WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2023 – 10:44 PM EDT

PDB ID	:	4ZDO
Title	:	The crystal structure of T325S mutant of human SepSecS in complex with selenocysteine tRNA (tRNASec)
Authors	:	French, R.L.; Simonovic, M.
Deposited on	:	2015-04-17
Resolution	:	2.65 Å(reported)

The following versions of software and data (see references ⓘ) 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	:	2.35.1
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)	:	2.35.1
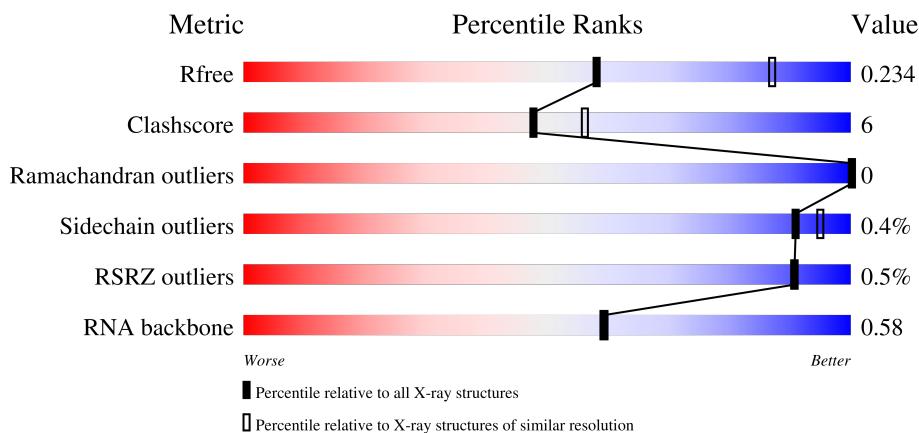
1   Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
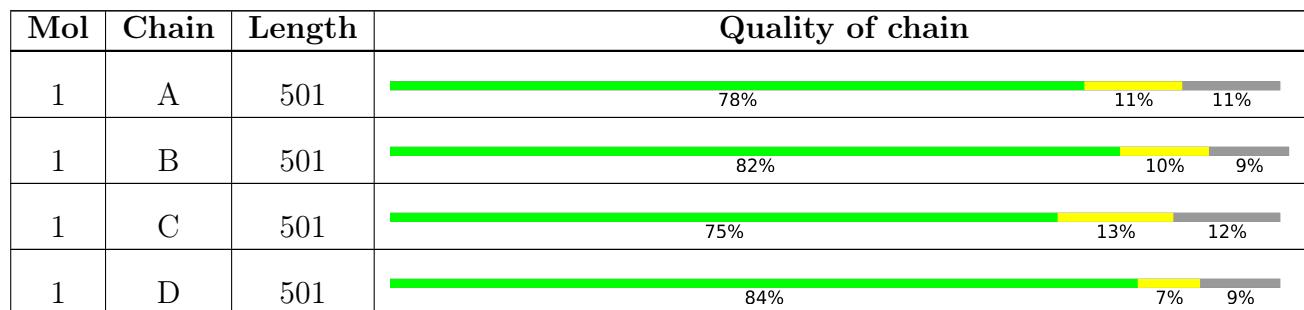
The reported resolution of this entry is 2.65 Å.

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		0.234
Clashscore		6
Ramachandran outliers		0
Sidechain outliers		0.4%
RSRZ outliers		0.5%
RNA backbone		0.58

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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)
RNA backbone	3102	1010 (2.96-2.36)

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 of 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	501	78% 11% 11%
1	B	501	82% 10% 9%
1	C	501	75% 13% 12%
1	D	501	84% 7% 9%

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Mol	Chain	Length	Quality of chain
2	E	87	10% 44% 43% 14%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 17260 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 O-phosphoseryl-tRNA(Sec) selenium transferase.

| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	0	0
			3349	2124	581	617	27			
1	B	458	Total	C	N	O	S	0	0	0
			3412	2161	595	629	27			
1	C	441	Total	C	N	O	S	0	0	0
			3343	2116	583	618	26			
1	D	458	Total	C	N	O	S	0	0	0
			3437	2173	604	632	28			
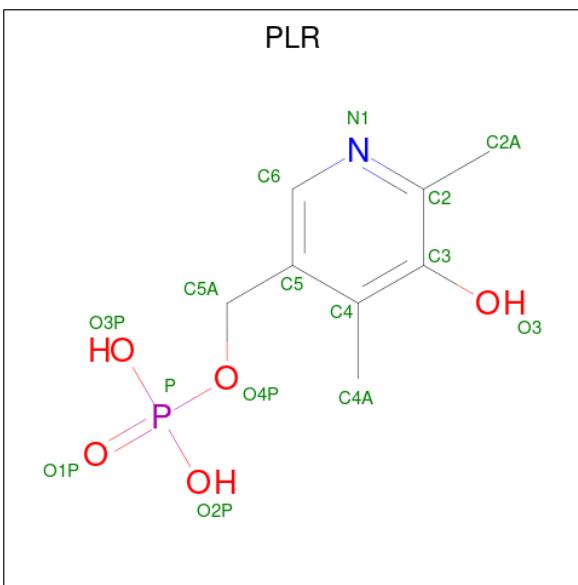
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	325	SER	THR	engineered mutation	UNP Q9HD40
B	325	SER	THR	engineered mutation	UNP Q9HD40
C	325	SER	THR	engineered mutation	UNP Q9HD40
D	325	SER	THR	engineered mutation	UNP Q9HD40

