Full wwPDB X-ray Structure Validation Report (i)

May 15, 2020 – 08:40 am BST

PDB ID	:	4JE5
Title	:	Crystal structure of the aromatic aminotransferase Aro8, a putative alpha-aminoadipate aminotransferase in Saccharomyces cerevisiae
Authors	:	Bulfer, S.L.; Brunzelle, J.S.; Trievel, R.C.
Deposited on	:	2013-02-26
Resolution	:	1.91 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

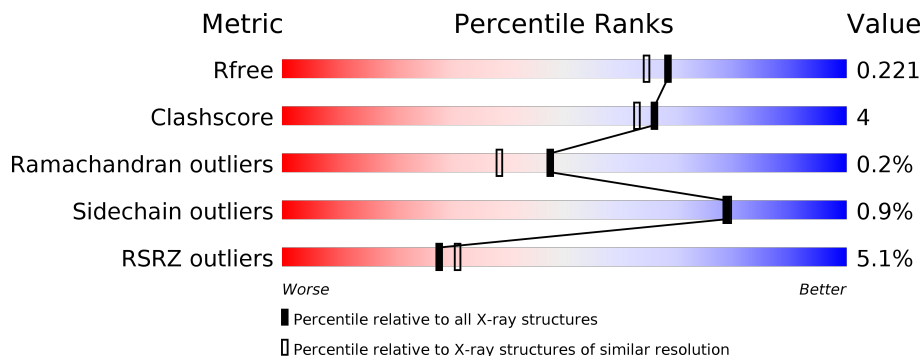|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.91 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	Percentile Ranks	Value
Rfree		0.221
Clashscore		4
Ramachandran outliers		0.2%
Sidechain outliers		0.9%
RSRZ outliers		5.1%

Worse ... *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	503	3% / 91% / 7% ·
1	B	503	10% / 89% / 9% ··
1	C	503	2% / 91% / 6% ·
2	D	503	4% / 90% / 9% ·

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 16855 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 Aromatic/aminoadipate aminotransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	26	0
			3978	2568	644	758	8			
1	B	497	Total	C	N	O	S	0	16	0
			3882	2511	630	732	9			
1	C	492	Total	C	N	O	S	0	18	0
			3899	2508	636	746	9			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP P53090
A	-1	HIS	-	EXPRESSION TAG	UNP P53090
A	0	MET	-	EXPRESSION TAG	UNP P53090
B	-2	GLY	-	EXPRESSION TAG	UNP P53090
B	-1	HIS	-	EXPRESSION TAG	UNP P53090
B	0	MET	-	EXPRESSION TAG	UNP P53090
C	-2	GLY	-	EXPRESSION TAG	UNP P53090
C	-1	HIS	-	EXPRESSION TAG	UNP P53090
C	0	MET	-	EXPRESSION TAG	UNP P53090

- Molecule 2 is a protein called Aromatic/aminoadipate aminotransferase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	496	Total	C	N	O	P	S	0	15	0
			3961	2545	645	761	1	9			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	GLY	-	EXPRESSION TAG	UNP P53090
D	-1	HIS	-	EXPRESSION TAG	UNP P53090
D	0	MET	-	EXPRESSION TAG	UNP P53090

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).
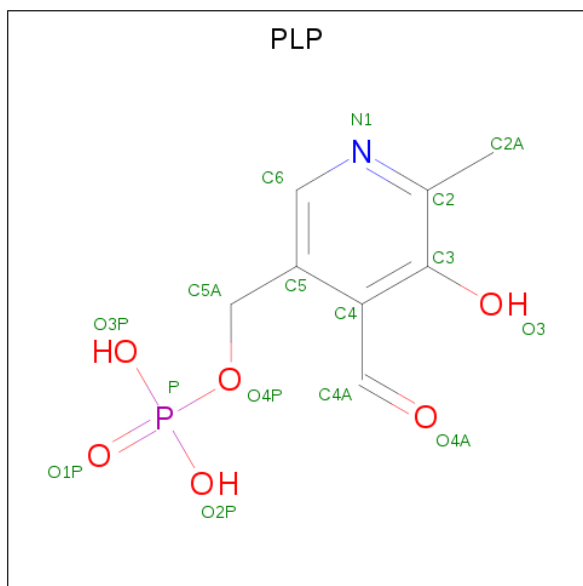
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	15	8	1	5	1	0	0

