Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:43 AM GMT

PDB ID	:	2IE4
Title	:	Structure of the Protein Phosphatase 2A Core Enzyme Bound to okadaic acid
Authors	:	Xing, Y.; Xu, Y.; Chen, Y.; Jeffrey, P.D.; Chao, Y.; Shi, Y.
Deposited on	:	2006-09-17
Resolution	:	2.60 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 (i)) were used in the production of this report:

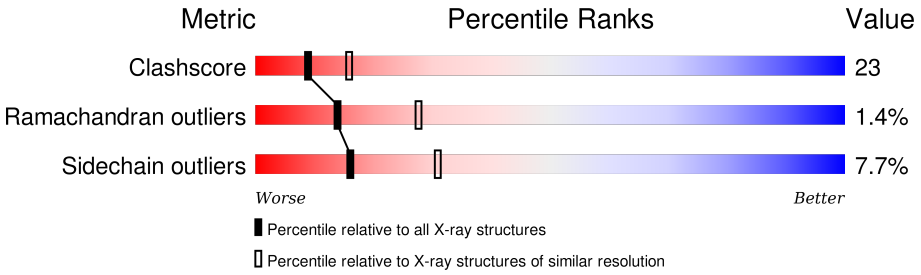
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	589	55% 40%
2	C	309	61% 28% 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6972 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 Protein Phosphatase 2, regulatory subunit A (PR 65), alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	581	4527	2877	763	860	27	0	0	0

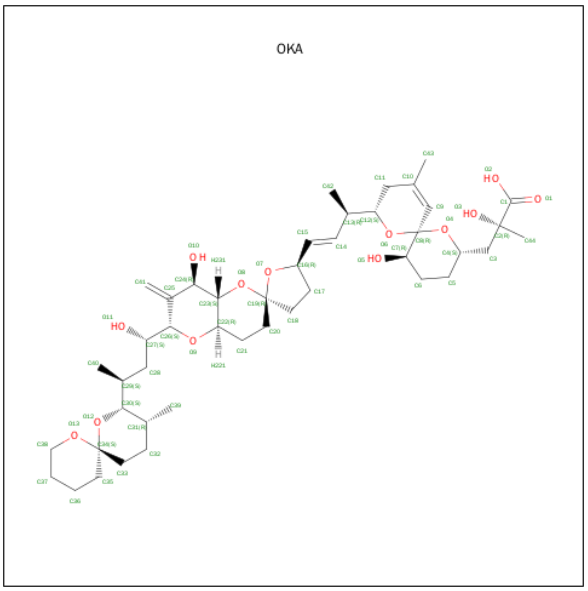
- Molecule 2 is a protein called Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	288	2322	1471	396	440	15	0	0	0

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
3	C	2	2	2	0	0

- Molecule 4 is OKADAIC ACID (three-letter code: OKA) (formula: $C_{44}H_{68}O_{13}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 57 44 13	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	27	Total O 27 27	0	0
5	C	37	Total O 37 37	0	0

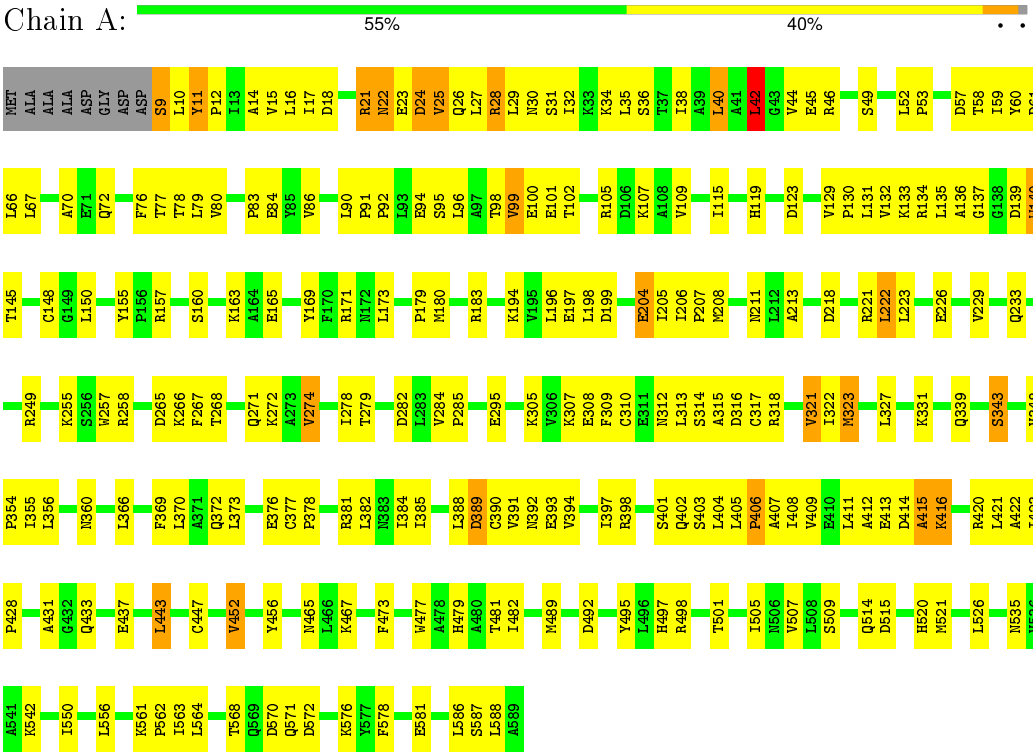
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