- Molecule 2 is a RNA chain called selenocysteine tRNA.
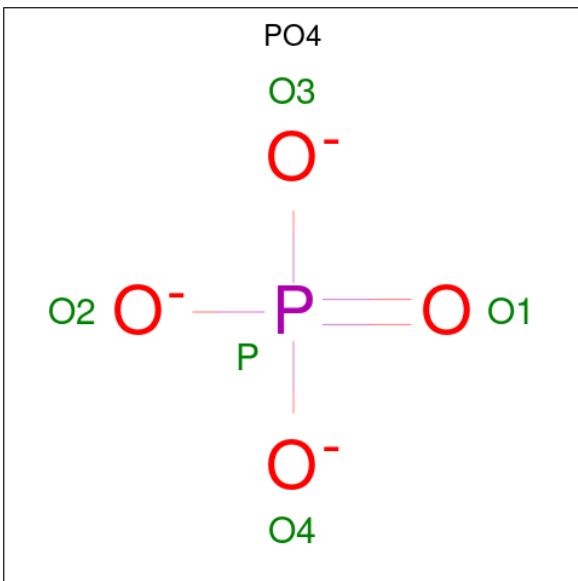
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	75	Total	C	N	O	P	0	75	0
			3170	1410	540	1070	150			

- Molecule 3 is (5-HYDROXY-4,6-DIMETHYLPYRIDIN-3-YL)METHYL DIHYDROGEN PHOSPHATE (three-letter code: PLR) (formula: $C_8H_{12}NO_5P$).

PLR

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

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

PO4

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 5	O 4	P 1	0	0
4	B	1	Total 5	O 4	P 1	0	0
4	C	1	Total 5	O 4	P 1	0	0
4	D	1	Total 5	O 4	P 1	0	0
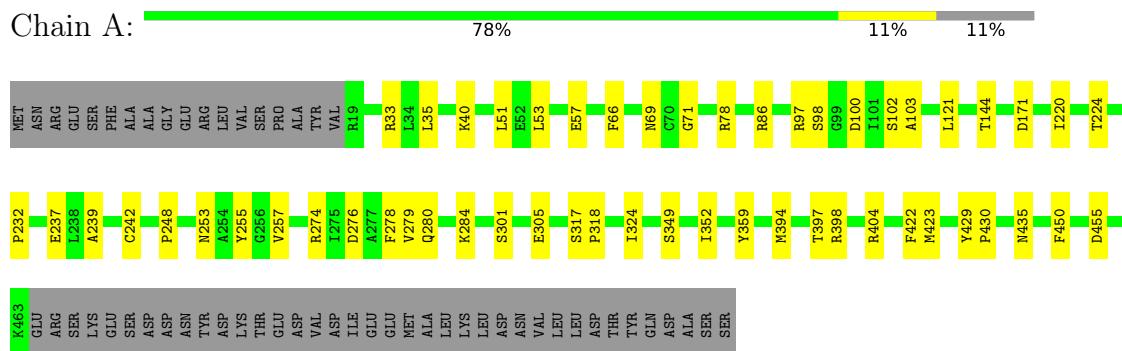
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	113	Total 113	O 113	0	0
5	B	118	Total 118	O 118	0	0
5	C	115	Total 115	O 115	0	0
5	D	121	Total 121	O 121	0	0
5	E	2	Total 2	O 2	0	0
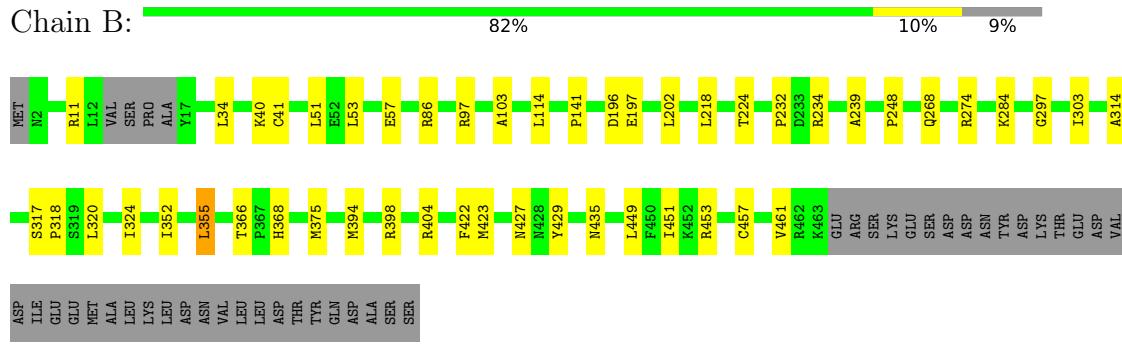
3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.
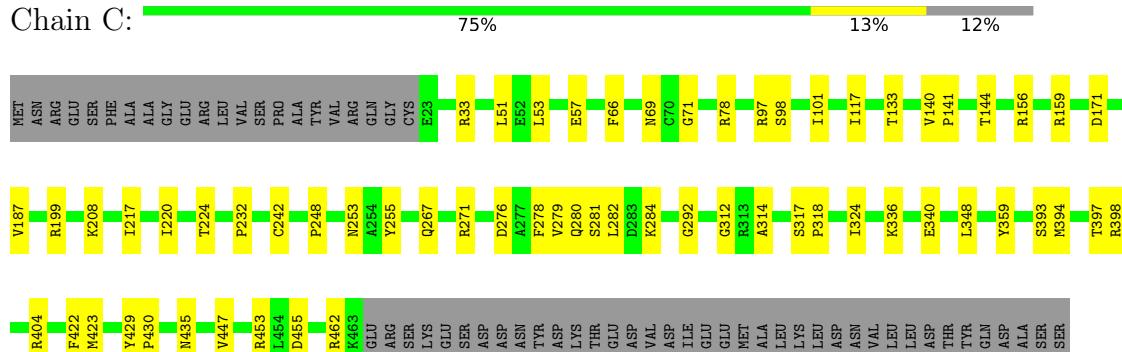
- Molecule 1: O-phosphoseryl-tRNA(Sec) selenium transferase

