Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:35 PM GMT

PDB ID	:	1UCX
Title	:	Crystal structure of proglycinin C12G mutant
Authors	:	Utsumi, S.; Adachi, M.
Deposited on	:	2003-04-24
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

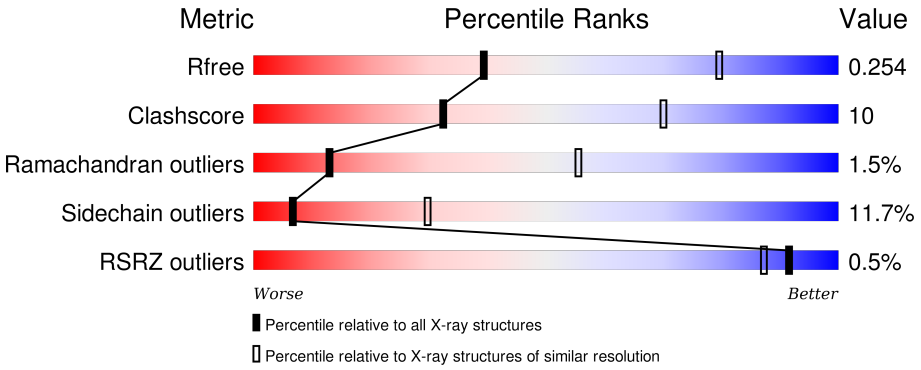
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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))
R_{free}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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.

Mol	Chain	Length	Quality of chain
1	A	476	50% 23% • 23%
1	B	476	% 49% 23% • 23%
1	C	476	49% 23% • 23%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 8643 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 Glycinin G1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	0	0
			2881	1821	509	540	11			
1	B	367	Total	C	N	O	S	0	0	0
			2881	1821	509	540	11			
1	C	367	Total	C	N	O	S	0	0	0
			2881	1821	509	540	11			

There are 3 discrepancies between the modelled and reference sequences:

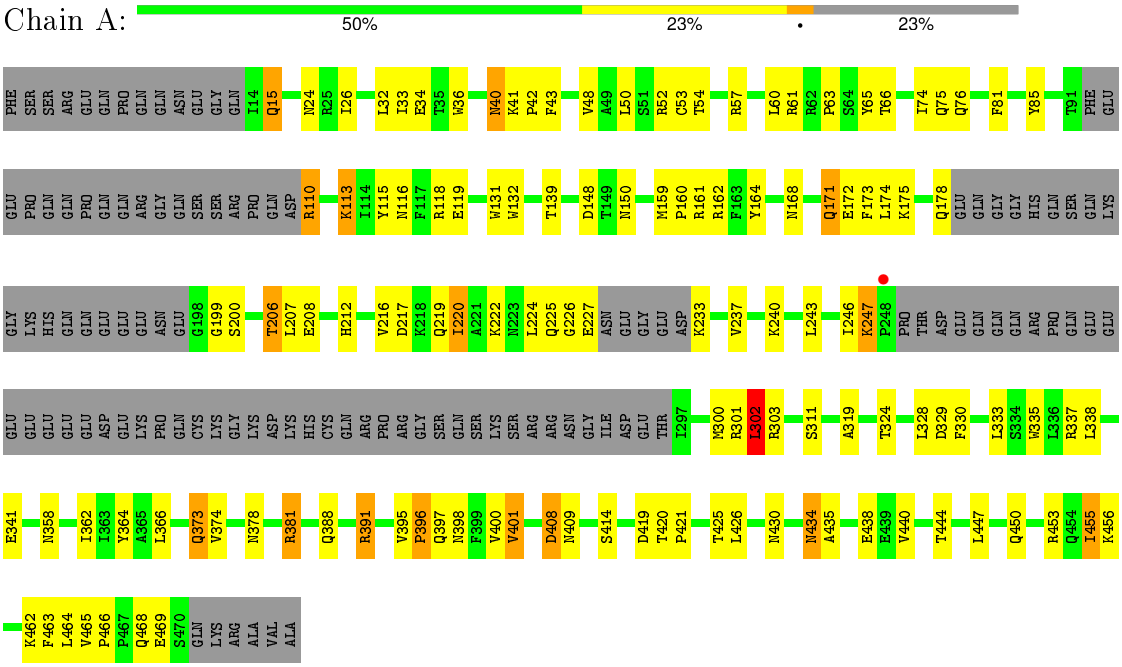
Chain	Residue	Modelled	Actual	Comment	Reference
A	12	GLY	CYS	ENGINEERED	UNP P04776
B	12	GLY	CYS	ENGINEERED	UNP P04776
C	12	GLY	CYS	ENGINEERED	UNP P04776

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.

