	199	LLP	C2'-C2-C3	6.23	128.55	121.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	199	LLP	2	0
1	B	199[A]	LLP	4	0
1	B	199[B]	LLP	3	0
1	C	199	LLP	1	0
1	D	199	LLP	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 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	TLP	B	1050[A]	-	20,23,23	4.44	8 (40%)	25,33,33	3.18	10 (40%)
5	PLP	B	1053[B]	-	15,15,16	5.16	7 (46%)	21,22,23	2.55	9 (42%)
4	TLP	C	1051	-	20,23,23	4.29	8 (40%)	25,33,33	3.10	9 (36%)
4	TLP	D	1052	-	20,23,23	4.29	7 (35%)	25,33,33	3.14	9 (36%)

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	TLP	B	1050[A]	-	-	0/15/19/19	0/1/1/1
5	PLP	B	1053[B]	-	-	0/6/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TLP	C	1051	-	-	0/15/19/19	0/1/1/1
4	TLP	D	1052	-	-	0/15/19/19	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1051	TLP	C9-N1	-3.14	1.36	1.46
4	B	1050[A]	TLP	C9-N1	-3.00	1.37	1.46
4	D	1052	TLP	C9-N1	-2.71	1.38	1.46
4	D	1052	TLP	P1-O7	-2.35	1.46	1.54
5	B	1053[B]	PLP	P-O3P	-2.29	1.46	1.54
5	B	1053[B]	PLP	C4A-C4	-2.27	1.47	1.51
4	C	1051	TLP	C9-C8	-2.27	1.49	1.51
4	B	1050[A]	TLP	P1-O7	-2.26	1.46	1.54
4	C	1051	TLP	P1-O7	-2.17	1.46	1.54
4	B	1050[A]	TLP	C9-C8	-2.01	1.49	1.51
5	B	1053[B]	PLP	C5A-C5	2.10	1.57	1.50
4	C	1051	TLP	C7-C8	2.29	1.43	1.40
4	B	1050[A]	TLP	C7-C8	2.54	1.44	1.40
4	D	1052	TLP	C7-C8	2.59	1.44	1.40
4	D	1052	TLP	C11-N2	3.02	1.40	1.34
4	C	1051	TLP	C11-N2	3.12	1.41	1.34
4	B	1050[A]	TLP	C11-N2	3.17	1.41	1.34
5	B	1053[B]	PLP	C6-N1	3.21	1.41	1.34
5	B	1053[B]	PLP	C2-N1	3.45	1.41	1.34
4	D	1052	TLP	C5-N2	3.61	1.41	1.34
4	B	1050[A]	TLP	C5-N2	3.70	1.41	1.34
4	C	1051	TLP	C5-N2	3.80	1.42	1.34
4	C	1051	TLP	C10-C8	11.03	1.56	1.40
4	D	1052	TLP	C10-C8	11.55	1.56	1.40
4	B	1050[A]	TLP	C10-C8	11.68	1.57	1.40
5	B	1053[B]	PLP	C3-C2	11.69	1.48	1.40
4	D	1052	TLP	C7-C5	13.42	1.50	1.40
4	C	1051	TLP	C7-C5	13.66	1.50	1.40
4	B	1050[A]	TLP	C7-C5	14.06	1.50	1.40
5	B	1053[B]	PLP	C5-C4	14.68	1.57	1.40

