WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2023 – 12:28 PM EDT

PDB ID	:	3KPS
Title	:	Crystal Structure of the LC13 TCR in complex with HLA B*4405 bound to EEYLQAFTY a self peptide from the ABCD3 protein
Authors	:	Macdonald, W.A.; Chen, Z.; Gras, S.; Archbold, J.K.; Tynan, F.E.; Clements, C.S.; Bharadwaj, M.; Kjer-Nielsen, L.; Saunders, P.M.; Wilce, M.C.; Crawford, F.; Stadinsky, B.; Jackson, D.; Brooks, A.G.; Purcell, A.W.; Kappler, J.W.; Burrows, S.R.; Rossjohn, J.; McCluskey, J.
Deposited on	:	2009-11-16
Resolution	:	2.70 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 ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
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
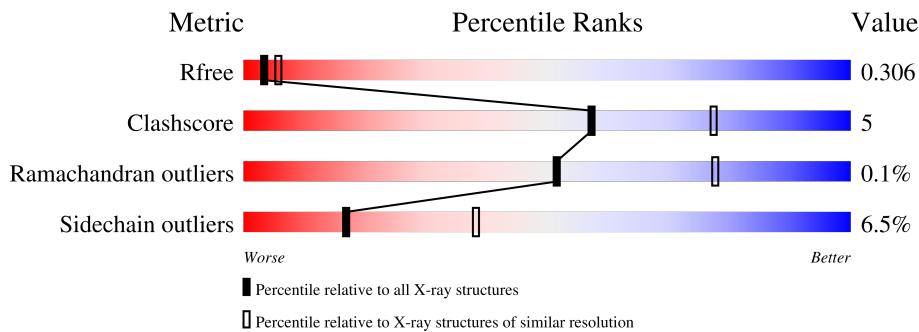
1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.70 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		0.306
Clashscore		5
Ramachandran outliers		0.1%
Sidechain outliers		6.5%

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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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%

Mol	Chain	Length	Quality of chain
1	A	276	87% 12% •
2	B	99	83% 17%
3	C	9	56% 33% 11%
4	D	201	83% 13% •
5	E	241	84% 15% •

2 Entity composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 6684 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 HLA class I histocompatibility antigen, B-44 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2259	1408	407	437	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	116	TYR	ASP	variant	UNP P30481

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			

- Molecule 3 is a protein called EEYLQAFTY, self peptide from the ATP binding cassette protein ABCD3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			83	55	10	18			

- Molecule 4 is a protein called LC13 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	201	Total	C	N	O	S	0	0	0
			1567	975	267	317	8			

- Molecule 5 is a protein called LC13 TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	241	Total	C	N	O	S	0	0	0
			1919	1209	335	371	4			
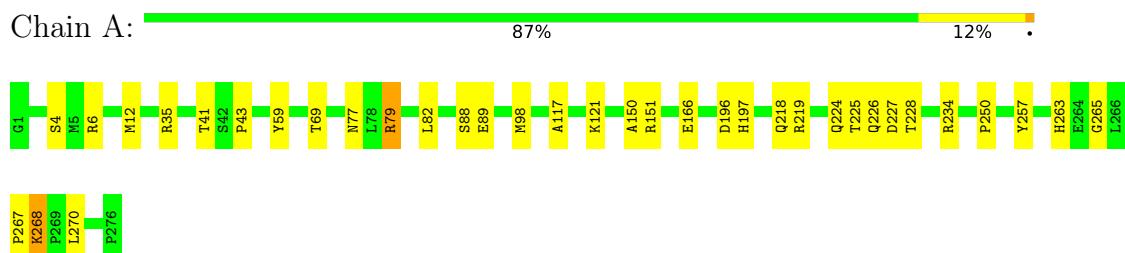
- Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total 3	O 3	0	0
6	B	4	Total 4	O 4	0	0
6	C	1	Total 1	O 1	0	0
6	D	6	Total 6	O 6	0	0
6	E	13	Total 13	O 13	0	0
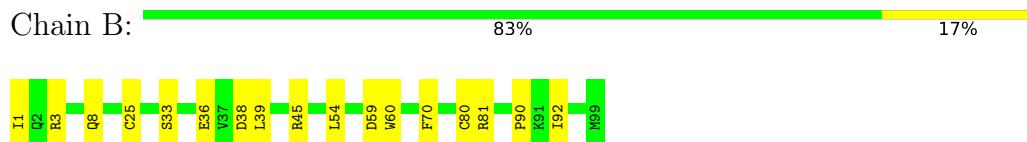
3 Residue-property plots (i)