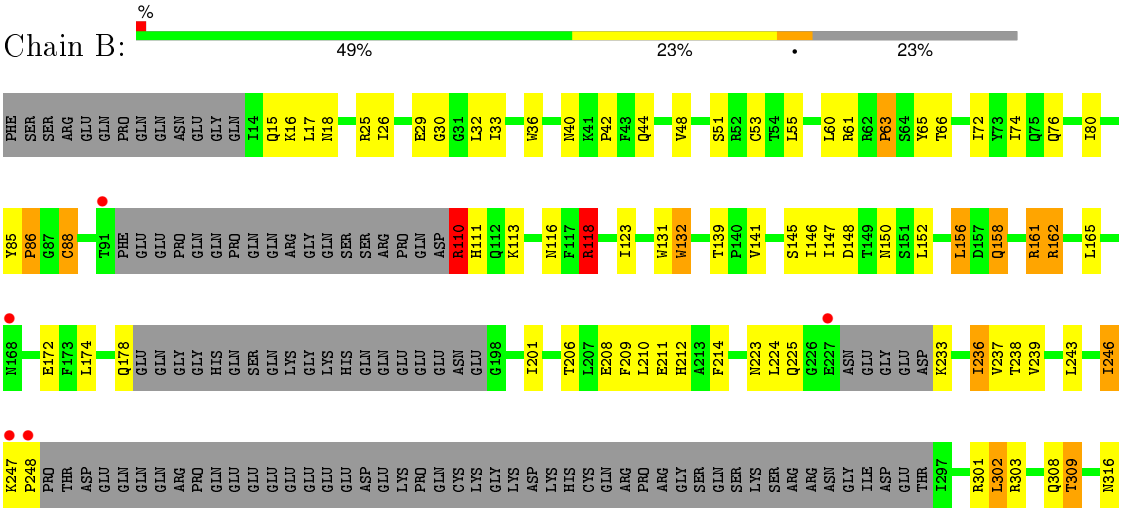
- Molecule 1: Glycinin G1

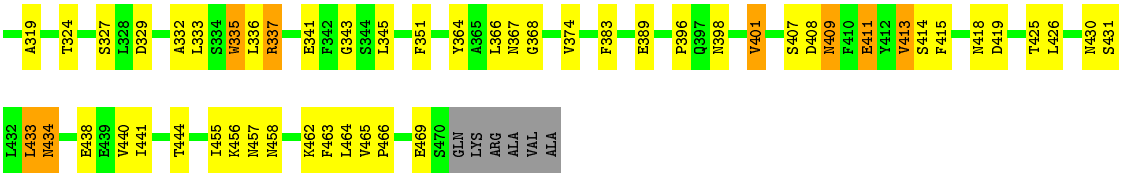
Chain A:



- Molecule 1: Glycinin G1

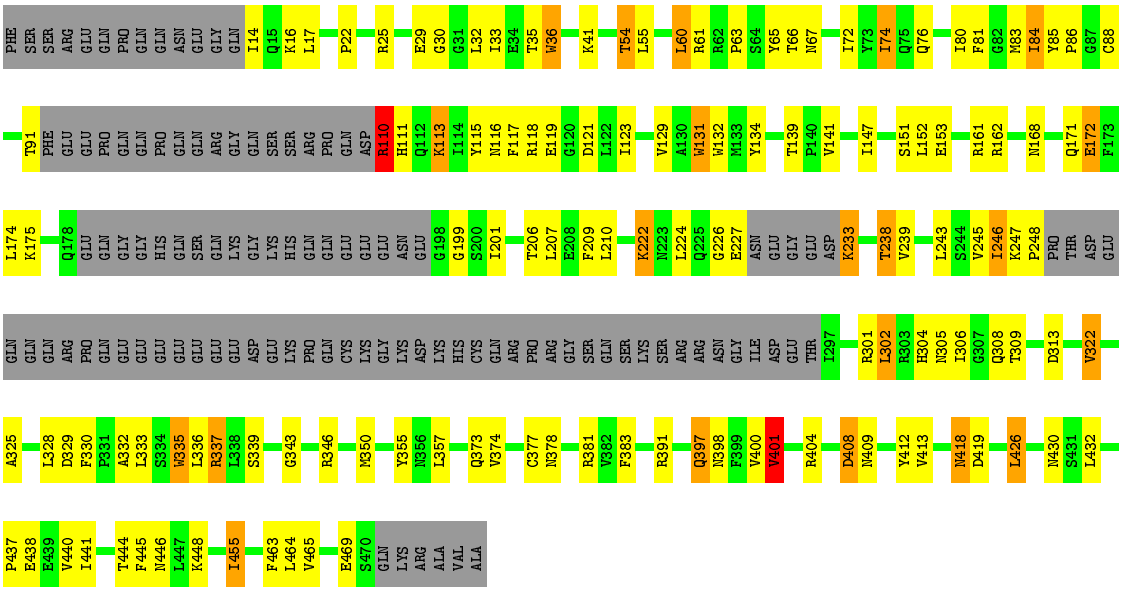
Chain B:





