Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:51 AM GMT

PDB ID	:	2V12
Title	:	CRYSTAL STRUCTURE OF RENIN WITH INHIBITOR 8
Authors	:	Rahuel, J.; Rasetti, V.; Maibaum, J.; Rueger, H.; Goschke, R.; Cohen, N.C.; Stutz, S.; Cumin, F.; Fuhrer, W.; Wood, J.M.; Grutter, M.G.
Deposited on	:	2007-05-21
Resolution	:	3.20 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 ⓘ symbol.

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

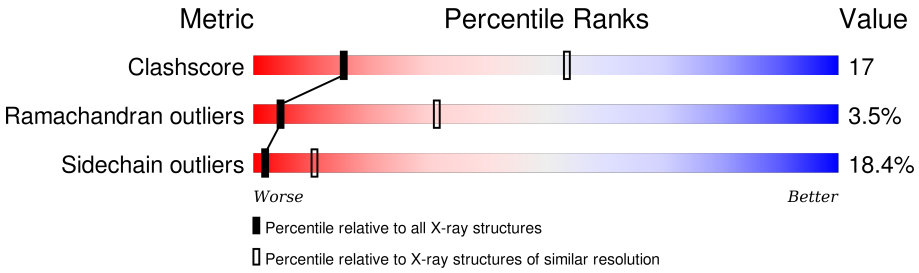
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.20 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	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)

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	C	340	52% 33% 11%
1	O	340	48% 35% 13%

2 Entry composition

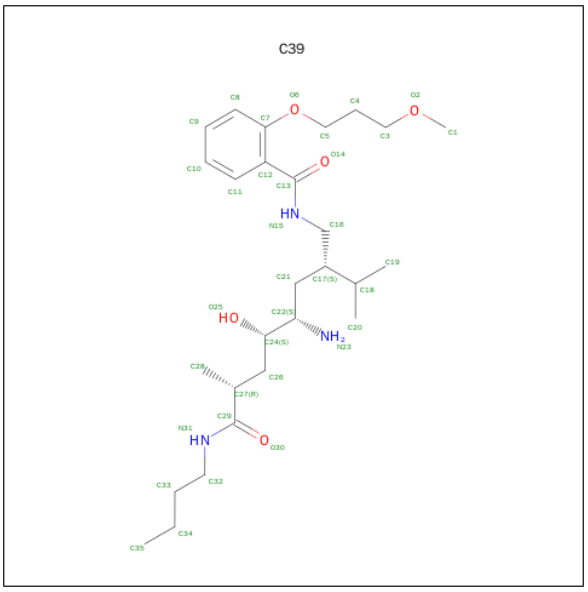
There are 2 unique types of molecules in this entry. The entry contains 5194 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RENIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	334	Total	C	N	O	S	0	0	1
			2567	1639	416	498	14			
1	O	332	Total	C	N	O	S	0	0	1
			2557	1634	414	495	14			

- Molecule 2 is N-[(2S,4S,5S,7R)-4-AMINO-8-(BUTYLAMINO)-5-HYDROXY-7-METHYL-2-(1-METHYLETHYL)-8-OXOOCTYL]-2-(3-METHOXYPROPOXY)BENZAMIDE (three-letter code: C39) (formula: $C_{27}H_{47}N_3O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			35	27	3	5		
2	O	1	Total	C	N	O	0	0
			35	27	3	5		

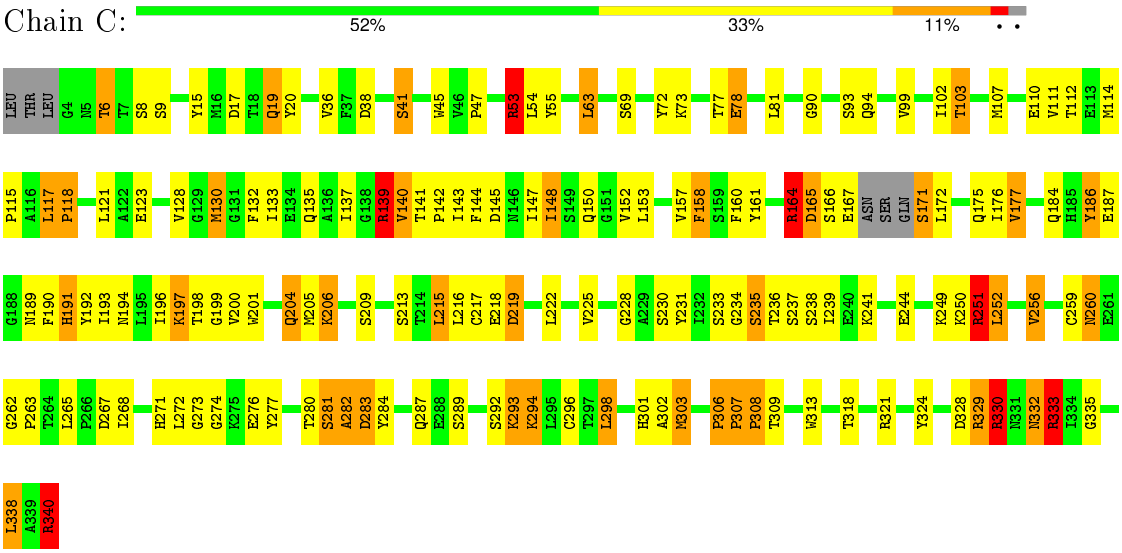
3 Residue-property plots (i)

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.