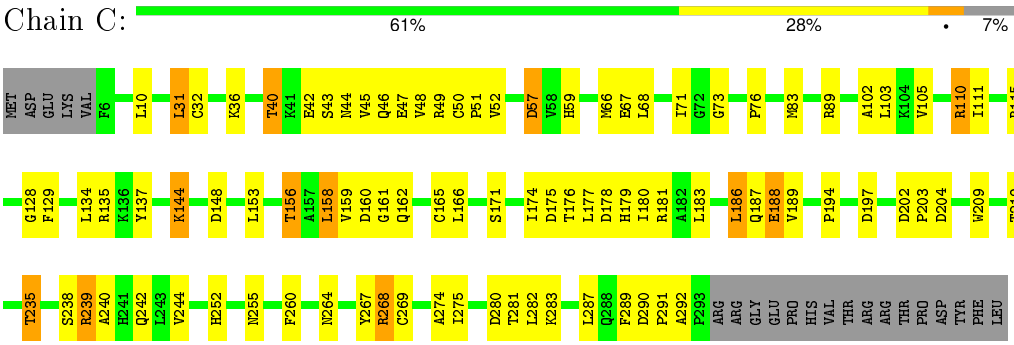
- Molecule 1: Protein Phosphatase 2, regulatory subunit A (PR 65), alpha isoform

Chain A:



- Molecule 2: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform

Chain C:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	92.54Å 194.85Å 201.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60	Depositor
% Data completeness (in resolution range)	94.0 (30.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.270 , 0.230	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6972	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OKA, MN

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	0.48	0/4601	0.72	5/6246 (0.1%)
2	C	0.53	0/2379	0.80	1/3227 (0.0%)
All	All	0.50	0/6980	0.75	6/9473 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	11	TYR	C-N-CA	-6.55	94.48	122.00
2	C	137	TYR	N-CA-C	-6.46	93.55	111.00
1	A	42	LEU	N-CA-C	-5.53	96.08	111.00
1	A	11	TYR	C-N-CD	5.37	139.68	128.40
1	A	11	TYR	N-CA-C	5.34	125.43	111.00
1	A	42	LEU	CA-CB-CG	5.17	127.20	115.30

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	4527	0	4633	227	0
2	C	2322	0	2224	97	0
3	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	57	0	67	1	0
5	A	27	0	0	0	0
5	C	37	0	0	2	0
All	All	6972	0	6924	322	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 23.