- Molecule 1: Glycinin G1

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	115.20Å 115.20Å 147.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.20 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-3.20) 68.5 (15.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 2.69Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.180 , 0.257 0.184 , 0.254	Depositor DCC
R_{free} test set	2479 reflections (9.99%)	DCC
Wilson B-factor (Å^2)	34.9	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 39.9	EDS
Estimated twinning fraction	0.046 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 35942 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	8643	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.71	0/2939	1.42	40/3982 (1.0%)
1	B	0.69	0/2939	1.43	36/3982 (0.9%)
1	C	0.71	0/2939	1.42	34/3982 (0.9%)
All	All	0.70	0/8817	1.42	110/11946 (0.9%)

There are no bond length outliers.

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	132	TRP	CD1-CG-CD2	9.65	114.02	106.30
1	A	110	ARG	NE-CZ-NH2	-9.14	115.73	120.30
1	A	408	ASP	CA-C-N	-8.99	97.41	117.20
1	C	110	ARG	NE-CZ-NH1	8.94	124.77	120.30
1	B	162	ARG	NE-CZ-NH2	-8.93	115.84	120.30
1	B	132	TRP	CD1-CG-CD2	8.89	113.41	106.30
1	B	335	TRP	CD1-CG-CD2	8.69	113.25	106.30
1	B	36	TRP	CD1-CG-CD2	8.62	113.19	106.30
1	B	408	ASP	CA-C-N	-8.62	98.24	117.20
1	A	335	TRP	CD1-CG-CD2	8.58	113.17	106.30
1	A	132	TRP	CE2-CD2-CG	-8.47	100.53	107.30
1	C	132	TRP	CD1-CG-CD2	8.33	112.96	106.30
1	A	131	TRP	CD1-CG-CD2	8.32	112.95	106.30
1	A	162	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	B	36	TRP	CE2-CD2-CG	-8.18	100.75	107.30
1	C	408	ASP	CA-C-N	-8.10	99.39	117.20
1	C	36	TRP	CD1-CG-CD2	7.88	112.61	106.30
1	C	36	TRP	CE2-CD2-CG	-7.84	101.03	107.30
1	A	52	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	A	301	ARG	NE-CZ-NH1	7.67	124.14	120.30
1	B	132	TRP	CE2-CD2-CG	-7.61	101.21	107.30
1	C	132	TRP	CE2-CD2-CG	-7.61	101.21	107.30
1	C	335	TRP	CD1-CG-CD2	7.53	112.33	106.30
1	A	335	TRP	CE2-CD2-CG	-7.52	101.28	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	36	TRP	CE2-CD2-CG	-7.50	101.30	107.30
1	C	162	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	A	131	TRP	CE2-CD2-CG	-7.49	101.31	107.30
1	A	36	TRP	CD1-CG-CD2	7.42	112.24	106.30
1	B	161	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	B	161	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	B	131	TRP	CD1-CG-CD2	7.29	112.13	106.30
1	B	131	TRP	CE2-CD2-CG	-7.26	101.50	107.30
1	B	335	TRP	CE2-CD2-CG	-7.25	101.50	107.30
1	C	335	TRP	CE2-CD2-CG	-7.23	101.51	107.30
1	C	131	TRP	CE2-CD2-CG	-7.17	101.57	107.30
1	C	131	TRP	CD1-CG-CD2	7.11	111.99	106.30
1	C	409	ASN	CA-C-N	-7.06	101.67	117.20
1	C	110	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	C	36	TRP	CG-CD2-CE3	6.96	140.16	133.90
1	B	301	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	B	337	ARG	NE-CZ-NH2	6.84	123.72	120.30
1	C	36	TRP	CB-CG-CD1	-6.77	118.20	127.00
1	B	36	TRP	CB-CG-CD1	-6.77	118.20	127.00
1	C	132	TRP	CG-CD2-CE3	6.70	139.93	133.90
1	A	132	TRP	CB-CG-CD1	-6.69	118.31	127.00
1	B	302	LEU	CA-CB-CG	6.61	130.51	115.30
1	B	36	TRP	CG-CD2-CE3	6.58	139.82	133.90
1	A	85	TYR	CB-CG-CD2	-6.57	117.06	121.00
1	A	132	TRP	CG-CD2-CE3	6.55	139.79	133.90
1	C	408	ASP	O-C-N	6.52	133.13	122.70
1	A	36	TRP	CB-CG-CD1	-6.50	118.55	127.00
1	A	408	ASP	O-C-N	6.49	133.09	122.70
1	C	132	TRP	CB-CG-CD1	-6.47	118.59	127.00
1	B	408	ASP	O-C-N	6.46	133.04	122.70
1	A	36	TRP	CG-CD2-CE3	6.38	139.64	133.90
1	A	409	ASN	CA-C-N	-6.37	103.19	117.20
1	A	57	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	B	131	TRP	CG-CD2-CE3	6.35	139.62	133.90
1	B	409	ASN	CA-C-N	-6.30	103.33	117.20
1	B	301	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	B	118	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	C	381	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	A	132	TRP	CG-CD1-NE1	-5.92	104.19	110.10
1	C	74	ILE	CG1-CB-CG2	-5.86	98.51	111.40
1	A	302	LEU	CA-CB-CG	5.81	128.67	115.30
1	B	131	TRP	CB-CG-CD1	-5.80	119.45	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	118	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	C	381	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	C	401	VAL	CB-CA-C	-5.67	100.63	111.40
1	A	60	LEU	CA-CB-CG	5.66	128.32	115.30
1	A	425	THR	CA-CB-CG2	5.65	120.31	112.40
1	A	162	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	A	110	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	A	52	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	C	302	LEU	CA-CB-CG	5.56	128.08	115.30
1	C	322	VAL	CG1-CB-CG2	-5.54	102.03	110.90
1	B	335	TRP	CG-CD1-NE1	-5.51	104.59	110.10
1	B	110	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	C	131	TRP	CG-CD2-CE3	5.44	138.79	133.90
1	A	408	ASP	CA-CB-CG	-5.41	101.49	113.40
1	B	25	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	335	TRP	CG-CD1-NE1	-5.37	104.73	110.10
1	A	61	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	C	61	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	C	25	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	B	303	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	C	346	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	A	131	TRP	CB-CG-CD1	-5.23	120.20	127.00
1	B	88	CYS	CA-CB-SG	-5.22	104.60	114.00
1	B	132	TRP	CB-CG-CD1	-5.21	120.23	127.00
1	A	455	ILE	CA-CB-CG1	-5.21	101.11	111.00
1	B	351	PHE	CA-CB-CG	5.19	126.36	113.90
1	A	381	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	B	110	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	C	245	VAL	CA-C-N	-5.18	105.80	117.20
1	B	36	TRP	CG-CD1-NE1	-5.18	104.92	110.10
1	A	131	TRP	CG-CD1-NE1	-5.17	104.93	110.10
1	A	330	PHE	CB-CG-CD2	-5.16	117.19	120.80
1	A	131	TRP	CG-CD2-CE3	5.14	138.53	133.90
1	B	457	ASN	N-CA-C	5.13	124.84	111.00
1	B	174	LEU	CA-CB-CG	5.12	127.08	115.30
1	A	453	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	C	404	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	A	206	THR	CA-CB-CG2	5.07	119.50	112.40
1	C	132	TRP	CG-CD1-NE1	-5.07	105.03	110.10
1	C	60	LEU	CA-CB-CG	5.06	126.94	115.30
1	B	132	TRP	CG-CD1-NE1	-5.05	105.05	110.10
1	B	401	VAL	CB-CA-C	-5.03	101.83	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	391	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	C	162	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2881	0	2847	66	0
1	B	2881	0	2847	66	0
1	C	2881	0	2847	78	0
All	All	8643	0	8541	180	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 10.