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1053[B]	PLP	C3-C2-N1	-3.24	116.14	120.61
4	B	1050[A]	TLP	C7-C5-N2	-3.15	116.26	120.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1051	TLP	C7-C5-N2	-3.15	116.26	120.61
4	D	1052	TLP	C7-C5-N2	-3.11	116.31	120.61
4	C	1051	TLP	C10-C11-N2	-3.09	118.50	123.86
4	D	1052	TLP	C10-C11-N2	-3.02	118.63	123.86
4	B	1050[A]	TLP	C10-C11-N2	-2.95	118.75	123.86
5	B	1053[B]	PLP	C4A-C4-C3	-2.70	115.46	120.36
5	B	1053[B]	PLP	C5-C6-N1	-2.69	119.19	123.86
5	B	1053[B]	PLP	O3-C3-C2	-2.45	113.40	117.66
4	B	1050[A]	TLP	O4-C7-C5	-2.35	113.58	117.66
4	D	1052	TLP	O4-C7-C5	-2.34	113.60	117.66
4	C	1051	TLP	O4-C7-C5	-2.26	113.72	117.66
4	B	1050[A]	TLP	O5-C12-C10	2.10	112.46	108.99
4	B	1050[A]	TLP	C11-C10-C8	2.50	119.96	118.09
4	C	1051	TLP	O4-C7-C8	2.53	125.66	118.11
4	B	1050[A]	TLP	O4-C7-C8	2.58	125.82	118.11
4	D	1052	TLP	O4-C7-C8	2.61	125.89	118.11
5	B	1053[B]	PLP	O3-C3-C4	2.64	125.55	118.12
4	D	1052	TLP	C11-C10-C8	2.72	120.12	118.09
4	C	1051	TLP	C11-C10-C8	3.00	120.33	118.09
4	C	1051	TLP	C11-N2-C5	3.60	126.62	119.28
4	B	1050[A]	TLP	C11-N2-C5	3.68	126.78	119.28
5	B	1053[B]	PLP	C6-N1-C2	3.68	126.79	119.28
5	B	1053[B]	PLP	O4P-C5A-C5	3.69	115.09	108.99
4	D	1052	TLP	C11-N2-C5	3.73	126.89	119.28
4	D	1052	TLP	C9-C8-C10	4.69	123.89	119.71
4	C	1051	TLP	C9-C8-C10	4.73	123.93	119.71
4	B	1050[A]	TLP	C9-C8-C10	4.88	124.06	119.71
5	B	1053[B]	PLP	C4A-C4-C5	5.31	126.42	120.88
5	B	1053[B]	PLP	C2A-C2-C3	6.01	128.29	121.04
4	B	1050[A]	TLP	C6-C5-C7	6.42	128.78	121.04
4	D	1052	TLP	C6-C5-C7	6.43	128.79	121.04
4	C	1051	TLP	C6-C5-C7	6.55	128.94	121.04
4	C	1051	TLP	C9-N1-C1	10.28	128.80	113.92
4	D	1052	TLP	C9-N1-C1	10.67	129.36	113.92
4	B	1050[A]	TLP	C9-N1-C1	10.87	129.66	113.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1050[A]	TLP	4	0
5	B	1053[B]	PLP	4	0
4	C	1051	TLP	1	0
4	D	1052	TLP	2	0

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

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	329/347 (94%)	-0.10	3 (0%)	85	87	13, 20, 30, 41	0
1	B	329/347 (94%)	-0.10	2 (0%)	90	91	11, 18, 32, 41	0
1	C	329/347 (94%)	-0.02	4 (1%)	81	83	10, 21, 33, 42	1 (0%)
1	D	329/347 (94%)	-0.08	4 (1%)	81	83	11, 18, 34, 46	0
All	All	1316/1388 (94%)	-0.07	13 (0%)	84	86	10, 19, 32, 46	1 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	137	THR	5.4
1	B	137	THR	5.3
1	D	137	THR	5.0
1	C	137	THR	4.7
1	C	72	ARG	3.4
1	D	290	LYS	2.7
1	A	122	ARG	2.6
1	C	85	PHE	2.4
1	B	106	LYS	2.3
1	D	343	SER	2.2
1	D	106	LYS	2.2
1	C	106	LYS	2.0
1	A	136	ASN	2.0

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

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
1	LLP	B	199[A]	9/25	0.95	0.39	-	13,14,19,23	9
1	LLP	D	199	9/25	0.96	0.14	-	12,14,23,29	0
1	LLP	B	199[B]	9/25	0.95	0.39	-	16,17,21,22	9
1	LLP	A	199	24/25	0.91	0.18	-	13,22,27,30	0
1	LLP	C	199	9/25	0.96	0.16	-	12,14,23,25	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	TLP	B	1050[A]	23/23	0.91	0.22	1.82	14,19,21,22	23
4	TLP	D	1052	23/23	0.92	0.16	0.76	13,19,28,32	0
5	PLP	B	1053[B]	15/16	0.94	0.16	0.56	18,24,27,27	15
4	TLP	C	1051	23/23	0.96	0.14	0.44	15,18,24,28	0
3	CL	C	1061	1/1	0.99	0.05	-1.08	24,24,24,24	0
3	CL	A	1060	1/1	1.00	0.03	-2.33	19,19,19,19	0
2	CA	B	1054	1/1	1.00	0.04	-2.68	17,17,17,17	0
2	CA	A	1056	1/1	0.99	0.05	-2.74	19,19,19,19	0
2	CA	D	1059	1/1	0.99	0.03	-3.85	18,18,18,18	0
2	CA	B	1057	1/1	1.00	0.04	-4.06	18,18,18,18	0
2	CA	D	1055	1/1	0.99	0.04	-4.08	17,17,17,17	0
3	CL	A	1064	1/1	0.99	0.03	-	31,31,31,31	0
3	CL	B	1063	1/1	0.98	0.04	-	29,29,29,29	0
3	CL	D	1062	1/1	0.96	0.07	-	31,31,31,31	0
3	CL	B	1065	1/1	0.98	0.07	-	28,28,28,28	0
2	CA	B	1058	1/1	0.98	0.12	-	27,27,27,27	0

6.5 Other polymers (i)

There are no such residues in this entry.