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. 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. 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: HLA class I histocompatibility antigen, B-44 alpha chain
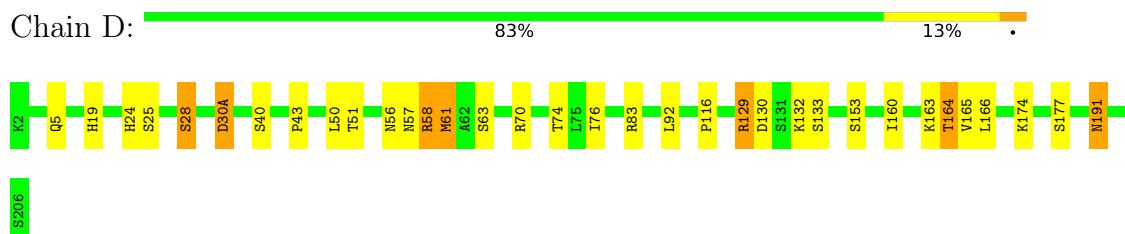
Chain A:

• Molecule 2: Beta-2-microglobulin
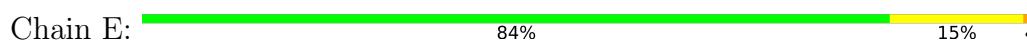
Chain B:

• Molecule 3: EEYLQAFTY, self peptide from the ATP binding cassette protein ABCD3
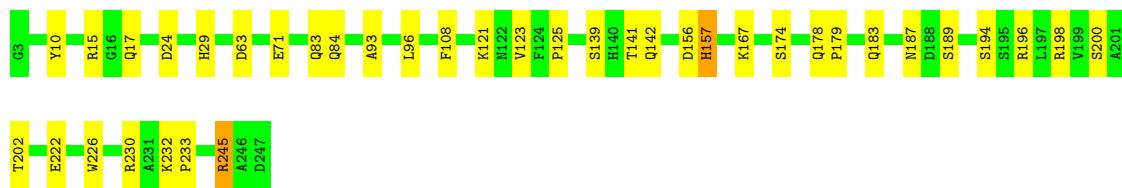
Chain C:

• Molecule 4: LC13 TCR alpha chain

Chain D:

• Molecule 5: LC13 TCR beta chain

Chain E:

G3 Y10 R15 G16 Q17 D24 H29 D63 E71 Q83 Q84 A93 L96 F108 K121 N122 V123 F124 P125 S139 H140 T141 Q142 D156 H157 K167 S174 Q178 P179 Q183 N187 D188 S189 S194 S195 R196 L197 R198 V199 S200 A201

T202 E222 W226 R230 A231 K232 P233 R245 A246 D247

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	142.52Å 54.24Å 121.77Å 90.00° 114.43° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.04 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.4 (50.00-2.70) 91.4 (50.04-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.52 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.193 , 0.269 0.240 , 0.306	Depositor DCC
R_{free} test set	1112 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å^2)	51.9	Xtriage
Anisotropy	0.563	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 35.9	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6684	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% 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 ⓘ

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	0.47	0/2320	0.59	0/3154
2	B	0.42	0/852	0.59	0/1152
3	C	0.57	0/85	0.65	0/113
4	D	0.47	0/1603	0.66	0/2181
5	E	0.49	0/1971	0.60	0/2681
All	All	0.47	0/6831	0.61	0/9281

There are no bond length outliers.

There are no bond angle outliers.