All (322) 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)
2:C:45:VAL:HA	2:C:156:THR:HG22	1.31	1.07
1:A:99:VAL:HG12	1:A:100:GLU:H	1.15	1.04
1:A:102:THR:HA	1:A:105:ARG:HG3	1.44	0.99
1:A:526:LEU:HD22	1:A:563:ILE:HG13	1.43	0.98
2:C:103:LEU:HB3	2:C:111:ILE:CD1	2.00	0.90
1:A:323:MET:HE3	1:A:327:LEU:HD22	1.56	0.88
1:A:99:VAL:HG12	1:A:100:GLU:N	1.91	0.86
1:A:183:ARG:HG3	1:A:183:ARG:HH11	1.42	0.85
1:A:205:ILE:HD13	1:A:208:MET:HE2	1.58	0.85
2:C:268:ARG:HH11	2:C:268:ARG:CB	1.90	0.84
2:C:175:ASP:H	2:C:179:HIS:HD2	1.28	0.80
1:A:77:THR:HG23	1:A:86:VAL:HG12	1.63	0.80
1:A:322:ILE:HG21	1:A:356:LEU:HD21	1.62	0.80
2:C:45:VAL:HA	2:C:156:THR:CG2	2.12	0.79
1:A:99:VAL:CG1	1:A:100:GLU:H	1.95	0.78
2:C:176:THR:CG2	2:C:179:HIS:H	1.97	0.78
1:A:94:GLU:OE1	1:A:131:LEU:HD13	1.84	0.77
1:A:102:THR:HA	1:A:105:ARG:CG	2.16	0.76
1:A:59:ILE:HG23	1:A:66:LEU:HD21	1.67	0.76
1:A:339:GLN:O	1:A:343:SER:HB2	1.86	0.75
1:A:274:VAL:HG13	1:A:278:ILE:HB	1.67	0.75
1:A:381:ARG:HD2	1:A:426:TYR:OH	1.87	0.74
1:A:70:ALA:HB2	1:A:96:LEU:HD13	1.68	0.74
2:C:158:LEU:HD21	2:C:161:GLY:HA2	1.71	0.73
1:A:405:LEU:HB3	1:A:406:PRO:HD3	1.71	0.73
1:A:180:MET:HG3	1:A:183:ARG:NH2	2.04	0.73
2:C:268:ARG:HH11	2:C:268:ARG:HB3	1.52	0.73
1:A:323:MET:CE	1:A:327:LEU:HD22	2.19	0.72
1:A:194:LYS:HD2	1:A:194:LYS:O	1.89	0.72
2:C:188:GLU:HG3	2:C:189:VAL:N	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ALA:O	1:A:221:ARG:HD2	1.89	0.72
1:A:561:LYS:HB3	1:A:562:PRO:HD3	1.71	0.72
1:A:102:THR:HG22	1:A:105:ARG:NH1	2.04	0.72
1:A:21:ARG:C	1:A:22:ASN:HD22	1.94	0.71
2:C:176:THR:HG23	2:C:179:HIS:H	1.54	0.71
1:A:514:GLN:HG3	1:A:550:ILE:O	1.90	0.71
2:C:281:THR:HG22	2:C:283:LYS:HE3	1.72	0.70
2:C:204:ASP:O	2:C:252:HIS:HE1	1.74	0.70
1:A:94:GLU:OE1	1:A:134:ARG:NH2	2.20	0.70
1:A:136:ALA:O	1:A:144:ARG:HD2	1.91	0.70
2:C:103:LEU:HB3	2:C:111:ILE:HD13	1.74	0.69
1:A:155:TYR:CE1	1:A:163:LYS:HB3	2.27	0.69
2:C:176:THR:HG22	2:C:179:HIS:CG	2.27	0.69
1:A:27:LEU:HD13	1:A:32:ILE:HD11	1.74	0.69
1:A:148:CYS:SG	1:A:173:LEU:HD13	2.34	0.68
1:A:131:LEU:O	1:A:131:LEU:HD12	1.93	0.68
1:A:414:ASP:CG	1:A:415:ALA:H	1.97	0.68
1:A:129:VAL:HB	1:A:130:PRO:HD3	1.74	0.68
2:C:176:THR:HG23	2:C:178:ASP:N	2.09	0.68
1:A:90:LEU:HB2	1:A:91:PRO:HD3	1.74	0.68
2:C:225:SER:OG	2:C:252:HIS:HD2	1.77	0.67
1:A:23:GLU:HG3	1:A:26:GLN:CD	2.15	0.67
2:C:174:ILE:HD11	2:C:183:LEU:HD11	1.77	0.67
1:A:388:LEU:H	1:A:433:GLN:HE22	1.43	0.67
1:A:29:LEU:C	1:A:31:SER:H	1.98	0.66
1:A:36:SER:O	1:A:40:LEU:HD23	1.96	0.65
1:A:467:LYS:HB2	1:A:507:VAL:CG1	2.27	0.65
1:A:12:PRO:HB2	1:A:42:LEU:HD11	1.77	0.65
2:C:68:LEU:HD21	2:C:275:ILE:CD1	2.27	0.65
1:A:389:ASP:O	1:A:393:GLU:HG3	1.97	0.65
2:C:275:ILE:HG22	2:C:287:LEU:HB2	1.77	0.64
1:A:323:MET:HE3	1:A:327:LEU:CD2	2.27	0.64
1:A:23:GLU:HG3	1:A:26:GLN:OE1	1.96	0.64
2:C:67:GLU:HB2	2:C:292:ALA:HB2	1.78	0.64
1:A:222:LEU:HD23	1:A:223:LEU:N	2.12	0.63
1:A:317:CYS:O	1:A:321:VAL:HG13	1.99	0.63
2:C:281:THR:HG22	2:C:281:THR:O	1.98	0.63
1:A:38:ILE:O	1:A:42:LEU:HD22	1.98	0.63
1:A:310:CYS:HB3	1:A:322:ILE:HD11	1.81	0.62
2:C:45:VAL:HG22	2:C:156:THR:HG21	1.81	0.62
2:C:264:ASN:ND2	2:C:267:TYR:HA	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:290:ASP:HB3	2:C:291:PRO:HD2	1.81	0.62
1:A:416:LYS:H	1:A:416:LYS:HD3	1.64	0.62
1:A:274:VAL:CG1	1:A:278:ILE:HB	2.29	0.62
1:A:183:ARG:NH1	1:A:183:ARG:HG3	2.12	0.61
1:A:427:MET:HE3	1:A:427:MET:HA	1.81	0.61
2:C:68:LEU:HD21	2:C:275:ILE:HD11	1.82	0.61
1:A:268:THR:HG21	1:A:308:GLU:HB3	1.82	0.61
1:A:105:ARG:HG3	1:A:105:ARG:HH11	1.65	0.61
1:A:32:ILE:O	1:A:35:LEU:HB2	2.00	0.60