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).
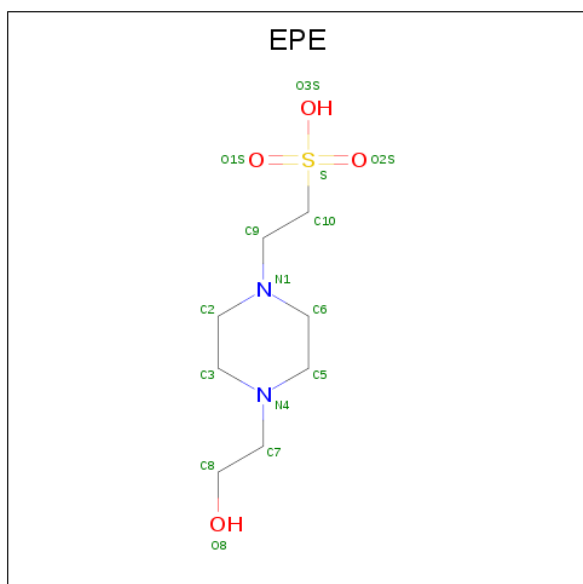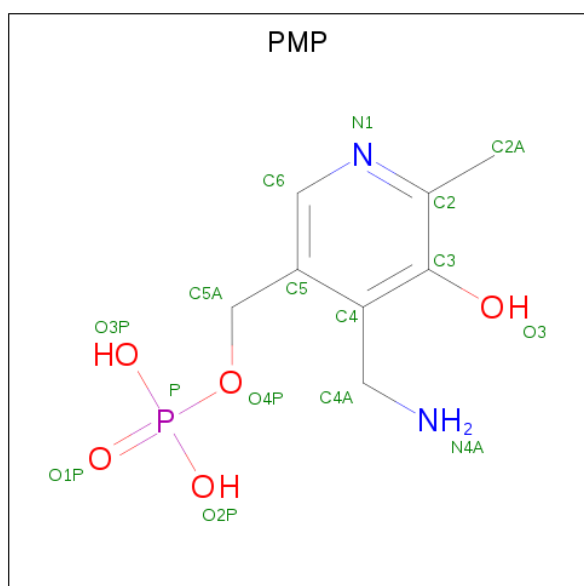

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	15	8	2	4	1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 15	C 8	N 2	O 4	S 1	0	0
4	B	1	Total 15	C 8	N 2	O 4	S 1	0	0
4	C	1	Total 15	C 8	N 2	O 4	S 1	0	0
4	C	1	Total 15	C 8	N 2	O 4	S 1	0	0