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	2259	0	2128	19	0
2	B	829	0	794	9	0
3	C	83	0	72	7	0
4	D	1567	0	1492	21	0
5	E	1919	0	1820	18	0
6	A	3	0	0	0	0
6	B	4	0	0	0	0
6	C	1	0	0	0	0
6	D	6	0	0	1	0
6	E	13	0	0	1	0
All	All	6684	0	6306	64	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 5.

All (64) 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)
4:D:164:THR:HB	5:E:174:SER:OG	1.77	0.82
4:D:57:ASN:HB3	4:D:58:ARG:O	1.85	0.75
1:A:267:PRO:HB2	1:A:268:LYS:HE2	1.68	0.73
1:A:263:HIS:CD2	1:A:265:GLY:H	2.11	0.68
4:D:56:ASN:ND2	4:D:63:SER:OG	2.30	0.65
4:D:163:LYS:HA	4:D:177:SER:O	1.97	0.63
1:A:59:TYR:CE1	3:C:1:GLU:HG2	2.36	0.61
4:D:57:ASN:CB	4:D:58:ARG:O	2.47	0.61
4:D:28:SER:O	4:D:70:ARG:NH2	2.34	0.61
5:E:156:ASP:OD1	5:E:179:PRO:HG2	2.02	0.60
5:E:178:GLN:NE2	5:E:178:GLN:HA	2.17	0.60
1:A:267:PRO:HB2	1:A:268:LYS:CE	2.32	0.59
4:D:153:SER:HB3	4:D:160:ILE:CD1	2.32	0.59
3:C:5:GLN:HA	3:C:5:GLN:HE21	1.68	0.59
1:A:197:HIS:O	1:A:250:PRO:HA	2.02	0.58
1:A:219:ARG:HB2	1:A:257:TYR:CE2	2.39	0.58
4:D:28:SER:HB2	4:D:30(A):ASP:OD2	2.03	0.58
4:D:153:SER:HB3	4:D:160:ILE:HD12	1.85	0.58
4:D:58:ARG:O	4:D:61:MET:HG2	2.04	0.57
1:A:77:ASN:ND2	3:C:9:TYR:H	2.04	0.56
1:A:59:TYR:HE1	3:C:1:GLU:HG2	1.70	0.55
2:B:25:CYS:HB2	2:B:39:LEU:HD21	1.89	0.54
1:A:234:ARG:HH11	2:B:8:GLN:NE2	2.05	0.54
2:B:38:ASP:HB2	2:B:81:ARG:HB3	1.90	0.54
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.43	0.54
2:B:3:ARG:NH2	2:B:59:ASP:O	2.41	0.53
4:D:51:THR:HG22	4:D:70:ARG:HD3	1.90	0.53
5:E:10:TYR:HB3	5:E:157:HIS:CD2	2.44	0.52
1:A:41:THR:O	1:A:43:PRO:HD3	2.10	0.52
3:C:5:GLN:HA	3:C:5:GLN:NE2	2.25	0.52
1:A:69:THR:HG21	3:C:4:LEU:HD21	1.92	0.51
4:D:43:PRO:HD2	5:E:108:PHE:CG	2.47	0.50
5:E:93:ALA:HB2	5:E:108:PHE:CD2	2.47	0.50
1:A:4:SER:HB2	1:A:6:ARG:NH1	2.27	0.50
2:B:80:CYS:O	2:B:92:ILE:HA	2.12	0.49
5:E:245:ARG:O	5:E:245:ARG:HG2	2.13	0.48
4:D:164:THR:HG23	6:D:212:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:123:VAL:O	5:E:230:ARG:NH2	2.48	0.47
5:E:141:THR:O	5:E:142:GLN:HB2	2.15	0.47
4:D:129:ARG:HH11	4:D:129:ARG:HG2	1.80	0.46
5:E:156:ASP:C	5:E:157:HIS:HD1	2.19	0.46
1:A:121:LYS:HG3	2:B:1:ILE:HG23	1.97	0.45
4:D:116:PRO:HG3	4:D:165:VAL:HG13	1.99	0.45
5:E:226:TRP:HB2	5:E:232:LYS:HG3	1.98	0.45
5:E:125:PRO:HD3	5:E:233:PRO:HB3	1.99	0.45
5:E:167:LYS:HB2	6:E:251:HOH:O	2.17	0.45
5:E:178:GLN:HA	5:E:179:PRO:HD3	1.87	0.45
3:C:5:GLN:NE2	3:C:5:GLN:CA	2.79	0.45
4:D:130:ASP:HB3	4:D:133:SER:O	2.17	0.44
4:D:166:LEU:O	4:D:174:LYS:HA	2.17	0.44
1:A:150:ALA:O	1:A:151:ARG:HB2	2.18	0.44
4:D:166:LEU:HD11	5:E:198:ARG:HB3	1.99	0.44
4:D:50:LEU:O	4:D:70:ARG:NH1	2.49	0.44
1:A:82:LEU:HD13	1:A:89:GLU:HG2	2.00	0.43
4:D:191:ASN:HD22	4:D:191:ASN:C	2.22	0.43
5:E:183:GLN:O	5:E:189:SER:HB2	2.19	0.43
1:A:218:GLN:O	1:A:257:TYR:HA	2.18	0.43
2:B:33:SER:HB2	2:B:54:LEU:HD21	2.00	0.42
2:B:38:ASP:OD1	2:B:45:ARG:NE	2.53	0.42
1:A:224:GLN:C	1:A:226:GLN:N	2.74	0.41
1:A:79:ARG:O	1:A:82:LEU:HB2	2.20	0.41
5:E:15:ARG:HD3	5:E:83:GLN:OE1	2.19	0.41
5:E:178:GLN:HA	5:E:178:GLN:HE21	1.85	0.41
4:D:19:HIS:HD2	4:D:76:ILE:HG12	1.86	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	274/276 (99%)	258 (94%)	16 (6%)	0	100	100
2	B	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
4	D	199/201 (99%)	185 (93%)	13 (6%)	1 (0%)	29	54
5	E	239/241 (99%)	224 (94%)	15 (6%)	0	100	100
All	All	816/826 (99%)	765 (94%)	50 (6%)	1 (0%)	51	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	61	MET