Chain A:

- Molecule 1: O-phosphoseryl-tRNA(Sec) selenium transferase
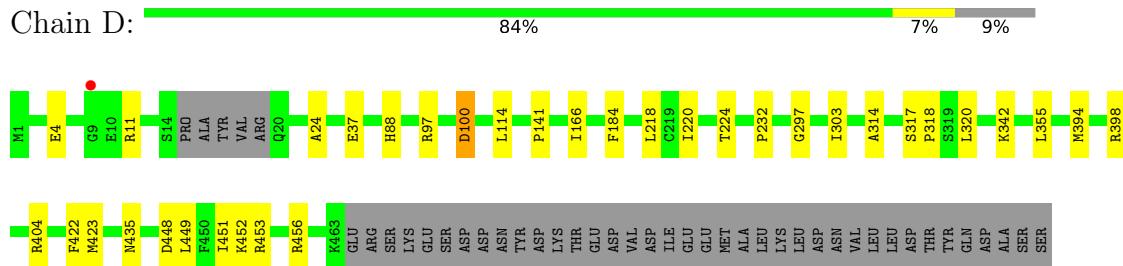
Chain B:

- Molecule 1: O-phosphoseryl-tRNA(Sec) selenium transferase
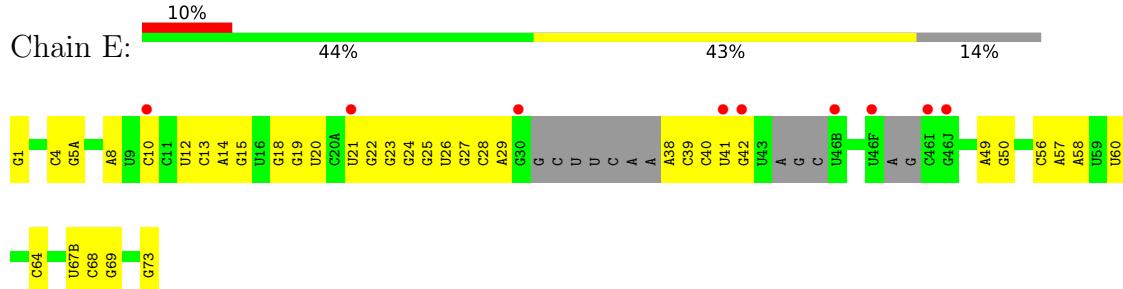
Chain C:

• Molecule 1: O-phosphoseryl-tRNA(Sec) selenium transferase

Chain D:

• Molecule 2: selenocysteine tRNA

Chain E:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α, β, γ	166.24Å 166.24Å 238.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.49 – 2.65 49.49 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.49-2.65) 79.1 (49.49-2.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.14 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.198 , 0.235 0.198 , 0.234	Depositor DCC
R_{free} test set	4978 reflections (3.73%)	wwPDB-VP
Wilson B-factor (Å^2)	41.9	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 24.0	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.470 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	17260	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% 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: PO4, PLR