- Molecule 5 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (three-letter code: PMP) (formula: $C_8H_{13}N_2O_5P$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total 16	C 8	N 2	O 5	P 1	0	0
5	C	1	Total 16	C 8	N 2	O 5	P 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	280	Total 280	O 280	0	0
6	B	213	Total 213	O 213	0	0
6	C	264	Total 264	O 264	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	256	Total O 256 256	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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
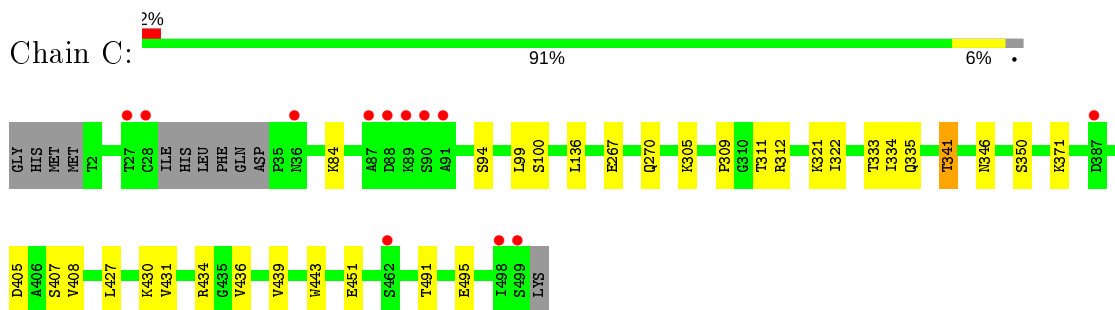
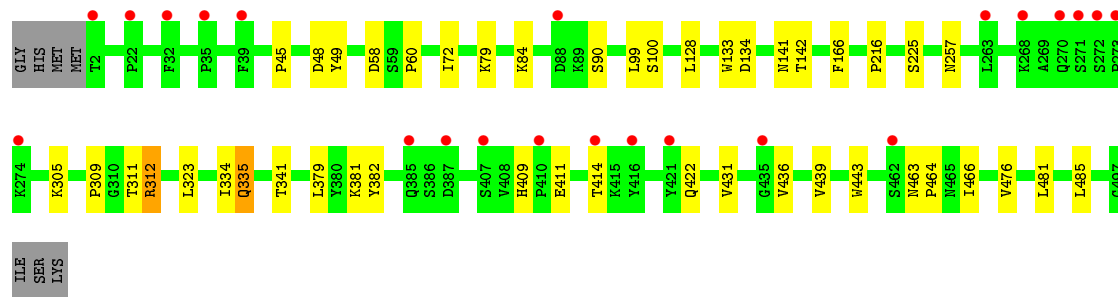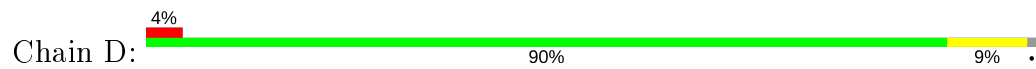• Molecule 1: Aromatic/aminoadipate aminotransferase 1
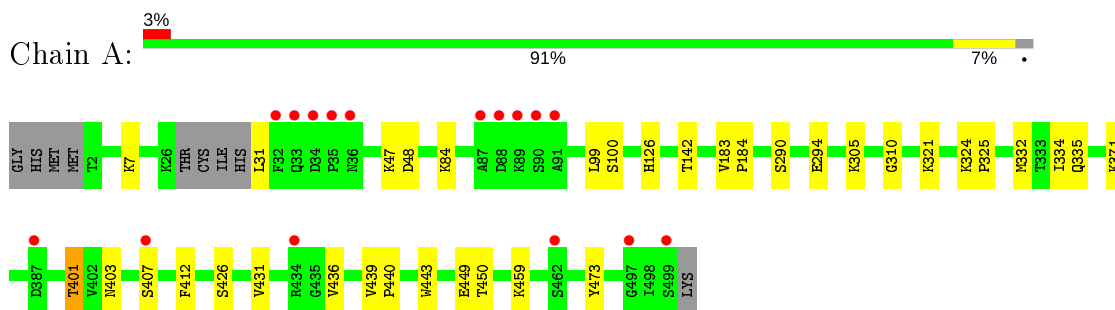
• Molecule 1: Aromatic/aminoadipate aminotransferase 1
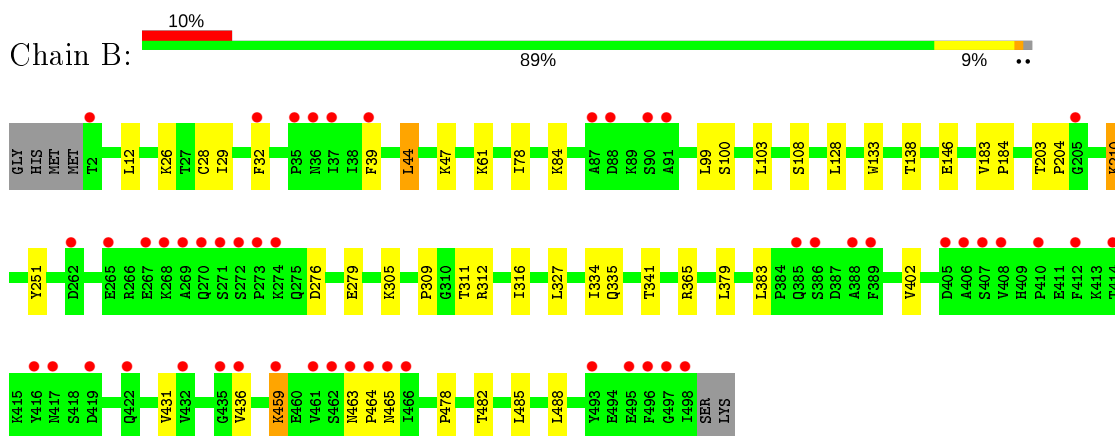
• Molecule 1: Aromatic/aminoadipate aminotransferase 1

• Molecule 2: Aromatic/aminoadipate aminotransferase 1

Chain D:

4   Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	227.44Å 159.83Å 70.64Å 90.00° 106.03° 90.00°	Depositor
Resolution (Å)	34.25 – 1.91 34.25 – 1.91	Depositor EDS
% Data completeness (in resolution range)	96.6 (34.25-1.91) 96.6 (34.25-1.91)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.182 , 0.217 0.186 , 0.221	Depositor DCC
R_{free} test set	9078 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	25.6	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 42.7	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16855	wwPDB-VP
Average B, all atoms (Å^2)	28.0	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.*

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[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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, PMP, LLP, PLP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.70	0/4149	0.65	0/5656
1	B	0.64	0/4041	0.65	1/5525 (0.0%)
1	C	0.69	0/4049	0.67	0/5527
2	D	0.69	0/4074	0.68	2/5566 (0.0%)
All	All	0.68	0/16313	0.66	3/22274 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	312[A]	ARG	NE-CZ-NH2	-5.25	117.67	120.30
2	D	312[B]	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	B	365	ARG	NE-CZ-NH2	-5.22	117.69	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	3978	0	3889	27	0
1	B	3882	0	3720	35	0
1	C	3899	0	3744	27	0
2	D	3961	0	3784	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	15	0	6	1	0
4	A	30	0	34	2	0
4	B	15	0	17	2	0
4	C	30	0	34	3	0
5	B	16	0	11	5	0
5	C	16	0	11	3	0
6	A	280	0	0	1	0
6	B	213	0	0	1	0
6	C	264	0	0	3	0
6	D	256	0	0	1	0
All	All	16855	0	15250	123	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 4.