1:A:339:GLN:NE2	1:A:377:CYS:HB2	2.16	0.60
1:A:412:ALA:O	1:A:420:ARG:HD2	2.01	0.60
1:A:52:LEU:HB2	1:A:53:PRO:HD3	1.83	0.60
1:A:307:LYS:NZ	1:A:307:LYS:HB3	2.17	0.59
1:A:180:MET:HG3	1:A:183:ARG:HH21	1.65	0.59
1:A:136:ALA:O	1:A:144:ARG:CD	2.51	0.59
1:A:509:SER:O	1:A:550:ILE:HD13	2.02	0.59
1:A:282:ASP:O	1:A:285:PRO:HD2	2.02	0.59
2:C:204:ASP:HB2	2:C:219:THR:HB	1.85	0.59
1:A:409:VAL:O	1:A:413:GLU:HG2	2.03	0.58
2:C:71:ILE:CD1	2:C:289:PHE:HB3	2.32	0.58
1:A:427:MET:CE	1:A:443:LEU:HG	2.32	0.58
1:A:115:ILE:O	1:A:119:HIS:HD2	1.85	0.58
2:C:118:HIS:HA	2:C:123:ILE:HG21	1.86	0.58
1:A:205:ILE:HD13	1:A:208:MET:CE	2.31	0.58
2:C:176:THR:HG23	2:C:178:ASP:H	1.67	0.58
1:A:77:THR:HG23	1:A:86:VAL:CG1	2.33	0.58
1:A:105:ARG:HH22	1:A:145:THR:HG21	1.69	0.57
1:A:29:LEU:HD11	1:A:64:GLU:HG2	1.85	0.57
1:A:431:ALA:HB1	1:A:473:PHE:CZ	2.38	0.57
2:C:103:LEU:HB3	2:C:111:ILE:HD11	1.81	0.57
1:A:427:MET:HG2	1:A:447:CYS:SG	2.45	0.57
1:A:58:THR:O	1:A:58:THR:HG22	2.05	0.57
2:C:10:LEU:HD11	2:C:105:VAL:HG12	1.87	0.57
1:A:29:LEU:O	1:A:31:SER:N	2.35	0.57
2:C:45:VAL:CA	2:C:156:THR:HG22	2.22	0.56
2:C:281:THR:CG2	2:C:281:THR:O	2.53	0.56
2:C:71:ILE:CG2	2:C:287:LEU:HD13	2.36	0.56
1:A:398:ARG:O	1:A:402:GLN:HB2	2.06	0.56
1:A:165:GLU:O	1:A:169:TYR:HD1	1.88	0.56
1:A:356:LEU:O	1:A:360:ASN:HB2	2.06	0.56
1:A:241:GLU:OE2	1:A:249:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:175:ASP:H	2:C:179:HIS:CD2	2.18	0.56
1:A:144:ARG:HG2	1:A:173:LEU:HD21	1.87	0.56
1:A:133:LYS:HE2	1:A:169:TYR:CE1	2.41	0.56
1:A:38:ILE:HD12	1:A:38:ILE:N	2.21	0.56
1:A:586:LEU:O	1:A:587:SER:HB2	2.05	0.55
1:A:38:ILE:H	1:A:38:ILE:HD12	1.71	0.55
1:A:271:GLN:HE22	1:A:309:PHE:HA	1.71	0.55
1:A:350:MET:HB3	1:A:391:VAL:CG2	2.36	0.55
1:A:12:PRO:HB2	1:A:42:LEU:CD1	2.36	0.55
1:A:204:GLU:O	1:A:208:MET:HG3	2.07	0.55
2:C:268:ARG:NH1	2:C:268:ARG:HB3	2.19	0.55
2:C:44:ASN:O	2:C:156:THR:HG22	2.07	0.55
1:A:179:PRO:C	1:A:183:ARG:HH12	2.10	0.54
2:C:76:PRO:HB2	2:C:110:ARG:HG3	1.90	0.54
2:C:229:ASN:ND2	2:C:255:ASN:HB3	2.22	0.54
1:A:136:ALA:O	1:A:144:ARG:CG	2.55	0.54
1:A:571:GLN:HG2	1:A:572:ASP:N	2.23	0.54
1:A:42:LEU:HB3	1:A:46:ARG:HB3	1.89	0.54
1:A:456:TYR:CG	2:C:73:GLY:HA2	2.42	0.54
1:A:21:ARG:C	1:A:22:ASN:ND2	2.61	0.54
2:C:162:GLN:HB3	2:C:235:THR:OG1	2.08	0.54
1:A:22:ASN:N	1:A:22:ASN:HD22	2.05	0.54
1:A:570:ASP:O	1:A:576:LYS:HE3	2.08	0.54
2:C:158:LEU:O	2:C:158:LEU:HD23	2.08	0.54
1:A:313:LEU:HD13	1:A:321:VAL:CG2	2.37	0.54
1:A:492:ASP:O	1:A:498:ARG:HD3	2.08	0.54
1:A:542:LYS:HE2	1:A:578:PHE:CD1	2.43	0.54
2:C:50:CYS:HB2	2:C:51:PRO:HA	1.90	0.54
1:A:60:TYR:O	1:A:62:GLU:N	2.41	0.53
1:A:427:MET:HE1	1:A:443:LEU:HG	1.90	0.53
2:C:124:THR:HB	2:C:129:PHE:HB3	1.89	0.53
2:C:203:PRO:HD2	2:C:239:ARG:CZ	2.39	0.53
1:A:373:LEU:HD11	1:A:385:ILE:CD1	2.39	0.53
1:A:206:ILE:HB	1:A:207:PRO:HD3	1.91	0.53
1:A:467:LYS:HB2	1:A:507:VAL:HG13	1.90	0.53
2:C:103:LEU:C	2:C:111:ILE:HD12	2.30	0.53
1:A:542:LYS:HE2	1:A:578:PHE:CE1	2.44	0.53
1:A:229:VAL:O	1:A:233:GLN:HG3	2.08	0.53
1:A:59:ILE:HG22	1:A:59:ILE:O	2.08	0.52
2:C:264:ASN:HA	2:C:269:CYS:O	2.10	0.52
1:A:100:GLU:O	1:A:101:GLU:C	2.48	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:281:THR:O	2:C:282:LEU:HB2	2.08	0.52
1:A:373:LEU:HD11	1:A:385:ILE:HD11	1.91	0.52
1:A:350:MET:CE	1:A:369:PHE:HB2	2.39	0.52
1:A:481:THR:HG22	1:A:481:THR:O	2.09	0.52
1:A:378:PRO:HA	1:A:381:ARG:NH1	2.24	0.52
2:C:264:ASN:HD22	2:C:267:TYR:HA	1.75	0.52
2:C:103:LEU:O	2:C:111:ILE:HD12	2.10	0.51
1:A:102:THR:HG22	1:A:105:ARG:HH12	1.75	0.51
1:A:136:ALA:O	1:A:144:ARG:HG3	2.10	0.51