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	0.77	0/3411	0.57	0/4622
1	B	0.74	1/3471 (0.0%)	0.53	0/4703
1	C	0.77	0/3404	0.55	0/4612
1	D	0.74	0/3497	0.56	2/4732 (0.0%)
2	E	0.36	2/3528 (0.1%)	0.71	0/5476
All	All	0.69	3/17311 (0.0%)	0.59	2/24145 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1[A]	G	OP3-P	-11.03	1.48	1.61
2	E	1[B]	G	OP3-P	-11.03	1.48	1.61
1	B	41	CYS	CB-SG	-5.15	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	37	GLU	CB-CA-C	-5.36	99.69	110.40
1	D	100	ASP	CB-CA-C	5.05	120.49	110.40

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	3349	0	3286	43	0
1	B	3412	0	3342	39	0
1	C	3343	0	3298	45	0
1	D	3437	0	3374	35	0
2	E	3170	0	1553	46	0
3	A	15	0	7	3	0
3	B	15	0	7	1	0
3	C	15	0	7	2	0
3	D	15	0	7	0	0
4	A	5	0	0	1	0
4	B	5	0	0	0	0
4	C	5	0	0	1	0
4	D	5	0	0	0	0
5	A	113	0	0	2	0
5	B	118	0	0	3	0
5	C	115	0	0	7	0
5	D	121	0	0	4	0
5	E	2	0	0	0	0
All	All	17260	0	14881	188	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 (188) 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:33:ARG:NH2	2:E:42[B]:G:OP1	1.72	1.22
1:D:398:ARG:HH22	2:E:38[A]:A:H4'	1.26	0.95
1:D:394:MET:O	1:D:398:ARG:HD2	1.67	0.94
1:D:88:HIS:HD2	5:D:1203:HOH:O	1.53	0.91
1:D:398:ARG:NH2	2:E:38[A]:A:H4'	1.87	0.89
1:D:97:ARG:O	1:D:100:ASP:O	1.94	0.86
1:D:398:ARG:HH22	2:E:38[A]:A:C4'	1.92	0.83
1:D:398:ARG:HH12	2:E:38[A]:A:H4'	1.43	0.82
1:A:398:ARG:HE	1:B:11:ARG:HH12	1.24	0.81
1:C:159:ARG:NH2	1:C:217:ILE:O	2.12	0.80
5:C:1134:HOH:O	1:D:24:ALA:CB	2.31	0.78
1:D:398:ARG:NH1	2:E:38[A]:A:H4'	1.99	0.77
1:A:144:THR:HB	3:A:1001:PLR:H5A1	1.66	0.77
1:C:271:ARG:NH1	2:E:56[A]:C:OP1	2.18	0.75
1:D:88:HIS:CD2	5:D:1203:HOH:O	2.33	0.75
1:D:398:ARG:O	1:D:453:ARG:NH1	2.19	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:ARG:O	1:B:453:ARG:NH1	2.21	0.74
1:A:253:ASN:HD22	1:A:280:GLN:HE21	1.35	0.73
1:B:355:LEU:HD13	1:B:451:ILE:HG23	1.69	0.73
1:C:144:THR:HG1	1:C:281:SER:HG	1.36	0.73
1:C:462:ARG:HG2	1:C:462:ARG:HH11	1.54	0.73
2:E:73[A]:G:OP2	2:E:73[A]:G:N2	2.19	0.72
1:C:267:GLN:HG3	5:C:1101:HOH:O	1.90	0.72
1:A:33:ARG:HH11	1:A:33:ARG:HG2	1.56	0.70
1:D:398:ARG:CZ	2:E:38[A]:A:H4'	2.21	0.70
1:D:394:MET:O	1:D:398:ARG:CD	2.39	0.70
2:E:50[B]:G:N1	2:E:64[B]:C:N3	2.36	0.69
1:C:278:PHE:CD2	1:C:280:GLN:NE2	2.61	0.69
1:D:456:ARG:HG2	1:D:456:ARG:HH11	1.58	0.68
1:A:33:ARG:HG2	1:A:33:ARG:NH1	2.09	0.67
1:B:355:LEU:CD1	1:B:451:ILE:HG23	2.23	0.67
1:C:398:ARG:NH1	1:D:4:GLU:OE1	2.27	0.67