All (123) 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:321:LYS:HA	1:A:324[A]:LYS:HE3	1.47	0.94
1:B:251:TYR:HH	5:B:1000:PMP:HO3	1.29	0.79
1:C:267:GLU:HA	1:C:270[B]:GLN:HG2	1.65	0.77
1:C:305:LYS:NZ	5:C:1000:PMP:H4A1	2.00	0.76
1:C:311:THR:O	1:C:341[B]:THR:HG21	1.85	0.74
1:A:401[A]:THR:CG2	1:A:403:ASN:OD1	2.37	0.73
1:A:431:VAL:HG13	1:A:436:VAL:HG13	1.71	0.72
2:D:311:THR:O	2:D:341[A]:THR:HG21	1.91	0.71
1:C:84:LYS:HG2	1:C:100[A]:SER:OG	1.91	0.70
1:C:431:VAL:HG13	1:C:436:VAL:HG13	1.72	0.70
1:C:305:LYS:HZ3	5:C:1000:PMP:H4A1	1.55	0.69
1:C:427:LEU:HD21	1:C:495:GLU:HG2	1.75	0.68
1:C:335:GLN:HG2	2:D:142[B]:THR:HG21	1.78	0.66
2:D:309:PRO:O	2:D:312[A]:ARG:HD2	1.95	0.65
1:A:431:VAL:HG12	1:A:436:VAL:O	1.96	0.65
1:A:334:ILE:HG22	1:B:334:ILE:HD13	1.80	0.64
2:D:463:ASN:HB3	2:D:466:ILE:HG13	1.80	0.63
2:D:166:PHE:CD2	2:D:305:LLP:H2'3	2.34	0.63
1:C:430:LYS:HE2	1:C:495:GLU:OE1	2.00	0.62
1:B:276:ASP:OD1	1:B:279:GLU:HG2	1.99	0.62
1:B:61[A]:LYS:HG3	1:B:78:ILE:HD11	1.81	0.62
1:C:346:ASN:O	1:C:350[B]:SER:HB2	2.00	0.61
1:B:311:THR:O	1:B:341[A]:THR:HG21	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:602:EPE:H32	4:A:602:EPE:O8	1.98	0.61
1:B:61[B]:LYS:HG3	1:B:78:ILE:HD11	1.83	0.60
2:D:84:LYS:HG2	2:D:100[A]:SER:OG	2.03	0.59
2:D:128:LEU:HD13	2:D:133:TRP:CE2	2.38	0.59
1:A:321:LYS:CA	1:A:324[A]:LYS:HE3	2.29	0.59
1:A:84:LYS:HA	1:A:99:LEU:HB2	1.86	0.58
1:A:332:MET:O	1:B:146[B]:GLU:HG3	2.04	0.57
2:D:439:VAL:HG13	2:D:443:TRP:CE3	2.38	0.57
4:A:603:EPE:H92	6:A:840:HOH:O	2.03	0.57
1:C:335:GLN:CG	2:D:142[B]:THR:HG21	2.35	0.57
2:D:60:PRO:HD3	2:D:72:ILE:HD11	1.86	0.56
1:A:439:VAL:HG13	1:A:443:TRP:CE3	2.41	0.56
1:C:333[B]:THR:O	2:D:142[B]:THR:HG23	2.06	0.56
2:D:476:VAL:HG23	2:D:481:LEU:HB2	1.88	0.55
2:D:431:VAL:HG12	2:D:436:VAL:O	2.07	0.55
1:B:431:VAL:HG13	1:B:436:VAL:HG13	1.88	0.54
1:B:128:LEU:HD13	1:B:133:TRP:CE2	2.43	0.54
2:D:84:LYS:HA	2:D:99:LEU:HB2	1.90	0.53
1:A:431:VAL:CG1	1:A:436:VAL:HG13	2.39	0.53
1:B:28:CYS:HB3	1:B:39:PHE:CZ	2.45	0.51
1:B:26:LYS:O	1:B:29:ILE:HG12	2.10	0.51
2:D:431:VAL:HG13	2:D:436:VAL:HG13	1.92	0.51
1:B:32:PHE:CZ	1:B:44:LEU:HG	2.45	0.51
1:C:334:ILE:O	1:C:335:GLN:HB2	2.11	0.51
1:A:47:LYS:HD2	1:A:100[B]:SER:HB2	1.93	0.50
4:B:604:EPE:H21	6:B:1214:HOH:O	2.10	0.50
2:D:422[A]:GLN:OE1	2:D:422[A]:GLN:HA	2.11	0.50
1:B:312[A]:ARG:HA	1:B:312[A]:ARG:NE	2.25	0.50
4:C:1002:EPE:H91	6:C:1238:HOH:O	2.12	0.50
2:D:463:ASN:N	2:D:464:PRO:HD3	2.26	0.49
2:D:312[A]:ARG:HD2	2:D:312[A]:ARG:H	1.77	0.49
1:A:305:LYS:HZ3	3:A:601:PLP:C4A	2.25	0.49
1:B:84:LYS:HA	1:B:99:LEU:HB2	1.95	0.49
1:C:84:LYS:HA	1:C:99:LEU:HB2	1.95	0.49
1:B:309:PRO:O	1:B:312[A]:ARG:HD2	2.13	0.48
1:C:305:LYS:HZ1	5:C:1000:PMP:H4A1	1.77	0.48
2:D:305:LLP:NZ	2:D:305:LLP:C5'	2.76	0.48