1:A:407:ALA:O	1:A:411:LEU:HG	2.09	0.51
1:A:556:LEU:HD22	1:A:588:LEU:HD11	1.91	0.51
1:A:180:MET:HA	1:A:183:ARG:CZ	2.40	0.51
1:A:194:LYS:CD	1:A:194:LYS:O	2.58	0.51
2:C:166:LEU:N	2:C:166:LEU:HD23	2.26	0.51
2:C:176:THR:HG22	2:C:179:HIS:H	1.73	0.51
1:A:94:GLU:CD	1:A:131:LEU:HD13	2.31	0.51
1:A:109:VAL:HG13	1:A:150:LEU:HD21	1.93	0.51
1:A:105:ARG:NH2	1:A:145:THR:CG2	2.74	0.51
1:A:356:LEU:HB3	1:A:360:ASN:HB3	1.92	0.51
2:C:68:LEU:CD2	2:C:275:ILE:HD12	2.41	0.51
2:C:209:TRP:CE2	2:C:224:ILE:HD13	2.46	0.51
1:A:381:ARG:O	1:A:385:ILE:HG12	2.10	0.51
1:A:98:THR:HG22	1:A:98:THR:O	2.10	0.51
1:A:452:VAL:HG22	1:A:497:HIS:CE1	2.47	0.50
1:A:197:GLU:CD	1:A:197:GLU:H	2.13	0.50
1:A:155:TYR:CZ	1:A:163:LYS:HB3	2.45	0.50
1:A:44:VAL:HG13	1:A:45:GLU:H	1.76	0.50
1:A:29:LEU:C	1:A:31:SER:N	2.65	0.50
2:C:48:VAL:O	2:C:159:VAL:HA	2.10	0.50
1:A:12:PRO:O	1:A:15:VAL:HG23	2.12	0.50
1:A:218:ASP:OD2	1:A:258:ARG:HD3	2.11	0.50
1:A:196:LEU:HD11	1:A:205:ILE:HD11	1.92	0.50
2:C:186:LEU:O	2:C:186:LEU:HD13	2.12	0.50
2:C:103:LEU:CB	2:C:111:ILE:HD13	2.42	0.50
2:C:36:LYS:O	2:C:40:THR:OG1	2.30	0.50
1:A:96:LEU:HA	1:A:99:VAL:HG23	1.94	0.49
1:A:421:LEU:HD12	1:A:421:LEU:O	2.12	0.49
1:A:18:ASP:C	1:A:18:ASP:OD1	2.50	0.49
1:A:370:LEU:HD21	1:A:403:SER:O	2.12	0.49
1:A:413:GLU:O	1:A:413:GLU:HG3	2.13	0.49
1:A:105:ARG:NH1	1:A:105:ARG:HG3	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:ALA:O	1:A:425:GLU:HG2	2.12	0.49
1:A:356:LEU:HB3	1:A:360:ASN:CB	2.43	0.49
1:A:428:PRO:HD3	1:A:465:ASN:HD21	1.77	0.49
1:A:392:ASN:HD21	1:A:397:ILE:HA	1.78	0.49
1:A:26:GLN:HG2	1:A:27:LEU:N	2.27	0.48
2:C:171:SER:HB2	2:C:197:ASP:CB	2.43	0.48
1:A:537:ARG:O	1:A:540:VAL:HB	2.12	0.48
2:C:268:ARG:NH1	2:C:268:ARG:CB	2.70	0.48
1:A:535:ASN:HA	1:A:538:PHE:CE2	2.49	0.48
1:A:401:SER:O	1:A:405:LEU:HB2	2.13	0.48
1:A:238:GLU:H	1:A:238:GLU:CD	2.15	0.48
1:A:265:ASP:O	1:A:305:LYS:HE2	2.13	0.48
2:C:45:VAL:HG22	2:C:156:THR:CG2	2.44	0.48
1:A:129:VAL:O	1:A:132:VAL:N	2.47	0.48
1:A:196:LEU:CD1	1:A:205:ILE:HD11	2.45	0.47
2:C:68:LEU:HD21	2:C:275:ILE:HD12	1.96	0.47
1:A:45:GLU:H	1:A:45:GLU:CD	2.17	0.47
1:A:155:TYR:CE2	1:A:163:LYS:HD3	2.50	0.47
1:A:373:LEU:HD13	1:A:384:ILE:HG21	1.95	0.47
2:C:68:LEU:HG	2:C:275:ILE:HD12	1.96	0.47
2:C:202:ASP:OD1	2:C:242:GLN:HG3	2.14	0.47
1:A:183:ARG:HH11	1:A:183:ARG:CG	2.20	0.47
1:A:130:PRO:O	1:A:134:ARG:HG3	2.14	0.47
2:C:115:ARG:HB2	2:C:153:LEU:HB2	1.96	0.47
1:A:24:ASP:C	1:A:25:VAL:HG23	2.34	0.47
1:A:414:ASP:CG	1:A:415:ALA:N	2.67	0.47
2:C:174:ILE:HD13	2:C:180:ILE:HG12	1.97	0.47
2:C:186:LEU:C	2:C:186:LEU:HD22	2.35	0.47
2:C:187:GLN:NE2	5:C:537:HOH:O	2.48	0.46
1:A:354:PRO:HD3	1:A:390:CYS:SG	2.55	0.46
1:A:405:LEU:HB3	1:A:406:PRO:CD	2.44	0.46
2:C:264:ASN:OD1	2:C:269:CYS:O	2.33	0.46
2:C:118:HIS:CE1	2:C:123:ILE:HD11	2.50	0.46
2:C:128:GLY:O	2:C:129:PHE:C	2.53	0.46
2:C:174:ILE:HD11	2:C:194:PRO:HB2	1.97	0.46
1:A:226:GLU:OE2	1:A:266:LYS:HE3	2.16	0.46
1:A:180:MET:HA	1:A:183:ARG:NH2	2.31	0.46
1:A:62:GLU:HB3	1:A:65:VAL:HB	1.98	0.46
1:A:279:THR:O	1:A:284:VAL:HG23	2.15	0.46
1:A:564:LEU:O	1:A:568:THR:HG23	2.15	0.46
2:C:32:CYS:O	2:C:36:LYS:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:83:MET:HE3	2:C:240:ALA:HB2	1.97	0.45
2:C:244:VAL:HG22	2:C:260:PHE:HB2	1.97	0.45
2:C:268:ARG:HH11	2:C:268:ARG:HB2	1.78	0.45
2:C:171:SER:HB2	2:C:197:ASP:HB2	1.97	0.45
1:A:42:LEU:HD13	1:A:42:LEU:N	2.32	0.45
1:A:313:LEU:HD13	1:A:321:VAL:HG22	1.99	0.45
2:C:42:GLU:HB3	2:C:46:GLN:OE1	2.17	0.45
1:A:99:VAL:CG1	1:A:100:GLU:N	2.62	0.45
1:A:505:ILE:HG23	1:A:521:MET:HB3	1.99	0.45