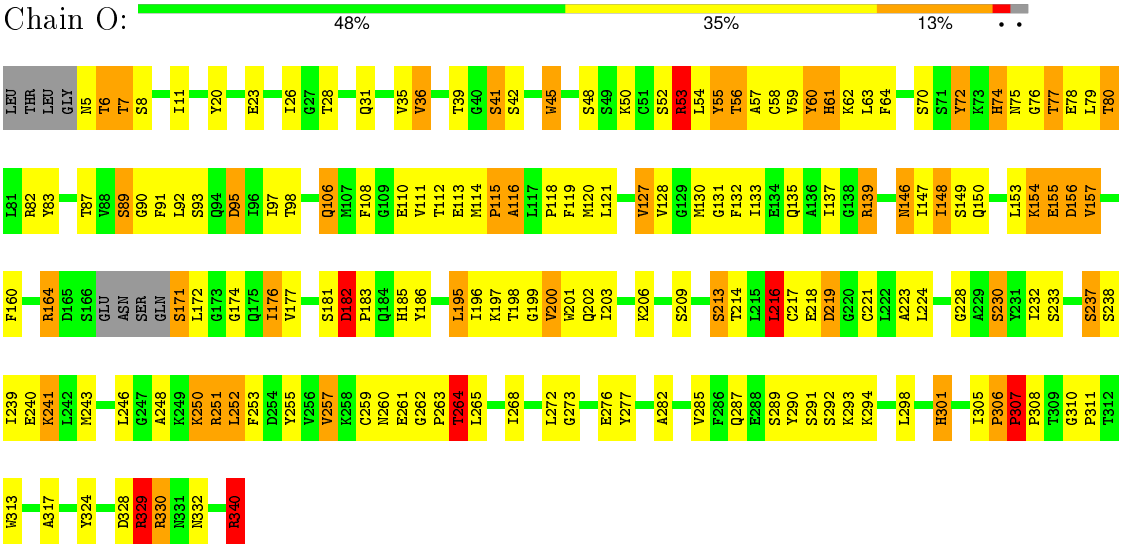
- Molecule 1: RENIN

Chain C:



- Molecule 1: RENIN

Chain O:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	142.90Å 142.90Å 142.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.20	Depositor
% Data completeness (in resolution range)	92.0 (10.00-3.20)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.236 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5194	wwPDB-VP
Average B, all atoms (Å^2)	15.0	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: C39

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	C	1.13	2/2626 (0.1%)	1.86	62/3560 (1.7%)
1	O	1.12	4/2616 (0.2%)	1.92	64/3547 (1.8%)
All	All	1.13	6/5242 (0.1%)	1.89	126/7107 (1.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	O	0	4
All	All	0	5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	171	SER	CA-CB	6.08	1.62	1.52
1	C	244	GLU	CG-CD	5.39	1.60	1.51
1	O	8	SER	CA-CB	-5.25	1.45	1.52
1	C	78	GLU	CG-CD	5.17	1.59	1.51
1	O	78	GLU	CG-CD	5.16	1.59	1.51
1	O	53	ARG	NE-CZ	5.04	1.39	1.33