1:A:449[B]:GLU:OE2	1:A:459:LYS:NZ	2.45	0.48
1:C:431:VAL:CG1	1:C:436:VAL:HG13	2.42	0.48
1:C:334:ILE:HG22	2:D:334:ILE:HD13	1.96	0.48
5:B:1000:PMP:C5A	5:B:1000:PMP:HNA1	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:LEU:HD21	1:B:485:LEU:HD22	1.96	0.48
1:B:47:LYS:HD2	1:B:100:SER:HB2	1.95	0.47
1:B:478:PRO:O	1:B:482:THR:HG23	2.14	0.47
1:B:312[A]:ARG:HD2	1:B:312[A]:ARG:H	1.79	0.47
1:C:434:ARG:HG3	1:C:491:THR:OG1	2.14	0.47
1:A:401[A]:THR:HG22	1:A:403:ASN:OD1	2.13	0.47
1:C:439:VAL:HG13	1:C:443:TRP:CE3	2.50	0.46
1:B:28:CYS:HB3	1:B:39:PHE:CE1	2.50	0.46
1:A:335:GLN:HB3	1:B:312[B]:ARG:NH2	2.30	0.46
2:D:379:LEU:HD21	2:D:485:LEU:HD22	1.96	0.46
1:C:408:VAL:HG12	1:C:408:VAL:O	2.15	0.46
4:C:1002:EPE:H61	6:C:1238:HOH:O	2.15	0.45
2:D:45:PRO:HB2	6:D:776:HOH:O	2.16	0.45
5:B:1000:PMP:C5A	5:B:1000:PMP:N4A	2.79	0.45
1:A:439:VAL:HA	1:A:440:PRO:HD3	1.79	0.45
1:B:383:LEU:HD21	1:B:402:VAL:HG13	1.97	0.45
1:A:449[B]:GLU:OE2	1:A:459:LYS:CE	2.64	0.45
1:C:309:PRO:O	1:C:312[B]:ARG:HD2	2.17	0.45
1:C:427:LEU:CD2	1:C:495:GLU:HG2	2.44	0.45
1:A:310:GLY:HA3	1:B:103:LEU:HA	1.99	0.45
1:B:108[B]:SER:OG	1:B:327:LEU:HD11	2.17	0.45
1:B:379:LEU:O	1:B:383:LEU:HB2	2.16	0.44
1:A:401[A]:THR:HG21	1:A:403:ASN:OD1	2.17	0.44
2:D:381:LYS:HD3	2:D:382:TYR:CZ	2.53	0.44
1:C:405:ASP:OD1	1:C:407:SER:HB2	2.18	0.43
4:B:604:EPE:H102	4:B:604:EPE:H61	1.73	0.43
1:A:142:THR:HG21	1:B:335[B]:GLN:HE21	1.84	0.43
1:B:459:LYS:HA	1:B:459:LYS:HD2	1.73	0.43
2:D:409:HIS:HE1	2:D:411:GLU:OE1	2.00	0.43
1:C:312[B]:ARG:HA	1:C:312[B]:ARG:NE	2.33	0.43
1:C:371:LYS:HZ1	2:D:49:TYR:HE2	1.66	0.43
5:B:1000:PMP:H5A1	5:B:1000:PMP:N4A	2.34	0.43
1:B:12:LEU:O	1:B:210:LYS:HE3	2.19	0.43
2:D:58:ASP:OD1	2:D:79:LYS:HG2	2.19	0.43
4:C:1001:EPE:H102	4:C:1001:EPE:H21	1.66	0.42
1:A:407:SER:HA	1:A:412:PHE:CD2	2.54	0.42
2:D:134:ASP:HB3	2:D:323:LEU:HD12	2.01	0.42
1:A:126:HIS:HB3	1:A:290[A]:SER:OG	2.19	0.42
2:D:141:ASN:HB2	2:D:305:LLP:H6	2.01	0.42
1:C:335:GLN:HB3	2:D:312[B]:ARG:NH1	2.34	0.42
1:A:371[B]:LYS:HD3	1:A:473:TYR:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:334:ILE:HG23	2:D:335:GLN:O	2.19	0.42
1:A:324[A]:LYS:HB2	1:A:325:PRO:CD	2.50	0.41
2:D:216:PRO:O	2:D:225[A]:SER:HA	2.20	0.41
1:A:7:LYS:HE2	1:A:294:GLU:HG2	2.03	0.41
2:D:312[A]:ARG:NE	2:D:312[A]:ARG:HA	2.34	0.41
1:B:305[A]:LYS:HZ3	5:B:1000:PMP:H4A1	1.85	0.41
1:B:251:TYR:CE1	1:B:305[B]:LYS:HE3	2.56	0.41
1:B:138:THR:CG2	1:B:316[A]:ILE:HG13	2.50	0.41
1:B:183:VAL:HA	1:B:184:PRO:HD3	1.94	0.41
1:C:321:LYS:HG3	6:C:1237:HOH:O	2.21	0.40
1:A:183:VAL:HA	1:A:184:PRO:HD3	1.93	0.40
1:B:203:THR:HA	1:B:204:PRO:HD2	1.79	0.40
1:B:463:ASN:C	1:B:465:ASN:H	2.25	0.40
1:A:449[B]:GLU:HG3	1:A:450:THR:N	2.37	0.40
2:D:216:PRO:O	2:D:225[B]:SER:HA	2.20	0.40