All (180) 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:398:ASN:HB3	1:C:65:TYR:HE1	1.39	0.87
1:C:33:ILE:HG21	1:C:172:GLU:HG2	1.65	0.78
1:A:65:TYR:HE1	1:B:398:ASN:HB3	1.50	0.77
1:B:324:THR:HG22	1:B:341:GLU:HG3	1.68	0.76
1:B:367:ASN:HB3	1:B:411:GLU:HG3	1.66	0.76
1:A:168:ASN:HA	1:A:199:GLY:HA2	1.68	0.75
1:B:333:LEU:HD12	1:B:336:LEU:HD12	1.70	0.73
1:A:75:GLN:HG3	1:A:366:LEU:HD22	1.69	0.73
1:A:373:GLN:HG2	1:A:381:ARG:HD2	1.75	0.68
1:B:65:TYR:HE1	1:C:398:ASN:HB3	1.59	0.66
1:A:447:LEU:HD11	1:A:455:ILE:HD12	1.78	0.65
1:A:110:ARG:NH2	1:B:438:GLU:HB2	2.13	0.64
1:C:60:LEU:HD23	1:C:134:TYR:HB2	1.80	0.62
1:B:72:ILE:HA	1:B:145:SER:HB3	1.81	0.62
1:A:395:VAL:HG11	1:A:401:VAL:HG22	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:VAL:HG12	1:B:383:PHE:HB3	1.82	0.61
1:A:430:ASN:ND2	1:A:462:LYS:HE2	2.17	0.59
1:B:201:ILE:HD11	1:C:426:LEU:HD21	1.85	0.59
1:A:110:ARG:HH22	1:B:438:GLU:HB2	1.66	0.59
1:A:400:VAL:HG21	1:C:201:ILE:HB	1.84	0.59
1:A:440:VAL:O	1:A:444:THR:HG23	2.03	0.59
1:B:80:ILE:HG22	1:B:116:ASN:HD22	1.69	0.58
1:A:233:LYS:HE2	1:A:237:VAL:HG13	1.83	0.58
1:B:364:TYR:HB3	1:B:413:VAL:HG23	1.85	0.58
1:C:339:SER:HB2	1:C:418:ASN:O	2.04	0.57
1:A:159:MET:SD	1:A:160:PRO:HD2	2.45	0.57
1:A:40:ASN:HB3	1:A:42:PRO:HD2	1.86	0.57
1:B:66:THR:HG22	1:B:161:ARG:O	2.05	0.57
1:B:33:ILE:HG13	1:B:236:ILE:HD11	1.87	0.56
1:C:66:THR:HG21	1:C:147:ILE:HD13	1.87	0.56
1:C:239:VAL:HG21	1:C:243:LEU:HD13	1.87	0.56
1:B:368:GLY:O	1:B:389:GLU:HG3	2.05	0.56
1:A:63:PRO:HD3	1:B:444:THR:HG21	1.87	0.56
1:A:302:LEU:H	1:A:302:LEU:HD22	1.71	0.55
1:A:66:THR:HG22	1:A:161:ARG:O	2.06	0.55
1:A:430:ASN:HD21	1:A:462:LYS:HE2	1.71	0.55
1:C:30:GLY:HA3	1:C:238:THR:HG23	1.88	0.54
1:C:207:LEU:HD21	1:C:222:LYS:HD2	1.88	0.54
1:A:333:LEU:HG	1:A:338:LEU:O	2.08	0.54
1:C:116:ASN:HD21	1:C:248:PRO:HD2	1.73	0.54
1:C:32:LEU:HB3	1:C:54:THR:HG23	1.90	0.54
1:C:85:TYR:HB3	1:C:88:CYS:SG	2.48	0.54
1:B:214:PHE:CD2	1:B:224:LEU:HD21	2.43	0.54
1:A:398:ASN:HB3	1:C:65:TYR:CE1	2.31	0.54
1:A:216:VAL:HG11	1:A:220:ILE:HD11	1.89	0.53
1:B:110:ARG:HH12	1:C:438:GLU:H	1.56	0.53
1:C:168:ASN:HD21	1:C:226:GLY:HA3	1.73	0.53
1:A:48:VAL:HG21	1:A:362:ILE:HG12	1.90	0.53
1:B:233:LYS:HB2	1:B:237:VAL:HG22	1.91	0.53
1:B:345:LEU:O	1:B:409:ASN:HA	2.10	0.52
1:C:35:THR:HG21	1:C:172:GLU:HB3	1.92	0.52
1:C:66:THR:HG23	1:C:161:ARG:O	2.09	0.51
1:B:63:PRO:HG3	1:B:132:TRP:HB3	1.90	0.51
1:B:53:CYS:SG	1:B:61:ARG:NH2	2.83	0.51
1:C:74:ILE:HG12	1:C:117:PHE:CD1	2.46	0.51
1:A:341:GLU:HB3	1:A:414:SER:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:374:VAL:CG1	1:C:383:PHE:HB3	2.41	0.51
1:A:26:ILE:O	1:A:32:LEU:HD12	2.10	0.51
1:A:113:LYS:HD2	1:A:115:TYR:CZ	2.46	0.51
1:B:156:LEU:HD21	1:C:397:GLN:H	1.74	0.51