1:B:197:GLU:OE1	1:B:368:HIS:ND1	2.27	0.66
1:A:257:VAL:HG23	1:A:280:GLN:HG2	1.77	0.66
1:A:398:ARG:NE	1:B:11:ARG:HH12	1.93	0.66
1:C:144:THR:HB	3:C:1001:PLR:H5A2	1.79	0.65
2:E:73[B]:G:OP2	2:E:73[B]:G:N2	2.20	0.64
1:B:457:CYS:O	1:B:461:VAL:HG23	1.98	0.63
1:C:66:PHE:HB2	1:C:69:ASN:HB2	1.80	0.62
1:B:141:PRO:HG2	1:B:314:ALA:HB1	1.82	0.62
1:B:449:LEU:HD22	1:B:453:ARG:HH21	1.65	0.62
2:E:38[B]:A:O2'	2:E:39[B]:C:OP2	2.17	0.62
1:A:100:ASP:OD1	1:A:102:SER:OG	2.17	0.61
2:E:18[B]:G:HO2'	2:E:57[B]:A:H2	1.48	0.60
1:C:282:LEU:HD12	1:C:292:GLY:HA3	1.83	0.60
1:D:355:LEU:HD12	1:D:451:ILE:HG23	1.82	0.60
1:C:398:ARG:HH21	1:D:11:ARG:NH2	2.00	0.60
1:B:427:ASN:ND2	5:B:1108:HOH:O	2.34	0.59
1:B:422:PHE:O	1:B:423:MET:HB2	2.04	0.58
5:C:1134:HOH:O	1:D:24:ALA:HB1	1.96	0.58
1:C:278:PHE:HD2	1:C:280:GLN:HE21	1.51	0.58
1:A:422:PHE:O	1:A:423:MET:HB2	2.04	0.58
1:D:398:ARG:HH12	2:E:38[A]:A:C4'	2.15	0.58
1:D:452:LYS:NZ	5:D:1112:HOH:O	2.38	0.57
1:A:66:PHE:HB2	1:A:69:ASN:HB2	1.87	0.56
1:D:449:LEU:O	1:D:453:ARG:HG3	2.05	0.56
1:B:449:LEU:O	1:B:453:ARG:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:LEU:HD11	1:D:320:LEU:HD13	1.87	0.56
2:E:19[B]:G:N1	2:E:56[B]:C:N3	2.48	0.56
1:A:171:ASP:OD2	1:A:423:MET:N	2.38	0.56
1:B:404:ARG:HB3	1:B:435:ASN:HB2	1.88	0.55
1:A:394:MET:HG2	1:B:11:ARG:HD2	1.88	0.55
1:C:359:TYR:OH	1:C:455:ASP:OD1	2.16	0.55
1:A:237:GLU:OE1	1:A:237:GLU:N	2.39	0.54
1:A:40:LYS:NZ	5:A:1113:HOH:O	2.40	0.54
1:A:352:ILE:HD11	1:A:450:PHE:HE2	1.73	0.54
1:C:33:ARG:NH2	2:E:42[A]:G:OP1	2.37	0.53
1:C:199:ARG:HB3	5:C:1162:HOH:O	2.09	0.52
1:A:33:ARG:HH11	1:A:33:ARG:CG	2.22	0.52
5:C:1134:HOH:O	1:D:24:ALA:HB2	2.04	0.52
2:E:4[B]:C:H2'	2:E:5(A)[B]:G:C8	2.44	0.52
1:C:284:LYS:NZ	3:C:1001:PLR:O3	2.41	0.52
1:A:97:ARG:HG3	1:A:103:ALA:HB3	1.91	0.52
1:B:51:LEU:HD21	1:B:324:ILE:HG23	1.90	0.52
1:A:144:THR:HG23	1:A:279:VAL:HG12	1.91	0.52
1:B:97:ARG:HG3	1:B:103:ALA:HB3	1.93	0.51
1:A:224:THR:O	1:A:232:PRO:HG3	2.10	0.51
2:E:12[B]:U:H2'	2:E:13[B]:C:C6	2.46	0.51
1:C:98:SER:HA	1:C:312:GLY:HA2	1.93	0.51
1:C:97:ARG:NH2	4:C:1002:PO4:O1	2.36	0.51
1:D:422:PHE:O	1:D:423:MET:HB2	2.10	0.51
1:C:253:ASN:HB3	1:C:280:GLN:HG3	1.93	0.50
2:E:12[A]:U:H2'	2:E:13[A]:C:C6	2.47	0.50
2:E:28[B]:C:H2'	2:E:29[B]:A:H8	1.76	0.50
1:B:224:THR:O	1:B:232:PRO:HG3	2.11	0.50
1:D:224:THR:O	1:D:232:PRO:HG3	2.12	0.49
1:A:278:PHE:HD2	1:A:280:GLN:NE2	2.11	0.49
1:B:352:ILE:HG23	1:B:375:MET:HE2	1.95	0.49
2:E:10[B]:C:O2	2:E:25[B]:G:N2	2.46	0.49