There are no symmetry-related clashes.

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	516/503 (103%)	502 (97%)	14 (3%)	0	100	100
1	B	511/503 (102%)	491 (96%)	19 (4%)	1 (0%)	47	38
1	C	506/503 (101%)	492 (97%)	14 (3%)	0	100	100
2	D	508/503 (101%)	494 (97%)	12 (2%)	2 (0%)	34	24
All	All	2041/2012 (101%)	1979 (97%)	59 (3%)	3 (0%)	47	43

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	414	THR
2	D	335	GLN
1	B	464	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	436/439 (99%)	431 (99%)	5 (1%)	73	73
1	B	411/439 (94%)	407 (99%)	4 (1%)	76	76
1	C	420/439 (96%)	413 (98%)	7 (2%)	60	57
2	D	425/438 (97%)	423 (100%)	2 (0%)	88	89
All	All	1692/1755 (96%)	1674 (99%)	18 (1%)	78	73

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	48	ASP
1	A	401[A]	THR
1	A	401[B]	THR
1	A	426	SER
1	B	44	LEU
1	B	210	LYS
1	B	459	LYS
1	B	488	LEU
1	C	94	SER
1	C	136	LEU
1	C	322	ILE
1	C	341[A]	THR
1	C	341[B]	THR
1	C	451[A]	GLU
1	C	451[B]	GLU
2	D	48	ASP
2	D	90	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	LLP	D	305	2	23,24,25	1.95	5 (21%)	25,32,34	1.65	4 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LLP	D	305	2	-	5/16/17/19	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	305	LLP	O3-C3	-5.47	1.24	1.37
2	D	305	LLP	C2-N1	3.57	1.40	1.33
2	D	305	LLP	C4-C4'	3.50	1.53	1.46
2	D	305	LLP	C4'-NZ	2.57	1.35	1.27
2	D	305	LLP	C6-N1	2.23	1.39	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	305	LLP	OP4-C5'-C5	3.83	116.66	109.35
2	D	305	LLP	C4-C4'-NZ	-3.53	108.10	124.31
2	D	305	LLP	OP2-P-OP4	-3.25	98.09	106.73
2	D	305	LLP	OP3-P-OP2	2.89	118.68	107.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	305	LLP	C5'-OP4-P-OP3
2	D	305	LLP	CA-CB-CG-CD
2	D	305	LLP	C5-C4-C4'-NZ
2	D	305	LLP	CD-CE-NZ-C4'
2	D	305	LLP	C3-C4-C4'-NZ

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	305	LLP	3	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	PLP	A	601	-	15,15,16	1.10	1 (6%)	20,22,23	1.23	2 (10%)
5	PMP	C	1000	-	16,16,16	1.09	1 (6%)	21,23,23	1.32	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	EPE	A	602	-	15,15,15	0.91	1 (6%)	18,20,20	2.14	5 (27%)
4	EPE	C	1001	-	15,15,15	0.87	1 (6%)	18,20,20	1.91	4 (22%)
4	EPE	C	1002	-	15,15,15	0.85	1 (6%)	18,20,20	2.09	5 (27%)
4	EPE	B	604	-	15,15,15	0.86	1 (6%)	18,20,20	2.11	6 (33%)
5	PMP	B	1000	-	16,16,16	1.01	1 (6%)	21,23,23	1.27	2 (9%)
4	EPE	A	603	-	15,15,15	0.99	1 (6%)	18,20,20	2.21	6 (33%)