1:C:74:ILE:HG22	1:C:119:GLU:HA	1.92	0.51
1:B:33:ILE:HG21	1:B:172:GLU:HG2	1.92	0.50
1:A:81:PHE:HZ	1:A:302:LEU:HD23	1.77	0.50
1:C:113:LYS:HD2	1:C:115:TYR:CZ	2.47	0.50
1:B:434:ASN:O	1:B:456:LYS:HE2	2.11	0.50
1:B:224:LEU:HD13	1:C:455:ILE:HD13	1.94	0.50
1:B:15:GLN:HG3	1:B:16:LYS:N	2.26	0.50
1:C:355:TYR:HE1	1:C:357:LEU:HG	1.77	0.50
1:A:118:ARG:HH11	1:A:303:ARG:HH22	1.59	0.50
1:A:164:TYR:O	1:A:200:SER:HB2	2.12	0.49
1:B:110:ARG:HH12	1:C:438:GLU:HB2	1.77	0.49
1:A:216:VAL:HG12	1:B:458:ASN:ND2	2.26	0.49
1:C:72:ILE:HB	1:C:123:ILE:HB	1.94	0.49
1:C:76:GLN:NE2	1:C:139:THR:HG22	2.28	0.49
1:A:15:GLN:HE22	1:A:41:LYS:HD3	1.77	0.48
1:C:116:ASN:ND2	1:C:248:PRO:HD2	2.28	0.48
1:A:337:ARG:HA	1:A:419:ASP:HB3	1.96	0.48
1:A:438:GLU:HB2	1:C:110:ARG:NH2	2.29	0.48
1:C:76:GLN:HA	1:C:119:GLU:HB3	1.96	0.48
1:C:14:ILE:HG12	1:C:41:LYS:HD3	1.95	0.48
1:B:463:PHE:HD2	1:B:464:LEU:HD13	1.79	0.47
1:B:430:ASN:ND2	1:B:462:LYS:HE2	2.29	0.47
1:A:110:ARG:HH12	1:B:438:GLU:H	1.63	0.47
1:B:343:GLY:O	1:B:411:GLU:HA	2.14	0.47
1:A:33:ILE:HG23	1:A:53:CYS:SG	2.54	0.47
1:A:434:ASN:O	1:A:456:LYS:HE2	2.14	0.47
1:A:438:GLU:H	1:C:110:ARG:HH12	1.62	0.47
1:B:165:LEU:HD12	1:B:201:ILE:HD11	1.95	0.47
1:C:80:ILE:HG22	1:C:116:ASN:ND2	2.30	0.47
1:B:118:ARG:NH2	1:B:309:THR:HG21	2.29	0.47
1:C:116:ASN:HD21	1:C:247:LYS:HD3	1.79	0.47
1:B:201:ILE:HD12	1:C:400:VAL:HG21	1.96	0.47
1:C:54:THR:HA	1:C:141:VAL:O	2.14	0.46
1:C:355:TYR:CE1	1:C:357:LEU:HG	2.50	0.46
1:A:24:ASN:O	1:A:34:GLU:HA	2.15	0.46
1:A:364:TYR:CE2	1:A:366:LEU:HD23	2.51	0.46
1:B:110:ARG:NH1	1:C:438:GLU:HB2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:LEU:HB2	1:B:383:PHE:HB2	1.97	0.46
1:B:374:VAL:CG1	1:B:383:PHE:HB3	2.45	0.46
1:C:80:ILE:HG22	1:C:116:ASN:HD22	1.80	0.46
1:C:121:ASP:HA	1:C:305:ASN:HA	1.97	0.46
1:A:300:MET:O	1:A:302:LEU:HD13	2.15	0.46
1:B:206:THR:HB	1:C:373:GLN:HE22	1.81	0.46
1:A:358:ASN:OD1	1:A:421:PRO:HA	2.16	0.46
1:C:29:GLU:HB2	1:C:233:LYS:HA	1.98	0.45
1:A:33:ILE:HG21	1:A:172:GLU:HG2	1.98	0.45
1:B:29:GLU:HB2	1:B:233:LYS:HA	1.97	0.45
1:A:364:TYR:HE2	1:A:366:LEU:HD23	1.82	0.45
1:A:76:GLN:HA	1:A:119:GLU:HG2	1.97	0.45
1:B:76:GLN:O	1:B:141:VAL:HA	2.17	0.45
1:B:147:ILE:HD11	1:B:162:ARG:NH2	2.32	0.45
1:B:366:LEU:HB2	1:B:411:GLU:HB2	1.99	0.45
1:A:373:GLN:HE22	1:C:206:THR:HB	1.82	0.45
1:B:40:ASN:O	1:B:44:GLN:HG2	2.17	0.45
1:C:377:CYS:SG	1:C:378:ASN:ND2	2.90	0.45
1:C:445:PHE:O	1:C:446:ASN:HB3	2.17	0.45
1:B:30:GLY:HA3	1:B:238:THR:HG23	1.99	0.44
1:B:425:THR:HG23	1:B:431:SER:HA	1.99	0.44
1:A:118:ARG:HD3	1:A:303:ARG:HH21	1.82	0.44
1:B:208:GLU:HA	1:B:211:GLU:HB2	1.99	0.44
1:C:301:ARG:NH2	1:C:304:HIS:ND1	2.66	0.44
1:B:327:SER:HB3	1:B:419:ASP:HB2	1.99	0.44
1:A:81:PHE:CE1	1:A:115:TYR:HB2	2.52	0.44
1:C:168:ASN:HA	1:C:199:GLY:HA2	1.99	0.44