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	53	ARG	NE-CZ-NH1	14.64	127.62	120.30
1	O	324	TYR	CB-CG-CD2	-12.55	113.47	121.00
1	C	139	ARG	NE-CZ-NH1	10.42	125.51	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	251	ARG	NE-CZ-NH1	9.46	125.03	120.30
1	C	139	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	C	330	ARG	NE-CZ-NH2	-8.55	116.03	120.30
1	O	75	ASN	CA-C-N	8.49	133.18	116.20
1	O	201	TRP	CD1-CG-CD2	8.48	113.08	106.30
1	C	165	ASP	O-C-N	8.39	136.13	122.70
1	C	72	TYR	CB-CG-CD2	-8.35	115.99	121.00
1	O	313	TRP	CD1-CG-CD2	8.29	112.93	106.30
1	O	72	TYR	CB-CG-CD1	-8.29	116.03	121.00
1	C	201	TRP	CD1-CG-CD2	8.27	112.92	106.30
1	O	53	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	O	45	TRP	CD1-CG-CD2	8.10	112.78	106.30
1	C	340	ARG	NE-CZ-NH2	-8.03	116.29	120.30
1	O	45	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	O	313	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	O	201	TRP	CE2-CD2-CG	-7.49	101.31	107.30
1	C	201	TRP	CE2-CD2-CG	-7.35	101.42	107.30
1	O	139	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	C	282	ALA	N-CA-C	-7.16	91.66	111.00
1	C	191	HIS	CA-CB-CG	-7.13	101.48	113.60
1	O	45	TRP	CB-CG-CD1	-7.11	117.76	127.00
1	C	251	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	O	83	TYR	CB-CG-CD1	-7.04	116.78	121.00
1	O	6	THR	CA-C-N	-6.99	101.82	117.20
1	O	324	TYR	CA-C-N	6.89	132.35	117.20
1	O	171	SER	CA-C-N	6.88	132.35	117.20
1	C	313	TRP	CE2-CD2-CG	-6.88	101.80	107.30
1	C	333	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	O	7	THR	N-CA-C	-6.75	92.77	111.00
1	C	165	ASP	CA-C-N	-6.75	102.36	117.20
1	C	6	THR	CA-CB-CG2	6.67	121.73	112.40
1	O	200	VAL	CG1-CB-CG2	-6.62	100.30	110.90
1	C	111	VAL	CG1-CB-CG2	-6.60	100.34	110.90
1	O	154	LYS	CA-CB-CG	-6.60	98.88	113.40
1	C	201	TRP	CG-CD2-CE3	6.51	139.76	133.90
1	O	156	ASP	CA-C-N	-6.48	102.94	117.20
1	O	213	SER	N-CA-CB	-6.48	100.78	110.50
1	C	15	TYR	CB-CG-CD1	-6.46	117.12	121.00
1	O	111	VAL	CA-CB-CG2	-6.44	101.24	110.90
1	C	313	TRP	CG-CD2-CE3	6.43	139.68	133.90
1	C	164	ARG	CB-CG-CD	6.40	128.25	111.60
1	C	340	ARG	NE-CZ-NH1	6.39	123.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	172	LEU	CA-C-N	6.32	128.83	116.20
1	C	45	TRP	CE2-CD2-CG	-6.28	102.28	107.30
1	C	139	ARG	CA-CB-CG	-6.21	99.74	113.40
1	C	130	MET	CG-SD-CE	-6.10	90.44	100.20
1	O	45	TRP	CG-CD2-CE3	6.10	139.39	133.90
1	O	201	TRP	CB-CG-CD1	-6.05	119.14	127.00
1	C	201	TRP	CB-CG-CD1	-6.04	119.15	127.00
1	O	155	GLU	CA-CB-CG	6.02	126.64	113.40
1	O	60	TYR	CB-CG-CD1	-5.98	117.41	121.00
1	C	55	TYR	CB-CG-CD2	-5.96	117.42	121.00
1	C	164	ARG	NE-CZ-NH2	-5.95	117.32	120.30
1	C	233	SER	N-CA-CB	5.93	119.40	110.50
1	C	313	TRP	CB-CG-CD1	-5.93	119.28	127.00
1	O	276	GLU	CA-CB-CG	-5.93	100.36	113.40
1	C	233	SER	CB-CA-C	-5.91	98.88	110.10
1	C	313	TRP	CD1-CG-CD2	5.90	111.02	106.30
1	O	290	TYR	O-C-N	-5.88	113.30	122.70
1	C	256	VAL	CA-CB-CG2	-5.84	102.14	110.90
1	O	201	TRP	CG-CD2-CE3	5.84	139.15	133.90
1	C	249	LYS	CB-CG-CD	5.83	126.75	111.60
1	C	298	LEU	CA-CB-CG	5.78	128.59	115.30
1	C	103	THR	CA-CB-CG2	5.77	120.48	112.40
1	O	340	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	O	201	TRP	CG-CD1-NE1	-5.71	104.39	110.10
1	C	45	TRP	CD1-CG-CD2	5.69	110.86	106.30
1	O	251	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	O	221	CYS	CA-CB-SG	-5.67	103.79	114.00
1	C	219	ASP	N-CA-CB	5.65	120.77	110.60
1	O	330	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	O	324	TYR	CB-CG-CD1	5.62	124.37	121.00
1	C	128	VAL	CG1-CB-CG2	-5.61	101.92	110.90
1	O	154	LYS	N-CA-C	5.58	126.08	111.00
1	O	157	VAL	CG1-CB-CG2	-5.58	101.97	110.90
1	C	36	VAL	CG1-CB-CG2	-5.57	101.99	110.90
1	O	340	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	C	15	TYR	CB-CG-CD2	5.53	124.32	121.00
1	C	148	ILE	CA-C-N	5.52	129.34	117.20
1	O	282	ALA	CB-CA-C	-5.52	101.82	110.10
1	C	103	THR	CA-CB-OG1	-5.51	97.43	109.00
1	C	6	THR	CA-CB-OG1	-5.51	97.43	109.00
1	O	176	ILE	CA-CB-CG1	-5.51	100.53	111.00
1	C	164	ARG	CA-CB-CG	5.47	125.44	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	64	PHE	CB-CG-CD1	-5.44	116.99	120.80
1	C	333	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	O	252	LEU	N-CA-C	-5.42	96.37	111.00
1	C	201	TRP	CG-CD1-NE1	-5.39	104.71	110.10
1	O	106	GLN	CG-CD-NE2	5.38	129.61	116.70
1	C	38	ASP	CA-C-N	5.37	129.02	117.20
1	O	216	LEU	CB-CG-CD2	-5.35	101.90	111.00
1	C	110	GLU	N-CA-C	-5.35	96.56	111.00
1	O	174	GLY	CA-C-N	5.32	128.90	117.20
1	O	328	ASP	CA-C-N	-5.30	105.54	117.20
1	O	313	TRP	CG-CD1-NE1	-5.29	104.81	110.10
1	O	264	THR	N-CA-CB	-5.29	100.25	110.30
1	C	340	ARG	CG-CD-NE	5.29	122.91	111.80
1	O	115	PRO	O-C-N	5.29	131.16	122.70
1	O	259	CYS	CA-CB-SG	-5.26	104.53	114.00
1	C	277	TYR	CB-CG-CD2	-5.26	117.85	121.00
1	C	8	SER	CA-CB-OG	-5.24	97.04	111.20
1	C	186	TYR	CA-CB-CG	5.24	123.35	113.40
1	C	225	VAL	CG1-CB-CG2	-5.23	102.53	110.90
1	O	55	TYR	N-CA-C	-5.23	96.88	111.00
1	O	219	ASP	N-CA-C	-5.20	96.97	111.00
1	O	115	PRO	CA-C-N	-5.18	105.79	117.20
1	C	171	SER	CA-C-N	5.16	128.56	117.20
1	O	59	VAL	CA-C-N	-5.16	105.85	117.20
1	O	201	TRP	NE1-CE2-CZ2	-5.15	124.73	130.40
1	C	19	GLN	CA-CB-CG	-5.15	102.08	113.40
1	C	99	VAL	N-CA-C	-5.15	97.10	111.00
1	O	313	TRP	CG-CD2-CE3	5.12	138.51	133.90
1	O	53	ARG	CA-CB-CG	5.12	124.66	113.40
1	C	69	SER	N-CA-C	-5.12	97.19	111.00
1	O	251	ARG	N-CA-C	-5.11	97.21	111.00
1	C	165	ASP	CA-CB-CG	5.10	124.61	113.40
1	O	329	ARG	CA-CB-CG	-5.08	102.22	113.40
1	C	53	ARG	CG-CD-NE	5.08	122.46	111.80
1	O	329	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	O	31	GLN	CA-C-N	5.05	128.32	117.20
1	C	177	VAL	N-CA-C	-5.04	97.40	111.00
1	C	272	LEU	CA-C-N	-5.01	106.17	116.20
1	O	301	HIS	CB-CA-C	-5.01	100.37	110.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	307	PRO	Peptide
1	O	182	ASP	Peptide
1	O	277	TYR	Sidechain
1	O	306	PRO	Peptide
1	O	307	PRO	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2567	0	2498	88	0
1	O	2557	0	2490	90	0
2	C	35	0	47	6	0
2	O	35	0	47	5	0
All	All	5194	0	5082	178	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 17.