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
3	PLP	A	601	-	-	0/6/6/8	0/1/1/1
5	PMP	C	1000	-	-	2/8/8/8	0/1/1/1
4	EPE	A	602	-	-	1/9/19/19	0/1/1/1
4	EPE	C	1001	-	-	7/9/19/19	0/1/1/1
4	EPE	C	1002	-	-	4/9/19/19	0/1/1/1
4	EPE	B	604	-	-	3/9/19/19	0/1/1/1
5	PMP	B	1000	-	-	4/8/8/8	0/1/1/1
4	EPE	A	603	-	-	2/9/19/19	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	EPE	C10-S	3.29	1.82	1.77
4	B	604	EPE	C10-S	3.04	1.81	1.77
4	A	602	EPE	C10-S	2.94	1.81	1.77
4	C	1002	EPE	C10-S	2.87	1.81	1.77
5	B	1000	PMP	C2-N1	2.76	1.39	1.33
5	C	1000	PMP	C2-N1	2.68	1.38	1.33
3	A	601	PLP	C2-N1	2.56	1.38	1.33
4	C	1001	EPE	C10-S	2.52	1.81	1.77

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	604	EPE	C5-N4-C3	5.65	121.55	108.83
4	C	1001	EPE	C5-N4-C3	5.54	121.31	108.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	EPE	C5-N4-C3	4.94	119.95	108.83
4	C	1002	EPE	C5-N4-C3	4.73	119.48	108.83
4	A	603	EPE	C5-N4-C3	4.52	119.00	108.83
4	C	1002	EPE	C6-N1-C2	4.26	118.41	108.83
4	A	602	EPE	O1S-S-C10	4.21	111.98	106.92
4	A	602	EPE	C7-N4-C3	4.10	121.71	111.23
4	A	603	EPE	C6-N1-C2	3.67	117.09	108.83
4	A	603	EPE	O2S-S-C10	3.49	111.11	106.92
4	B	604	EPE	C7-N4-C5	3.44	120.03	111.23
4	C	1001	EPE	C7-N4-C3	3.43	120.00	111.23
4	B	604	EPE	O3S-S-C10	3.25	111.02	105.77
4	A	603	EPE	C7-N4-C5	3.04	119.01	111.23
4	A	603	EPE	O1S-S-C10	2.96	110.47	106.92
4	A	603	EPE	C7-N4-C3	2.89	118.62	111.23
4	C	1001	EPE	C7-N4-C5	2.79	118.37	111.23
4	A	602	EPE	O2S-S-C10	-2.74	103.62	106.92
4	B	604	EPE	C7-N4-C3	2.64	117.97	111.23
4	C	1002	EPE	C7-N4-C5	2.58	117.83	111.23
5	B	1000	PMP	O3P-P-O4P	-2.56	99.91	106.73
4	C	1001	EPE	C6-C5-N4	2.53	115.83	110.64
4	C	1002	EPE	C9-N1-C2	-2.52	104.78	111.23
4	C	1002	EPE	O2S-S-C10	2.44	109.85	106.92
4	B	604	EPE	O2S-S-C10	2.32	109.71	106.92
4	A	602	EPE	C7-N4-C5	2.31	117.13	111.23
3	A	601	PLP	C6-C5-C4	2.31	119.97	118.16
5	C	1000	PMP	C5-C6-N1	-2.24	120.08	123.82
5	B	1000	PMP	C6-C5-C4	2.15	119.64	118.12
3	A	601	PLP	O3P-P-O2P	2.09	115.62	107.64
5	C	1000	PMP	C6-C5-C4	2.09	119.59	118.12
4	B	604	EPE	C6-C5-N4	2.06	114.86	110.64

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1000	PMP	C5-C4-C4A-N4A
4	A	602	EPE	C8-C7-N4-C3
4	C	1001	EPE	C10-C9-N1-C2
4	B	604	EPE	C10-C9-N1-C6
4	B	604	EPE	C8-C7-N4-C5
5	B	1000	PMP	C3-C4-C4A-N4A
5	B	1000	PMP	C5-C4-C4A-N4A

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Mol	Chain	Res	Type	Atoms
5	B	1000	PMP	C5A-O4P-P-O2P
5	B	1000	PMP	C5A-O4P-P-O3P
4	C	1001	EPE	N4-C7-C8-O8
4	C	1001	EPE	C9-C10-S-O3S
4	A	603	EPE	S-C10-C9-N1
4	C	1001	EPE	C10-C9-N1-C6
4	B	604	EPE	C10-C9-N1-C2
4	C	1002	EPE	C9-C10-S-O3S
4	C	1002	EPE	C9-C10-S-O1S
4	C	1002	EPE	C9-C10-S-O2S
4	A	603	EPE	C8-C7-N4-C5
4	C	1002	EPE	C10-C9-N1-C2
5	C	1000	PMP	C3-C4-C4A-N4A
4	C	1001	EPE	C8-C7-N4-C5
4	C	1001	EPE	C9-C10-S-O1S
4	C	1001	EPE	C9-C10-S-O2S