1:C:91:THR:HG23	1:C:111:HIS:O	2.17	0.44
1:A:174:LEU:O	1:A:178:GLN:HG2	2.18	0.44
1:B:201:ILE:CD1	1:C:426:LEU:HD21	2.48	0.44
1:B:316:ASN:HB3	1:B:319:ALA:HB3	2.00	0.44
1:C:332:ALA:O	1:C:335:TRP:HB2	2.18	0.44
1:C:374:VAL:HB	1:C:401:VAL:CG1	2.48	0.44
1:A:15:GLN:H	1:A:15:GLN:CD	2.21	0.44
1:B:74:ILE:HD11	1:B:123:ILE:CD1	2.48	0.43
1:C:333:LEU:HD12	1:C:336:LEU:HD12	2.00	0.43
1:A:116:ASN:HD21	1:A:247:LYS:HG2	1.82	0.43
1:A:319:ALA:HB2	1:A:466:PRO:HA	2.00	0.43
1:A:456:LYS:NZ	1:C:110:ARG:NH2	2.66	0.43
1:C:83:MET:HE3	1:C:129:VAL:HG11	2.01	0.43
1:B:48:VAL:HG12	1:B:148:ASP:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:ILE:HB	1:C:400:VAL:HG21	2.00	0.43
1:C:441:ILE:HD11	1:C:455:ILE:HG22	2.00	0.43
1:A:171:GLN:HE21	1:A:173:PHE:HB2	1.83	0.43
1:B:26:ILE:O	1:B:32:LEU:HD12	2.19	0.43
1:C:17:LEU:HB2	1:C:383:PHE:HB2	2.01	0.42
1:B:438:GLU:HA	1:B:441:ILE:HG22	2.01	0.42
1:B:332:ALA:O	1:B:335:TRP:HB2	2.19	0.42
1:A:74:ILE:HG22	1:A:119:GLU:HA	2.01	0.42
1:C:304:HIS:HB3	1:C:330:PHE:CD2	2.54	0.42
1:B:85:TYR:HB3	1:B:88:CYS:SG	2.60	0.42
1:A:435:ALA:HB3	1:C:84:ILE:CG2	2.50	0.42
1:A:456:LYS:HZ2	1:C:110:ARG:NH2	2.16	0.42
1:C:322:VAL:HG21	1:C:463:PHE:HE2	1.85	0.42
1:C:337:ARG:HD3	1:C:419:ASP:OD1	2.19	0.42
1:A:217:ASP:OD2	1:A:219:GLN:HB2	2.19	0.42
1:C:374:VAL:HB	1:C:401:VAL:HG13	2.01	0.42
1:B:16:LYS:HB2	1:B:16:LYS:HE3	1.83	0.42
1:B:239:VAL:HG11	1:B:243:LEU:HD12	2.02	0.42
1:C:343:GLY:HA3	1:C:412:TYR:CE1	2.55	0.41
1:C:374:VAL:HA	1:C:400:VAL:O	2.21	0.41
1:C:22:PRO:HD3	1:C:36:TRP:CZ2	2.56	0.41
1:B:146:ILE:HD13	1:B:415:PHE:HB3	2.03	0.41
1:B:246:ILE:HG23	1:B:248:PRO:HD3	2.03	0.41
1:B:465:VAL:HA	1:B:466:PRO:HD3	1.92	0.41
1:C:306:ILE:HG21	1:C:325:ALA:HB2	2.02	0.41
1:A:444:THR:HG21	1:C:63:PRO:HD3	2.02	0.41
1:C:63:PRO:HA	1:C:131:TRP:O	2.21	0.41
1:A:233:LYS:HB2	1:A:237:VAL:HG22	2.02	0.41
1:A:148:ASP:HB2	1:A:338:LEU:HD21	2.02	0.41
1:A:206:THR:HG22	1:A:208:GLU:HG2	2.03	0.41
1:A:243:LEU:HD21	1:B:440:VAL:HG12	2.02	0.41
1:B:111:HIS:CD2	1:C:437:PRO:HA	2.56	0.41
1:A:465:VAL:HA	1:A:466:PRO:HD3	1.91	0.41
1:A:447:LEU:CD1	1:A:455:ILE:HD12	2.49	0.40
1:C:66:THR:HG22	1:C:67:ASN:N	2.36	0.40
1:C:85:TYR:HA	1:C:86:PRO:HD2	1.87	0.40
1:C:440:VAL:O	1:C:444:THR:HG23	2.20	0.40
1:A:440:VAL:HG12	1:C:243:LEU:HD21	2.03	0.40
1:C:246:ILE:O	1:C:248:PRO:HD3	2.21	0.40
1:B:433:LEU:HD12	1:B:455:ILE:HG21	2.02	0.40
1:C:350:MET:HB3	1:C:465:VAL:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:PHE:HD1	1:A:48:VAL:HG23	1.86	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	357/476 (75%)	327 (92%)	24 (7%)	6 (2%)	11	52
1	B	357/476 (75%)	323 (90%)	28 (8%)	6 (2%)	11	52
1	C	357/476 (75%)	328 (92%)	25 (7%)	4 (1%)	17	62
All	All	1071/1428 (75%)	978 (91%)	77 (7%)	16 (2%)	13	55