All (178) 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:O:5:ASN:HA	1:O:154:LYS:HD3	1.28	1.07
1:O:148:ILE:HD11	1:O:156:ASP:HB3	1.56	0.87
1:C:293:LYS:HG3	1:C:294:LYS:HG2	1.58	0.85
1:O:285:VAL:HG22	1:O:298:LEU:HD22	1.64	0.79
1:C:260:ASN:OD1	1:C:292:SER:HA	1.87	0.74
1:O:55:TYR:HB2	1:O:58:CYS:SG	2.30	0.71
1:O:80:THR:HG23	1:O:89:SER:HB3	1.73	0.70
1:O:6:THR:HB	1:O:153:LEU:HA	1.73	0.70
1:C:197:LYS:N	1:C:197:LYS:HD2	2.08	0.68
1:O:53:ARG:HB3	1:O:53:ARG:HH11	1.59	0.67
1:C:20:TYR:HD1	2:C:350:C39:H1C1	1.60	0.67
1:C:197:LYS:HD2	1:C:197:LYS:H	1.60	0.66
1:C:53:ARG:NE	1:C:53:ARG:H	1.94	0.66
1:C:204:GLN:HE21	1:C:205:MET:N	1.93	0.65
1:C:144:PHE:HB3	1:C:329:ARG:NH2	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:ILE:HD12	1:C:273:GLY:HA3	1.79	0.63
1:O:230:SER:O	1:O:317:ALA:HB3	1.99	0.63
1:O:200:VAL:HG12	1:O:202:GLN:HB2	1.81	0.62
1:C:81:LEU:HD23	1:C:137:ILE:HD12	1.81	0.61
1:C:157:VAL:HG12	1:C:328:ASP:HA	1.81	0.60
1:C:204:GLN:HE21	1:C:205:MET:H	1.49	0.60
1:C:186:TYR:HA	1:C:338:LEU:O	2.01	0.60
1:O:5:ASN:OD1	1:O:154:LYS:HE2	2.02	0.60
1:O:216:LEU:HB3	1:O:241:LYS:HE2	1.83	0.59
1:O:147:ILE:O	1:O:150:GLN:HG2	2.02	0.59
1:O:228:GLY:HA2	2:O:350:C39:H3C1	1.84	0.59
1:C:239:ILE:HB	1:C:302:ALA:HB2	1.85	0.59
1:C:164:ARG:H	1:C:164:ARG:NH1	2.00	0.59
1:C:196:ILE:HD11	1:C:204:GLN:HB2	1.85	0.58
1:C:139:ARG:HG2	1:C:139:ARG:HH11	1.69	0.58
1:O:233:SER:HA	1:O:301:HIS:O	2.03	0.58
1:O:53:ARG:HB3	1:O:53:ARG:NH1	2.17	0.58
1:O:139:ARG:NH1	1:O:139:ARG:H	2.02	0.57
1:O:216:LEU:N	1:O:241:LYS:HZ3	2.02	0.57
1:O:209:SER:HA	1:O:214:THR:HA	1.87	0.57
1:O:216:LEU:HB3	1:O:241:LYS:NZ	2.20	0.57
1:C:53:ARG:N	1:C:53:ARG:HE	2.03	0.56
1:C:293:LYS:HE3	1:C:294:LYS:HD2	1.88	0.56
1:O:139:ARG:HG2	1:O:139:ARG:HH11	1.71	0.56
1:O:307:PRO:HA	1:O:310:GLY:O	2.06	0.56
1:O:26:ILE:HG23	1:O:97:ILE:HG12	1.86	0.56
1:O:202:GLN:HA	1:O:223:ALA:O	2.06	0.56
1:O:72:TYR:HE1	1:O:93:SER:HG	1.53	0.56
1:O:11:ILE:HD12	1:O:11:ILE:H	1.71	0.55
1:O:41:SER:HB3	2:O:350:C39:H331	1.89	0.54
1:C:213:SER:O	1:C:215:LEU:HD23	2.07	0.54
1:O:291:SER:HB3	1:O:294:LYS:HG3	1.90	0.54
1:C:259:CYS:SG	1:C:296:CYS:N	2.82	0.53
1:O:79:LEU:HD13	1:O:92:LEU:HD13	1.90	0.53
1:C:133:ILE:HG12	1:C:139:ARG:HH12	1.73	0.53
1:C:187:GLU:HB3	1:C:340:ARG:HE	1.74	0.53
1:C:192:TYR:HB3	1:C:333:ARG:HD3	1.91	0.52
1:C:330:ARG:O	1:C:330:ARG:HD3	2.09	0.52
1:O:155:GLU:HB3	1:O:157:VAL:HG22	1.91	0.52
1:O:248:ALA:HA	1:O:257:VAL:HG23	1.92	0.52
1:C:167:GLU:N	1:C:171:SER:N	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:216:LEU:HB3	1:O:241:LYS:CE	2.40	0.52
1:C:53:ARG:HE	1:C:53:ARG:H	1.57	0.52
1:O:132:PHE:HD2	1:O:199:GLY:C	2.13	0.52