1:A:404:LEU:HD11	1:A:408:ILE:HD11	1.98	0.45
1:A:477:TRP:CH2	1:A:482:ILE:HD12	2.52	0.45
2:C:274:ALA:HA	2:C:287:LEU:O	2.17	0.44
1:A:80:VAL:CG1	1:A:80:VAL:O	2.66	0.44
1:A:141:PHE:CD1	1:A:141:PHE:C	2.89	0.44
1:A:92:PRO:O	1:A:95:SER:HB3	2.18	0.44
1:A:66:LEU:HD22	1:A:96:LEU:HD21	1.99	0.44
1:A:34:LYS:O	1:A:38:ILE:CD1	2.65	0.44
2:C:71:ILE:HG23	2:C:287:LEU:HD13	2.00	0.44
1:A:255:LYS:HD3	1:A:255:LYS:HA	1.78	0.44
1:A:107:LYS:HD3	1:A:107:LYS:HA	1.85	0.44
1:A:388:LEU:H	1:A:433:GLN:NE2	2.11	0.44
1:A:570:ASP:O	1:A:576:LYS:CE	2.65	0.44
1:A:378:PRO:O	1:A:382:LEU:HB2	2.18	0.44
2:C:174:ILE:HG13	2:C:194:PRO:HB3	1.99	0.44
1:A:427:MET:HE2	1:A:443:LEU:HG	1.98	0.43
1:A:353:SER:N	1:A:354:PRO:HD2	2.33	0.43
2:C:89:ARG:HH21	4:C:401:OKA:H32	1.83	0.43
1:A:42:LEU:HB3	1:A:46:ARG:CB	2.48	0.43
1:A:9:SER:HB2	1:A:14:ALA:HB2	1.99	0.43
1:A:62:GLU:O	1:A:64:GLU:N	2.51	0.43
1:A:572:ASP:OD2	2:C:110:ARG:NH2	2.51	0.43
1:A:35:LEU:HB3	1:A:72:GLN:HG2	2.01	0.43
1:A:21:ARG:HD2	1:A:26:GLN:OE1	2.18	0.43
1:A:135:LEU:O	1:A:143:SER:O	2.36	0.43
2:C:144:LYS:HE3	2:C:148:ASP:OD2	2.19	0.43
1:A:381:ARG:CD	1:A:426:TYR:OH	2.61	0.43
1:A:489:MET:HB2	1:A:501:THR:OG1	2.18	0.43
2:C:57:ASP:N	2:C:57:ASP:OD1	2.52	0.43
2:C:31:LEU:HD21	2:C:102:ALA:HA	2.01	0.43
2:C:165:CYS:HA	2:C:238:SER:O	2.19	0.43
1:A:416:LYS:HD3	1:A:416:LYS:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:59:HIS:HE1	2:C:118:HIS:CD2	2.37	0.42
1:A:204:GLU:C	1:A:207:PRO:HD2	2.39	0.42
1:A:381:ARG:HG3	1:A:426:TYR:OH	2.19	0.42
1:A:17:ILE:HG22	1:A:18:ASP:N	2.34	0.42
2:C:103:LEU:CB	2:C:111:ILE:CD1	2.84	0.42
1:A:179:PRO:C	1:A:183:ARG:NH1	2.72	0.42
1:A:28:ARG:HB3	1:A:31:SER:CB	2.49	0.42
2:C:176:THR:HG23	2:C:179:HIS:N	2.28	0.42
1:A:46:ARG:HA	1:A:49:SER:OG	2.19	0.42
2:C:176:THR:CG2	2:C:179:HIS:N	2.73	0.42
2:C:158:LEU:CD2	2:C:161:GLY:HA2	2.45	0.42
1:A:405:LEU:HD12	1:A:405:LEU:HA	1.89	0.42
2:C:66:MET:HA	2:C:66:MET:HE2	2.01	0.42
1:A:67:LEU:HA	1:A:67:LEU:HD12	1.86	0.42
1:A:372:GLN:OE1	1:A:384:ILE:HD11	2.20	0.42
1:A:411:LEU:CB	1:A:423:ILE:HG13	2.49	0.42
2:C:158:LEU:HD21	2:C:161:GLY:CA	2.43	0.42
1:A:390:CYS:O	1:A:394:VAL:HG23	2.19	0.42
1:A:139:ASP:O	1:A:140:TRP:C	2.59	0.42
1:A:171:ARG:HH22	1:A:204:GLU:HG2	1.85	0.41
1:A:9:SER:HB2	1:A:10:LEU:H	1.69	0.41
1:A:105:ARG:NH2	1:A:142:THR:HB	2.35	0.41
1:A:66:LEU:HD22	1:A:96:LEU:CD2	2.50	0.41
1:A:83:PRO:HA	1:A:86:VAL:HG13	2.02	0.41
1:A:327:LEU:HG	1:A:331:LYS:HE3	2.01	0.41
2:C:283:LYS:HA	2:C:283:LYS:HE2	2.03	0.41
1:A:44:VAL:HG23	1:A:80:VAL:C	2.41	0.41
1:A:413:GLU:O	1:A:414:ASP:HB2	2.21	0.41
1:A:349:ILE:HG23	1:A:350:MET:N	2.36	0.41
1:A:355:ILE:HG22	1:A:355:ILE:O	2.21	0.41
1:A:100:GLU:O	1:A:102:THR:N	2.54	0.41
1:A:373:LEU:HD13	1:A:384:ILE:CG2	2.51	0.41
1:A:481:THR:O	1:A:481:THR:CG2	2.68	0.41
1:A:479:HIS:CE1	1:A:520:HIS:CD2	3.09	0.41
1:A:40:LEU:CD2	1:A:40:LEU:N	2.83	0.40
1:A:498:ARG:O	1:A:501:THR:HB	2.21	0.40
1:A:171:ARG:HH22	1:A:204:GLU:CG	2.34	0.40
2:C:177:LEU:O	2:C:181:ARG:HG3	2.20	0.40
1:A:133:LYS:O	1:A:137:GLY:N	2.49	0.40
2:C:49:ARG:NH2	5:C:504:HOH:O	2.41	0.40
1:A:373:LEU:HD12	1:A:373:LEU:HA	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:THR:HG21	1:A:308:GLU:CG	2.52	0.40
1:A:272:LYS:HE3	1:A:312:ASN:ND2	2.36	0.40
1:A:314:SER:O	1:A:315:ALA:C	2.60	0.40
1:A:257:TRP:CB	1:A:295:GLU:HG3	2.51	0.40
1:A:42:LEU:H	1:A:42:LEU:HD13	1.85	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	579/589 (98%)	511 (88%)	56 (10%)	12 (2%)	9 16
2	C	286/309 (93%)	256 (90%)	30 (10%)	0	100 100
All	All	865/898 (96%)	767 (89%)	86 (10%)	12 (1%)	14 28