1:B:366:THR:O	1:B:366:THR:OG1	2.26	0.49
1:D:317:SER:HB3	1:D:318:PRO:HD3	1.94	0.49
2:E:58[B]:A:H2	2:E:60[B]:U:HO2'	1.60	0.49
1:C:71:GLY:O	1:C:78:ARG:NH2	2.46	0.49
1:B:394:MET:O	1:B:398:ARG:HG3	2.13	0.48
1:A:278:PHE:HD2	1:A:280:GLN:HE22	1.61	0.48
1:C:141:PRO:HG2	1:C:314:ALA:HB1	1.95	0.48
2:E:19[B]:G:H1'	2:E:20[B]:U:H5	1.78	0.48
1:B:218:LEU:O	1:B:248:PRO:HG2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:GLY:HA3	1:B:303:ILE:HD11	1.95	0.48
2:E:28[A]:C:H2'	2:E:29[A]:A:H8	1.78	0.48
1:C:422:PHE:O	1:C:423:MET:HB2	2.13	0.48
2:E:21[A]:U:H2'	2:E:22[A]:G:O4'	2.13	0.48
1:C:220:ILE:HD12	1:C:242:CYS:SG	2.54	0.48
1:A:51:LEU:HD21	1:A:324:ILE:HG23	1.96	0.47
1:A:53:LEU:O	1:A:57:GLU:HG2	2.14	0.47
1:A:239:ALA:HB1	1:A:274:ARG:H	1.79	0.47
1:A:404:ARG:HB3	1:A:435:ASN:HB2	1.97	0.47
1:B:284:LYS:NZ	3:B:1001:PLR:O3	2.48	0.47
1:B:317:SER:HB3	1:B:318:PRO:HD3	1.95	0.47
1:B:398:ARG:HH22	2:E:38[B]:A:H4'	1.80	0.47
1:D:448:ASP:O	1:D:452:LYS:HG2	2.15	0.47
2:E:41[A]:U:H2'	2:E:42[A]:G:C8	2.50	0.47
1:A:429:TYR:CG	1:A:430:PRO:HD2	2.50	0.47
1:C:53:LEU:O	1:C:57:GLU:HG3	2.15	0.47
1:D:456:ARG:HG2	1:D:456:ARG:NH1	2.27	0.46
1:B:114:LEU:HD11	1:B:320:LEU:HD13	1.97	0.46
1:C:462:ARG:HG2	1:C:462:ARG:NH1	2.24	0.46
2:E:14[A]:A:H2'	2:E:15[A]:G:H8	1.81	0.46
1:D:342:LYS:NZ	5:D:1121:HOH:O	2.47	0.46
2:E:19[B]:G:N2	2:E:56[B]:C:O2	2.34	0.46
1:B:40:LYS:HE2	1:B:40:LYS:HB3	1.80	0.45
1:B:239:ALA:HB1	1:B:274:ARG:H	1.80	0.45
1:C:398:ARG:O	1:C:453:ARG:NH1	2.50	0.45
1:A:253:ASN:O	1:A:280:GLN:HG3	2.16	0.45
1:B:202:LEU:HD11	1:B:234:ARG:HD3	1.98	0.45
2:E:14[A]:A:H2'	2:E:15[A]:G:C8	2.52	0.45
3:A:1001:PLR:H5A2	3:A:1001:PLR:H4A1	1.47	0.45
1:A:255:TYR:HB3	1:A:284:LYS:HB3	1.99	0.45
2:E:39[A]:C:H2'	2:E:40[A]:C:H6	1.82	0.45
1:A:98:SER:OG	4:A:1002:PO4:O3	2.26	0.45
1:A:220:ILE:HD12	1:A:242:CYS:SG	2.57	0.45
2:E:26[A]:U:H2'	2:E:27[A]:G:C8	2.52	0.44
2:E:28[A]:C:H2'	2:E:29[A]:A:C8	2.52	0.44
1:A:35:LEU:HD11	1:A:121:LEU:HD21	1.99	0.44
2:E:68[A]:C:H2'	2:E:69[A]:G:C8	2.53	0.44
1:A:397:THR:OG1	1:B:11:ARG:HD3	2.18	0.44
1:B:196:ASP:O	1:B:429:TYR:OH	2.26	0.44
1:C:255:TYR:HB3	1:C:284:LYS:HB3	2.00	0.44
1:C:394:MET:O	1:C:398:ARG:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:SER:HB3	1:C:318:PRO:HD3	1.99	0.44
1:B:268:GLN:NE2	5:B:1119:HOH:O	2.50	0.44
1:D:141:PRO:HG2	1:D:314:ALA:HB1	2.00	0.44
2:E:8[A]:A:O2'	2:E:49[A]:A:O2'	2.04	0.43
2:E:28[B]:C:H2'	2:E:29[B]:A:C8	2.53	0.43