1:C:47:PRO:HB2	1:C:63:LEU:HD23	1.92	0.52
1:C:102:ILE:HG21	1:C:147:ILE:HG23	1.92	0.52
1:O:250:LYS:HA	1:O:255:TYR:HA	1.91	0.51
1:O:127:VAL:HG11	2:O:350:C39:H201	1.91	0.51
1:C:206:LYS:HD2	1:C:206:LYS:H	1.76	0.51
1:C:144:PHE:HB3	1:C:329:ARG:HH21	1.76	0.51
1:O:246:LEU:HD21	1:O:268:ILE:HD11	1.92	0.51
1:O:5:ASN:HA	1:O:154:LYS:CD	2.20	0.51
1:C:107:MET:HB2	1:C:140:VAL:HG13	1.92	0.51
1:C:271:HIS:CD2	1:C:276:GLU:HG3	2.46	0.50
1:C:267:ASP:OD1	1:C:280:THR:HG22	2.10	0.50
1:C:293:LYS:HZ2	1:C:293:LYS:HB2	1.76	0.50
1:C:20:TYR:CD1	2:C:350:C39:H1C1	2.45	0.50
1:C:301:HIS:HE1	1:C:303:MET:HG3	1.76	0.50
1:C:216:LEU:HD13	1:C:241:LYS:CE	2.42	0.50
1:C:234:GLY:O	1:C:302:ALA:HA	2.11	0.49
1:O:95:ASP:HB2	1:O:108:PHE:HE2	1.77	0.49
1:O:156:ASP:OD1	1:O:330:ARG:HB3	2.13	0.49
1:O:261:GLU:O	1:O:264:THR:HB	2.13	0.49
1:O:185:HIS:HA	1:O:340:ARG:O	2.11	0.49
1:C:150:GLN:O	1:C:152:VAL:HG23	2.13	0.49
1:O:196:ILE:HB	1:O:197:LYS:HG2	1.94	0.49
1:C:301:HIS:CE1	1:C:303:MET:HG3	2.48	0.48
1:C:250:LYS:HD3	1:C:250:LYS:O	2.14	0.48
1:O:182:ASP:HA	1:O:183:PRO:HD3	1.56	0.48
1:O:183:PRO:HA	1:O:186:TYR:CE1	2.49	0.48
1:C:132:PHE:HB2	1:C:199:GLY:O	2.13	0.48
1:C:191:HIS:O	1:C:335:GLY:HA2	2.14	0.48
1:O:257:VAL:HG21	1:O:265:LEU:HD21	1.95	0.48
1:O:195:LEU:HB2	1:O:332:ASN:O	2.13	0.48
1:O:56:THR:HB	1:O:120:MET:SD	2.53	0.47
1:O:74:HIS:HA	1:O:93:SER:HB2	1.96	0.47
1:C:17:ASP:HB3	1:C:321:ARG:CZ	2.44	0.47
1:C:293:LYS:HZ2	1:C:294:LYS:H	1.62	0.47
1:O:57:ALA:HB2	1:O:116:ALA:HA	1.97	0.47
1:O:305:ILE:O	1:O:310:GLY:HA3	2.14	0.47
1:O:216:LEU:HB3	1:O:241:LYS:HZ3	1.80	0.47
1:C:148:ILE:HD13	1:C:153:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:ILE:HG22	1:C:177:VAL:N	2.30	0.47
1:C:41:SER:HB2	2:C:350:C39:H353	1.95	0.47
1:C:216:LEU:HD12	1:C:217:CYS:H	1.80	0.47
1:C:135:GLN:O	2:C:350:C39:H352	2.15	0.46
2:C:350:C39:H193	2:C:350:C39:H15	1.80	0.46
1:O:237:SER:HA	1:O:240:GLU:HB2	1.97	0.46
1:O:61:HIS:HE1	1:O:119:PHE:O	1.98	0.46
1:O:216:LEU:HD21	1:O:238:SER:OG	2.16	0.46
1:C:340:ARG:NH2	1:O:7:THR:HG22	2.31	0.46
1:C:139:ARG:HH11	1:C:139:ARG:CG	2.28	0.46
1:O:90:GLY:HA2	1:O:112:THR:HB	1.96	0.46
1:O:164:ARG:HD2	1:O:164:ARG:HH11	1.63	0.46
1:O:5:ASN:CA	1:O:154:LYS:HD3	2.20	0.46
1:C:340:ARG:HG3	1:C:340:ARG:HH11	1.81	0.46
1:O:243:MET:CE	1:O:298:LEU:HD12	2.46	0.45
2:O:350:C39:H15	2:O:350:C39:H193	1.80	0.45
1:C:268:ILE:HG12	1:C:284:TYR:CE2	2.51	0.45
1:C:280:THR:O	1:C:283:ASP:HB2	2.16	0.45
1:O:82:ARG:HA	1:O:87:THR:OG1	2.16	0.45
1:C:338:LEU:HD23	1:C:338:LEU:HA	1.72	0.45
1:C:228:GLY:HA2	2:C:350:C39:H3C1	1.98	0.45
1:C:308:PRO:HB2	1:C:309:THR:HG23	1.99	0.45
1:C:73:LYS:HB2	1:C:94:GLN:HB3	1.97	0.45
1:O:139:ARG:NH1	1:O:139:ARG:N	2.65	0.45