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	158	GLN
1	B	246	ILE
1	B	396	PRO
1	C	397	GLN
1	C	246	ILE
1	A	226	GLY
1	A	396	PRO
1	A	397	GLN
1	A	463	PHE
1	B	418	ASN
1	A	240	LYS
1	B	86	PRO
1	B	156	LEU
1	C	418	ASN
1	C	469	GLU
1	A	246	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	A	315/413 (76%)	278 (88%)	37 (12%)	7	30
1	B	315/413 (76%)	279 (89%)	36 (11%)	7	31
1	C	315/413 (76%)	277 (88%)	38 (12%)	6	28
All	All	945/1239 (76%)	834 (88%)	111 (12%)	7	30

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	40	ASN
1	A	50	LEU
1	A	54	THR
1	A	113	LYS
1	A	139	THR
1	A	150	ASN
1	A	171	GLN
1	A	175	LYS
1	A	207	LEU
1	A	212	HIS
1	A	220	ILE
1	A	222	LYS
1	A	224	LEU
1	A	225	GLN
1	A	227	GLU
1	A	247	LYS
1	A	302	LEU
1	A	311	SER
1	A	324	THR
1	A	328	LEU
1	A	329	ASP
1	A	373	GLN
1	A	374	VAL
1	A	378	ASN
1	A	388	GLN