1:A:317:SER:HB3	1:A:318:PRO:HD3	2.00	0.43
1:C:187:VAL:HG11	1:C:208:LYS:HG2	2.00	0.43
1:B:449:LEU:HD22	1:B:453:ARG:NH2	2.33	0.43
1:D:404:ARG:HB2	1:D:435:ASN:HB2	1.99	0.43
1:D:297:GLY:HA3	1:D:303:ILE:HD11	2.00	0.43
1:B:398:ARG:NH2	2:E:38[B]:A:H4'	2.33	0.43
1:A:278:PHE:CD2	1:A:280:GLN:NE2	2.82	0.43
2:E:12[A]:U:H2'	2:E:13[A]:C:H6	1.83	0.43
1:C:140:VAL:HA	1:C:141:PRO:HD3	1.87	0.43
2:E:68[B]:C:H2'	2:E:69[B]:G:C8	2.53	0.43
1:A:71:GLY:O	1:A:78:ARG:NH2	2.51	0.43
1:C:51:LEU:HD21	1:C:324:ILE:HG23	2.00	0.43
2:E:4[A]:C:H2'	2:E:5(A)[A]:G:C8	2.54	0.42
1:B:355:LEU:HD12	1:B:451:ILE:HG23	2.01	0.42
1:C:156:ARG:HD2	5:C:1154:HOH:O	2.19	0.42
1:C:429:TYR:CG	1:C:430:PRO:HD2	2.53	0.42
2:E:68[A]:C:H2'	2:E:69[A]:G:H8	1.83	0.42
1:A:86:ARG:HH12	1:B:86:ARG:NH2	2.16	0.42
1:A:398:ARG:HH21	1:B:11:ARG:HH22	1.66	0.42
1:C:348:LEU:HD13	1:C:447:VAL:HG22	2.02	0.42
1:C:393:SER:O	1:C:397:THR:HG23	2.19	0.42
2:E:13[B]:C:H2'	2:E:14[B]:A:C8	2.54	0.42
1:C:394:MET:HA	1:D:11:ARG:HD3	2.02	0.42
1:A:359:TYR:OH	1:A:455:ASP:OD1	2.30	0.42
1:C:144:THR:HG23	1:C:279:VAL:HG12	2.01	0.41
1:C:171:ASP:OD2	1:C:423:MET:N	2.52	0.41
1:C:224:THR:O	1:C:232:PRO:HG3	2.19	0.41
1:D:184:PHE:CE2	1:D:218:LEU:HD22	2.55	0.41
1:A:284:LYS:NZ	3:A:1001:PLR:O3	2.52	0.41
2:E:19[A]:G:H1'	2:E:20[A]:U:H5	1.83	0.41
2:E:67(B)[B]:U:H2'	2:E:68[B]:C:C6	2.55	0.41
1:B:53:LEU:O	1:B:57:GLU:HG2	2.21	0.41
1:B:404:ARG:NH2	5:B:1107:HOH:O	2.54	0.41
2:E:23[B]:G:H2'	2:E:24[B]:G:C8	2.55	0.41
1:D:166:ILE:HB	1:D:220:ILE:HG12	2.02	0.41
1:A:301:SER:O	1:A:305:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:MET:HG2	5:A:1151:HOH:O	2.20	0.40
1:C:336:LYS:HE2	1:C:340:GLU:OE1	2.20	0.40
1:C:248:PRO:HA	1:C:276:ASP:OD2	2.21	0.40
1:C:267:GLN:CG	5:C:1101:HOH:O	2.58	0.40
2:E:39[A]:C:H2'	2:E:40[A]:C:C6	2.56	0.40
1:A:248:PRO:HA	1:A:276:ASP:OD2	2.21	0.40
1:C:117:ILE:HA	1:C:117:ILE:HD13	1.82	0.40
1:C:404:ARG:HB3	1:C:435:ASN:HB2	2.02	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	443/501 (88%)	427 (96%)	16 (4%)	0	100	100
1	B	454/501 (91%)	440 (97%)	14 (3%)	0	100	100
1	C	439/501 (88%)	425 (97%)	14 (3%)	0	100	100
1	D	454/501 (91%)	437 (96%)	17 (4%)	0	100	100
All	All	1790/2004 (89%)	1729 (97%)	61 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	348/430 (81%)	347 (100%)	1 (0%)	92	96
1	B	351/430 (82%)	349 (99%)	2 (1%)	86	92
1	C	352/430 (82%)	350 (99%)	2 (1%)	86	92
1	D	354/430 (82%)	354 (100%)	0	100	100
All	All	1405/1720 (82%)	1400 (100%)	5 (0%)	91	95