1:C:340:ARG:HH22	1:O:7:THR:HG22	1.82	0.45
1:O:11:ILE:N	1:O:11:ILE:HD12	2.32	0.44
1:C:328:ASP:HB3	1:C:333:ARG:O	2.18	0.44
1:O:36:VAL:HG11	2:O:350:C39:H192	2.00	0.44
1:C:53:ARG:H	1:C:53:ARG:CD	2.29	0.44
1:O:39:THR:HG22	1:O:130:MET:HB2	2.00	0.44
1:C:196:ILE:HD12	1:C:222:LEU:HD23	1.99	0.44
1:O:48:SER:HB2	1:O:110:GLU:HB3	2.00	0.44
1:C:90:GLY:HA2	1:C:112:THR:OG1	2.17	0.44
1:C:141:THR:HA	1:C:142:PRO:HD3	1.56	0.44
1:O:154:LYS:HA	1:O:154:LYS:HD2	1.43	0.43
1:O:203:ILE:HG13	1:O:223:ALA:HB3	1.99	0.43
1:C:194:ASN:HA	1:C:333:ARG:HB3	2.00	0.43
1:C:239:ILE:HA	1:C:239:ILE:HD13	1.69	0.43
1:C:250:LYS:O	1:C:252:LEU:N	2.51	0.43
1:O:90:GLY:HA3	1:O:110:GLU:O	2.18	0.43
1:C:161:TYR:HB2	1:C:324:TYR:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:60:TYR:HD1	1:O:120:MET:HG3	1.83	0.43
1:C:19:GLN:OE1	1:C:123:GLU:N	2.52	0.43
1:O:243:MET:SD	1:O:246:LEU:HD12	2.59	0.43
1:C:265:LEU:HB2	1:C:281:SER:OG	2.19	0.43
1:C:289:SER:OG	1:C:294:LYS:HG3	2.19	0.43
1:O:305:ILE:HA	1:O:306:PRO:HD3	1.84	0.43
1:O:146:ASN:O	1:O:149:SER:HB3	2.17	0.43
1:O:114:MET:HA	1:O:115:PRO:HD3	1.84	0.43
1:C:194:ASN:HD22	1:C:194:ASN:N	2.17	0.42
1:O:77:THR:O	1:O:91:PHE:HA	2.18	0.42
1:O:7:THR:HG23	1:O:177:VAL:CG1	2.49	0.42
1:C:192:TYR:HA	1:C:335:GLY:HA2	2.01	0.42
1:O:62:LYS:C	1:O:63:LEU:HD12	2.40	0.42
1:C:213:SER:O	1:C:215:LEU:N	2.52	0.42
1:O:35:VAL:HG21	1:O:128:VAL:HG23	2.02	0.42
1:O:132:PHE:HE1	1:O:329:ARG:CZ	2.33	0.42
1:C:306:PRO:HG2	1:C:308:PRO:HG2	2.02	0.42
1:O:217:CYS:SG	1:O:217:CYS:O	2.78	0.42
1:O:45:TRP:NE1	1:O:127:VAL:HG13	2.36	0.41
1:C:158:PHE:HD2	1:C:160:PHE:HE2	1.69	0.41
1:C:117:LEU:HA	1:C:118:PRO:HA	1.80	0.41
1:O:42:SER:OG	1:O:135:GLN:HB2	2.21	0.41
1:C:239:ILE:CB	1:C:302:ALA:HB2	2.51	0.41
1:C:139:ARG:O	1:C:141:THR:N	2.54	0.41
1:O:292:SER:HB2	1:O:293:LYS:NZ	2.36	0.41
1:O:160:PHE:CE1	1:O:176:ILE:HD11	2.55	0.41
1:O:89:SER:OG	1:O:113:GLU:HB2	2.21	0.41
1:O:262:GLY:HA2	1:O:265:LEU:HD12	2.03	0.41
1:C:206:LYS:NZ	1:C:274:GLY:H	2.19	0.41
1:O:251:ARG:HB3	1:O:252:LEU:H	1.60	0.41
1:O:239:ILE:HA	1:O:239:ILE:HD13	1.88	0.41
1:C:217:CYS:SG	1:C:217:CYS:O	2.79	0.40
1:O:146:ASN:HA	1:O:146:ASN:HD22	1.71	0.40
1:O:79:LEU:HD22	1:O:92:LEU:HD12	2.02	0.40
1:C:47:PRO:HG3	1:C:114:MET:CE	2.51	0.40
1:C:231:TYR:HD2	1:C:301:HIS:CD2	2.40	0.40
1:O:285:VAL:HG22	1:O:298:LEU:CD2	2.45	0.40
1:C:282:ALA:O	1:C:283:ASP:C	2.59	0.40
1:C:198:THR:OG1	1:C:332:ASN:ND2	2.54	0.40
1:C:81:LEU:HA	1:C:137:ILE:HD12	2.04	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	C	330/340 (97%)	296 (90%)	23 (7%)	11 (3%)	5	32
1	O	328/340 (96%)	281 (86%)	35 (11%)	12 (4%)	4	29
All	All	658/680 (97%)	577 (88%)	58 (9%)	23 (4%)	4	31