There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	PLP	1	0
5	C	1000	PMP	3	0
4	A	602	EPE	1	0
4	C	1001	EPE	1	0
4	C	1002	EPE	2	0
4	B	604	EPE	2	0
5	B	1000	PMP	5	0
4	A	603	EPE	1	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 (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	494/503 (98%)	-0.08	16 (3%)	47	50	14, 24, 45, 69	2 (0%)
1	B	497/503 (98%)	0.38	51 (10%)	6	7	15, 29, 66, 80	0
1	C	492/503 (97%)	-0.09	12 (2%)	59	62	14, 24, 49, 67	0
2	D	495/503 (98%)	0.06	22 (4%)	34	37	13, 24, 54, 65	0
All	All	1978/2012 (98%)	0.07	101 (5%)	28	31	13, 25, 57, 80	2 (0%)

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	271	SER	7.7
1	B	273	PRO	7.6
2	D	271	SER	6.6
1	B	87	ALA	6.6
1	B	91	ALA	6.5
1	B	272	SER	6.3
1	C	87	ALA	6.2
2	D	273	PRO	5.9
1	A	88	ASP	5.9
1	C	28	CYS	5.8
1	A	32	PHE	5.8
1	B	462	SER	5.8
1	C	90	SER	5.4
1	B	464	PRO	5.2
1	C	88	ASP	5.0
1	B	88	ASP	4.7
1	B	407	SER	4.7
1	B	388	ALA	4.6
1	B	412	PHE	4.5
1	A	90	SER	4.5
1	B	386	SER	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	35	PRO	4.4
1	A	87	ALA	4.4
1	A	91	ALA	4.2
1	B	269	ALA	4.2
1	B	32	PHE	4.2
1	C	462	SER	4.2
2	D	272	SER	4.1
1	B	498	ILE	4.1
1	B	461	VAL	4.1
1	B	268	LYS	3.8
1	C	27	THR	3.8
2	D	414	THR	3.8
2	D	270	GLN	3.8
1	C	91	ALA	3.7
1	B	389	PHE	3.5
1	B	35	PRO	3.5
1	B	406	ALA	3.3
1	C	387	ASP	3.3
1	A	89	LYS	3.3
1	B	463	ASN	3.3
1	B	410	PRO	3.3
2	D	387	ASP	3.2
1	B	465	ASN	3.2
1	A	497	GLY	3.2
2	D	435	GLY	3.2
1	A	499	SER	3.1
1	B	274	LYS	3.1
1	A	34	ASP	3.0
2	D	2	THR	3.0
1	A	33	GLN	3.0
2	D	32	PHE	2.9
1	A	387	ASP	2.9
1	B	262	ASP	2.9
1	B	90	SER	2.9
1	B	493	TYR	2.9
1	C	89	LYS	2.9
2	D	385	GLN	2.8
1	B	2	THR	2.8
1	B	414	THR	2.8
1	B	422	GLN	2.8
1	B	265	GLU	2.8
2	D	407	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	416	TYR	2.7
1	B	408	VAL	2.7
1	B	496	PHE	2.6
1	B	497	GLY	2.6
1	B	205	GLY	2.6
1	C	498	ILE	2.6
1	C	499	SER	2.6
2	D	416	TYR	2.6
2	D	263	LEU	2.6
2	D	410	PRO	2.6
1	B	432	VAL	2.6
1	B	39	PHE	2.5
1	A	36	ASN	2.5
1	A	462	SER	2.4
1	B	405	ASP	2.4
1	B	37	ILE	2.4
2	D	462	SER	2.3
1	B	267	GLU	2.3
1	B	417	ASN	2.3
1	B	435	GLY	2.3
1	B	495	GLU	2.3
2	D	35	PRO	2.2
2	D	274	LYS	2.2
2	D	22	PRO	2.2
2	D	88	ASP	2.2
2	D	268	LYS	2.1
1	B	36	ASN	2.1
1	B	270	GLN	2.1
1	B	459	LYS	2.1
1	C	36	ASN	2.1
1	B	385	GLN	2.1
1	A	407	SER	2.1
1	B	466	ILE	2.1
2	D	39	PHE	2.0
2	D	421	TYR	2.0
1	A	434	ARG	2.0
1	B	436	VAL	2.0
1	B	419	ASP	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LLP	D	305	24/25	0.91	0.15	16,32,38,39	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EPE	C	1002	15/15	0.76	0.20	44,58,75,75	0
4	EPE	A	603	15/15	0.85	0.16	47,56,69,70	0
4	EPE	C	1001	15/15	0.91	0.18	42,58,67,67	0
3	PLP	A	601	15/16	0.92	0.15	31,38,41,41	0
4	EPE	B	604	15/15	0.93	0.30	32,34,39,40	11
5	PMP	C	1000	16/16	0.94	0.12	24,39,44,47	0
5	PMP	B	1000	16/16	0.96	0.10	31,40,43,45	0
4	EPE	A	602	15/15	0.96	0.13	35,40,50,51	0

6.5 Other polymers (i)

There are no such residues in this entry.