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	349	SER
1	B	34	LEU
1	B	355	LEU
1	C	101	ILE
1	C	133	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
1	A	253	ASN
1	A	264	HIS
1	B	56	HIS
1	D	88	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	E	0/87	-	-

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

WORLDWIDE
wwPDB
PROTEIN DATA BANK

5.5　Carbohydrates (i)

There are no monosaccharides 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	PLR	A	1001	1	15,15,15	1.50	2 (13%)	20,22,22	1.67	3 (15%)
3	PLR	C	1001	1	15,15,15	1.24	1 (6%)	20,22,22	1.22	2 (10%)
4	PO4	C	1002	-	4,4,4	0.93	0	6,6,6	0.44	0
3	PLR	B	1001	1	15,15,15	1.38	2 (13%)	20,22,22	1.18	3 (15%)
4	PO4	B	1002	-	4,4,4	0.87	0	6,6,6	0.67	0
4	PO4	A	1002	-	4,4,4	1.01	0	6,6,6	0.41	0
4	PO4	D	1002	-	4,4,4	0.98	0	6,6,6	0.37	0
3	PLR	D	1001	1	15,15,15	1.56	3 (20%)	20,22,22	1.57	4 (20%)

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	PLR	C	1001	1	-	0/6/6/6	0/1/1/1
3	PLR	A	1001	1	-	3/6/6/6	0/1/1/1
3	PLR	B	1001	1	-	0/6/6/6	0/1/1/1
3	PLR	D	1001	1	-	3/6/6/6	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1001	PLR	C3-C2	-3.26	1.37	1.40
3	B	1001	PLR	C3-C2	-2.97	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	PLR	C3-C2	-2.94	1.38	1.40
3	A	1001	PLR	C5-C4	-2.71	1.37	1.40
3	C	1001	PLR	C3-C2	-2.66	1.38	1.40
3	D	1001	PLR	C5-C4	-2.32	1.37	1.40
3	B	1001	PLR	C5-C4	-2.03	1.38	1.40
3	D	1001	PLR	P-O3P	-2.02	1.47	1.54

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1001	PLR	C6-C5-C4	4.69	121.85	118.16
3	D	1001	PLR	C6-C5-C4	4.21	121.47	118.16
3	A	1001	PLR	C4A-C4-C5	-3.61	117.21	120.94
3	C	1001	PLR	C6-C5-C4	3.07	120.57	118.16
3	B	1001	PLR	O4P-C5A-C5	2.89	114.87	109.35
3	D	1001	PLR	C5-C6-N1	-2.86	119.05	123.82
3	A	1001	PLR	C5-C6-N1	-2.80	119.16	123.82
3	B	1001	PLR	C6-C5-C4	2.56	120.17	118.16
3	D	1001	PLR	C4A-C4-C5	-2.31	118.56	120.94
3	B	1001	PLR	C5-C6-N1	-2.24	120.09	123.82
3	D	1001	PLR	C2A-C2-C3	-2.22	118.14	120.89
3	C	1001	PLR	C4A-C4-C5	-2.04	118.83	120.94

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	PLR	C5A-O4P-P-O1P
3	A	1001	PLR	C5A-O4P-P-O2P
3	A	1001	PLR	C5A-O4P-P-O3P
3	D	1001	PLR	C5A-O4P-P-O2P
3	D	1001	PLR	C5A-O4P-P-O1P
3	D	1001	PLR	C5A-O4P-P-O3P

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	PLR	3	0
3	C	1001	PLR	2	0
4	C	1002	PO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1001	PLR	1	0
4	A	1002	PO4	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	445/501 (88%)	-0.86	0	100	100	25, 36, 59, 94	0
1	B	458/501 (91%)	-0.82	0	100	100	25, 38, 82, 129	0
1	C	441/501 (88%)	-0.85	0	100	100	26, 37, 59, 109	0
1	D	458/501 (91%)	-0.79	1 (0%)	95	96	24, 38, 78, 129	0
2	E	75/87 (86%)	0.90	9 (12%)	4	3	52, 82, 100, 103	0
All	All	1877/2091 (89%)	-0.76	10 (0%)	91	91	24, 38, 81, 129	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	46(I)[A]	C	4.3
2	E	42[A]	G	3.5
2	E	41[A]	U	3.4
2	E	46(J)[A]	G	3.4
2	E	46(F)[A]	U	3.4
2	E	30[A]	G	3.0
2	E	46(B)[A]	U	2.4
2	E	21[A]	U	2.4
2	E	10[A]	C	2.3
1	D	9	GLY	2.2

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	PO4	C	1002	5/5	0.90	0.09	75,79,84,97	0
4	PO4	B	1002	5/5	0.91	0.07	64,72,78,95	0
4	PO4	A	1002	5/5	0.92	0.08	68,69,73,96	0
4	PO4	D	1002	5/5	0.92	0.10	68,78,81,98	0
3	PLR	A	1001	15/15	0.98	0.11	30,33,37,38	0
3	PLR	D	1001	15/15	0.98	0.13	28,34,39,40	0
3	PLR	C	1001	15/15	0.99	0.11	34,37,41,41	0
3	PLR	B	1001	15/15	0.99	0.11	30,35,37,38	0

6.5 Other polymers ⓘ

There are no such residues in this entry.