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	166	SER
1	C	251	ARG
1	O	50	LYS
1	O	116	ALA
1	C	140	VAL
1	C	219	ASP
1	C	262	GLY
1	O	53	ARG
1	O	61	HIS
1	O	273	GLY
1	O	289	SER
1	O	308	PRO
1	C	235	SER
1	C	294	LYS
1	C	283	ASP
1	O	76	GLY
1	O	77	THR
1	C	287	GLN
1	O	131	GLY
1	C	308	PRO
1	C	263	PRO
1	O	307	PRO
1	O	137	ILE

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	C	283/290 (98%)	228 (81%)	55 (19%)	2 9
1	O	282/290 (97%)	233 (83%)	49 (17%)	2 12
All	All	565/580 (97%)	461 (82%)	104 (18%)	2 10

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	6	THR
1	C	9	SER
1	C	41	SER
1	C	53	ARG
1	C	54	LEU
1	C	63	LEU
1	C	77	THR
1	C	78	GLU
1	C	93	SER
1	C	103	THR
1	C	115	PRO
1	C	117	LEU
1	C	118	PRO
1	C	121	LEU
1	C	130	MET
1	C	139	ARG
1	C	143	ILE
1	C	145	ASP
1	C	158	PHE
1	C	164	ARG
1	C	165	ASP
1	C	172	LEU
1	C	175	GLN
1	C	184	GLN
1	C	189	ASN
1	C	190	PHE
1	C	197	LYS