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	237/237 (100%)	225 (95%)	12 (5%)	24	50
2	B	94/94 (100%)	91 (97%)	3 (3%)	39	68
3	C	8/8 (100%)	7 (88%)	1 (12%)	4	10
4	D	180/180 (100%)	166 (92%)	14 (8%)	12	29
5	E	207/207 (100%)	190 (92%)	17 (8%)	11	26
All	All	726/726 (100%)	679 (94%)	47 (6%)	17	38

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	MET
1	A	35	ARG
1	A	79	ARG
1	A	88	SER
1	A	98	MET
1	A	166	GLU
1	A	196	ASP

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Mol	Chain	Res	Type
1	A	225	THR
1	A	227	ASP
1	A	228	THR
1	A	268	LYS
1	A	270	LEU
2	B	36	GLU
2	B	70	PHE
2	B	90	PRO
3	C	5	GLN
4	D	5	GLN
4	D	24	HIS
4	D	25	SER
4	D	28	SER
4	D	30(A)	ASP
4	D	40	SER
4	D	58	ARG
4	D	74	THR
4	D	83	ARG
4	D	92	LEU
4	D	129	ARG
4	D	132	LYS
4	D	164	THR
4	D	191	ASN
5	E	17	GLN
5	E	24	ASP
5	E	29	HIS
5	E	63	ASP
5	E	71	GLU
5	E	84	GLN
5	E	96	LEU
5	E	121	LYS
5	E	139	SER
5	E	157	HIS
5	E	187	ASN
5	E	194	SER
5	E	196	ARG
5	E	200	SER
5	E	202	THR
5	E	222	GLU
5	E	245	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	77	ASN
1	A	263	HIS
2	B	8	GLN
3	C	5	GLN
4	D	19	HIS
4	D	33	HIS
4	D	56	ASN
4	D	115	HIS
4	D	191	ASN
5	E	29	HIS
5	E	51	ASN
5	E	80	GLN
5	E	122	ASN
5	E	223	ASN
5	E	236	GLN

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 monosaccharides in this entry.

5.6   Ligand geometry ⓘ

There are no ligands in this entry.

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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.