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Mol	Chain	Res	Type
1	A	391	ARG
1	A	396	PRO
1	A	401	VAL
1	A	408	ASP
1	A	420	THR
1	A	426	LEU
1	A	434	ASN
1	A	450	GLN
1	A	464	LEU
1	A	468	GLN
1	A	469	GLU
1	B	18	ASN
1	B	42	PRO
1	B	51	SER
1	B	55	LEU
1	B	60	LEU
1	B	63	PRO
1	B	86	PRO
1	B	110	ARG
1	B	113	LYS
1	B	118	ARG
1	B	139	THR
1	B	150	ASN
1	B	152	LEU
1	B	158	GLN
1	B	178	GLN
1	B	209	PHE
1	B	210	LEU
1	B	212	HIS
1	B	223	ASN
1	B	225	GLN
1	B	236	ILE
1	B	247	LYS
1	B	302	LEU
1	B	308	GLN
1	B	309	THR
1	B	329	ASP
1	B	337	ARG
1	B	401	VAL
1	B	407	SER
1	B	411	GLU
1	B	413	VAL

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Mol	Chain	Res	Type
1	B	414	SER
1	B	426	LEU
1	B	433	LEU
1	B	434	ASN
1	B	469	GLU
1	C	16	LYS
1	C	54	THR
1	C	55	LEU
1	C	81	PHE
1	C	84	ILE
1	C	110	ARG
1	C	113	LYS
1	C	151	SER
1	C	152	LEU
1	C	153	GLU
1	C	171	GLN
1	C	172	GLU
1	C	174	LEU
1	C	175	LYS
1	C	209	PHE
1	C	210	LEU
1	C	222	LYS
1	C	224	LEU
1	C	227	GLU
1	C	233	LYS
1	C	238	THR
1	C	302	LEU
1	C	308	GLN
1	C	309	THR
1	C	313	ASP
1	C	328	LEU
1	C	329	ASP
1	C	337	ARG
1	C	391	ARG
1	C	401	VAL
1	C	408	ASP
1	C	413	VAL
1	C	426	LEU
1	C	430	ASN
1	C	432	LEU
1	C	448	LYS
1	C	455	ILE

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Mol	Chain	Res	Type
1	C	464	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	116	ASN
1	A	135	ASN
1	A	223	ASN
1	A	378	ASN
1	A	450	GLN
1	A	454	GLN
1	B	116	ASN
1	B	171	GLN
1	B	177	GLN
1	B	212	HIS
1	B	443	HIS
1	B	451	GLN
1	B	454	GLN
1	C	39	ASN
1	C	76	GLN
1	C	116	ASN
1	C	171	GLN
1	C	177	GLN
1	C	178	GLN
1	C	212	HIS
1	C	367	ASN
1	C	378	ASN
1	C	458	ASN

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

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

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, 95^{th} 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	367/476 (77%)	-0.82	1 (0%) 94 93	2, 14, 32, 39	0
1	B	367/476 (77%)	-0.71	5 (1%) 78 65	4, 16, 33, 41	0
1	C	367/476 (77%)	-0.81	0 100 100	3, 14, 31, 42	0
All	All	1101/1428 (77%)	-0.78	6 (0%) 91 87	2, 15, 32, 42	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	168	ASN	3.0
1	B	247	LYS	2.8
1	B	91	THR	2.2
1	B	227	GLU	2.1
1	A	248	PRO	2.1
1	B	248	PRO	2.0

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 carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.