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Mol	Chain	Res	Type
1	C	200	VAL
1	C	204	GLN
1	C	206	LYS
1	C	209	SER
1	C	215	LEU
1	C	218	GLU
1	C	230	SER
1	C	235	SER
1	C	236	THR
1	C	237	SER
1	C	238	SER
1	C	251	ARG
1	C	252	LEU
1	C	256	VAL
1	C	260	ASN
1	C	281	SER
1	C	293	LYS
1	C	298	LEU
1	C	303	MET
1	C	306	PRO
1	C	307	PRO
1	C	318	THR
1	C	329	ARG
1	C	330	ARG
1	C	332	ASN
1	C	333	ARG
1	C	338	LEU
1	C	340	ARG
1	O	20	TYR
1	O	23	GLU
1	O	28	THR
1	O	36	VAL
1	O	41	SER
1	O	52	SER
1	O	53	ARG
1	O	54	LEU
1	O	56	THR
1	O	70	SER
1	O	74	HIS
1	O	80	THR
1	O	89	SER
1	O	95	ASP

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Mol	Chain	Res	Type
1	O	98	THR
1	O	106	GLN
1	O	118	PRO
1	O	121	LEU
1	O	127	VAL
1	O	133	ILE
1	O	146	ASN
1	O	148	ILE
1	O	164	ARG
1	O	171	SER
1	O	181	SER
1	O	182	ASP
1	O	195	LEU
1	O	198	THR
1	O	206	LYS
1	O	213	SER
1	O	216	LEU
1	O	218	GLU
1	O	219	ASP
1	O	224	LEU
1	O	230	SER
1	O	232	ILE
1	O	237	SER
1	O	241	LYS
1	O	250	LYS
1	O	253	PHE
1	O	257	VAL
1	O	260	ASN
1	O	263	PRO
1	O	264	THR
1	O	272	LEU
1	O	287	GLN
1	O	311	PRO
1	O	329	ARG
1	O	340	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	189	ASN
1	C	191	HIS
1	C	194	ASN

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Mol	Chain	Res	Type
1	C	204	GLN
1	C	301	HIS
1	C	332	ASN
1	O	31	GLN
1	O	146	ASN
1	O	175	GLN
1	O	194	ASN
1	O	271	HIS
1	O	332	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
2	C39	C	350	-	35,35,35	1.33	2 (5%)	36,44,44	1.88	8 (22%)
2	C39	O	350	-	35,35,35	1.23	2 (5%)	36,44,44	2.07	8 (22%)

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	C39	C	350	-	-	0/40/40/40	0/1/1/1
2	C39	O	350	-	-	0/40/40/40	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	350	C39	C12-C13	-5.65	1.38	1.50
2	O	350	C39	C12-C13	-5.20	1.39	1.50
2	C	350	C39	C11-C12	-2.04	1.36	1.39
2	O	350	C39	O6-C7	2.15	1.41	1.37

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	350	C39	O6-C7-C8	-5.18	113.17	124.01
2	O	350	C39	O6-C7-C8	-4.52	114.55	124.01
2	O	350	C39	C7-C12-C13	-4.13	119.35	126.18
2	C	350	C39	C7-C12-C13	-3.79	119.92	126.18
2	O	350	C39	O25-C24-C22	-3.77	103.90	109.49
2	C	350	C39	O25-C24-C22	-3.53	104.25	109.49
2	O	350	C39	C28-C27-C26	-3.10	105.22	111.42
2	C	350	C39	O30-C29-N31	-2.26	118.55	123.08
2	C	350	C39	C21-C17-C18	-2.21	107.07	112.47
2	O	350	C39	C21-C17-C18	-2.16	107.19	112.47
2	C	350	C39	C11-C12-C7	2.39	121.32	118.24
2	O	350	C39	C11-C12-C7	3.73	123.04	118.24
2	C	350	C39	C27-C29-N31	3.90	122.37	116.84
2	C	350	C39	O6-C7-C12	4.55	127.28	116.86
2	O	350	C39	O6-C7-C12	4.68	127.57	116.86
2	O	350	C39	C27-C26-C24	5.46	121.03	114.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	350	C39	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	350	C39	5	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.