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	ASP
1	A	63	ASP
1	A	99	VAL
1	A	318	ARG
1	A	415	ALA
1	A	21	ARG
1	A	30	ASN
1	A	84	GLU
1	A	140	TRP
1	A	376	GLU
1	A	348	VAL
1	A	25	VAL

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	508/512 (99%)	468 (92%)	40 (8%)	15 30
2	C	254/274 (93%)	235 (92%)	19 (8%)	17 33
All	All	762/786 (97%)	703 (92%)	59 (8%)	16 31

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	11	TYR
1	A	16	LEU
1	A	22	ASN
1	A	24	ASP
1	A	28	ARG
1	A	40	LEU
1	A	42	LEU
1	A	57	ASP
1	A	76	PHE
1	A	78	THR
1	A	79	LEU
1	A	123	ASP
1	A	141	PHE
1	A	157	ARG
1	A	160	SER
1	A	198	LEU
1	A	199	ASP
1	A	204	GLU
1	A	211	ASN
1	A	222	LEU
1	A	237	GLN
1	A	267	PHE
1	A	274	VAL
1	A	316	ASP
1	A	321	VAL
1	A	323	MET

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Mol	Chain	Res	Type
1	A	343	SER
1	A	366	LEU
1	A	389	ASP
1	A	406	PRO
1	A	416	LYS
1	A	425	GLU
1	A	427	MET
1	A	437	GLU
1	A	443	LEU
1	A	452	VAL
1	A	495	TYR
1	A	515	ASP
1	A	581	GLU
2	C	31	LEU
2	C	40	THR
2	C	43	SER
2	C	47	GLU
2	C	52	VAL
2	C	57	ASP
2	C	110	ARG
2	C	134	LEU
2	C	135	ARG
2	C	144	LYS
2	C	156	THR
2	C	158	LEU
2	C	160	ASP
2	C	186	LEU
2	C	188	GLU
2	C	235	THR
2	C	239	ARG
2	C	268	ARG
2	C	280	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	119	HIS
1	A	237	GLN
1	A	271	GLN
1	A	288	GLN
1	A	339	GLN

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Mol	Chain	Res	Type
1	A	364	HIS
1	A	392	ASN
1	A	402	GLN
1	A	433	GLN
1	A	465	ASN
1	A	479	HIS
1	A	506	ASN
1	A	520	HIS
2	C	12	GLN
2	C	16	GLN
2	C	122	GLN
2	C	179	HIS
2	C	187	GLN
2	C	191	HIS
2	C	252	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	OKA	C	401	-	57,63,63	1.29	4 (7%)	60,97,97	1.59	11 (18%)

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	OKA	C	401	-	-	0/26/129/129	0/7/7/7

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	401	OKA	C8-C9	-7.57	1.39	1.50
4	C	401	OKA	C16-C15	-2.18	1.39	1.50
4	C	401	OKA	C15-C14	2.31	1.39	1.32
4	C	401	OKA	C41-C25	3.54	1.39	1.32

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	401	OKA	C11-C12-C13	-6.37	106.93	116.58
4	C	401	OKA	C21-C20-C19	-3.38	107.51	111.73
4	C	401	OKA	C29-C30-C31	-3.35	110.32	116.37
4	C	401	OKA	C38-O13-C34	-2.80	111.38	114.05
4	C	401	OKA	C19-O7-C16	-2.75	102.45	107.66
4	C	401	OKA	O13-C34-C35	-2.55	109.22	111.26
4	C	401	OKA	C19-O8-C23	-2.45	110.75	114.31
4	C	401	OKA	C5-C6-C7	-2.01	109.05	111.52
4	C	401	OKA	C43-C10-C11	2.12	120.56	116.22
4	C	401	OKA	O12-C30-C29	2.34	109.97	106.27
4	C	401	OKA	O8-C23-C22	2.57	113.31	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	401	OKA	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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.