Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:38 PM GMT

PDB ID	:	1ULA
Title	:	APPLICATION OF CRYSTALLOGRAPHIC AND MODELING METHODS IN THE DESIGN OF PURINE NUCLEOSIDE PHOSPHORYLASE INHIBITORS
Authors	:	Ealick, S.E.; Rule, S.A.; Carter, D.C.; Greenhough, T.J.; Babu, Y.S.; Cook, W.J.; Habash, J.; Helliwell, J.R.; Stoeckler, J.D.; Parksjunior, R.E.; Chen, S.-F.; Bugg, C.E.
Deposited on	:	1991-11-05
Resolution	:	2.75 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:

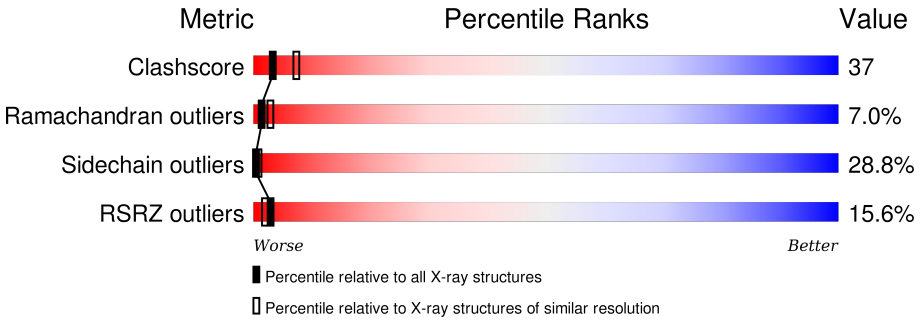
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.75 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	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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	289	16%, 21%, 44%, 28%, 7%

2 Entry composition

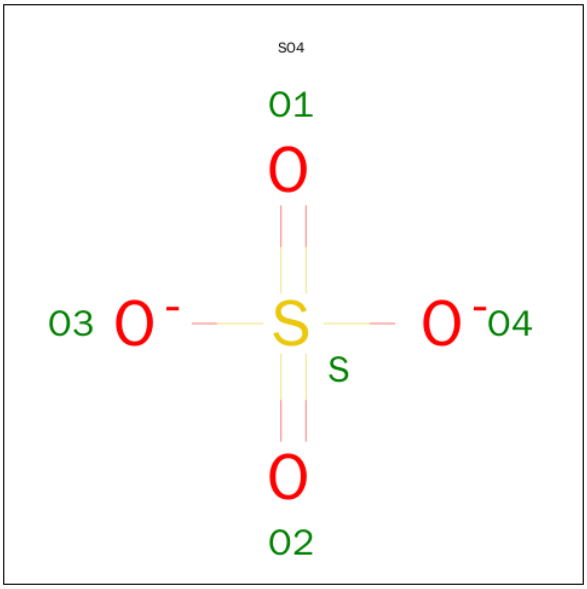
There are 2 unique types of molecules in this entry. The entry contains 2268 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PURINE NUCLEOSIDE PHOSPHORYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	0
			2258	1434	395	413	16			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



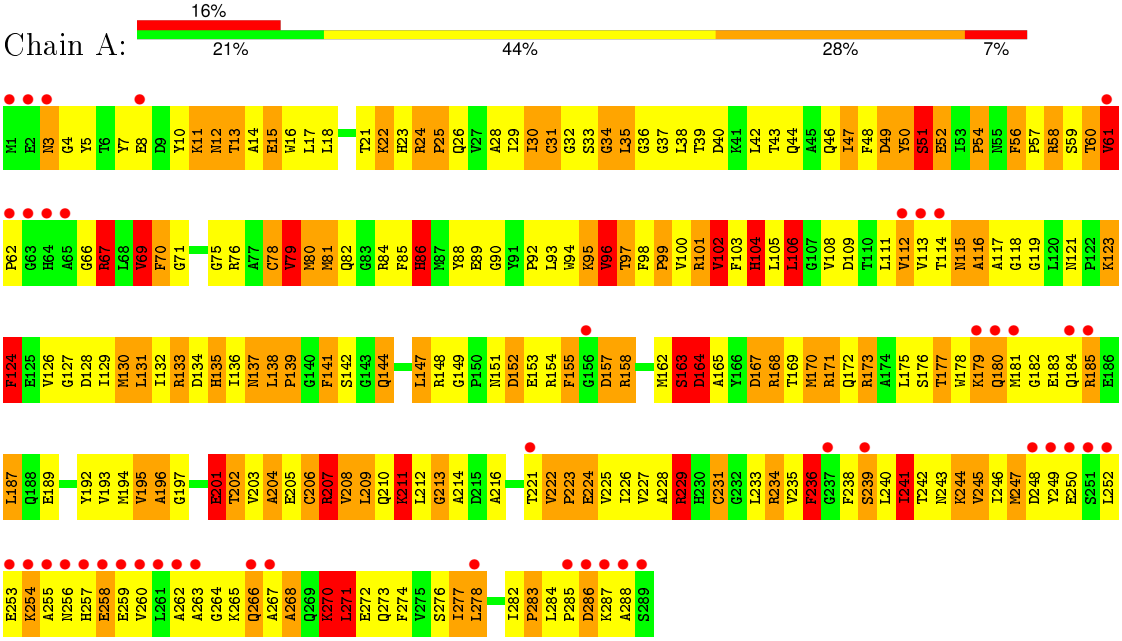
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	O	S		0	0
			5	4	1			
2	A	1	Total	O	S		0	0
			5	4	1			

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: PURINE NUCLEOSIDE PHOSPHORYLASE

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	142.90Å 142.90Å 165.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.75 33.61 – 2.75	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.75) 97.8 (33.61-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.31 (at 2.76Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.202 , (Not available) 0.234 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	53.8	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 58.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 16752 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	2268	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	1.36	9/2310 (0.4%)	2.52	141/3125 (4.5%)

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	A	0	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	GLU	CG-CD	-6.58	1.42	1.51
1	A	119	GLY	N-CA	6.24	1.55	1.46
1	A	164	ASP	CA-CB	6.21	1.67	1.53
1	A	224	GLU	CD-OE1	-5.91	1.19	1.25
1	A	231	CYS	CB-SG	-5.79	1.72	1.81
1	A	78	CYS	CB-SG	-5.68	1.72	1.81
1	A	205	GLU	CD-OE1	-5.66	1.19	1.25
1	A	36	GLY	N-CA	5.51	1.54	1.46
1	A	54	PRO	C-O	5.13	1.33	1.23

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	154	ARG	NE-CZ-NH2	23.65	132.13	120.30
1	A	101	ARG	NE-CZ-NH1	17.49	129.04	120.30
1	A	168	ARG	NE-CZ-NH1	13.93	127.27	120.30
1	A	185	ARG	NE-CZ-NH1	-13.80	113.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	154	ARG	NE-CZ-NH1	-12.72	113.94	120.30
1	A	168	ARG	CD-NE-CZ	12.70	141.38	123.60
1	A	171	ARG	NE-CZ-NH2	12.54	126.57	120.30
1	A	196	ALA	C-N-CA	11.64	146.74	122.30
1	A	76	ARG	NE-CZ-NH1	11.26	125.93	120.30
1	A	181	MET	CA-CB-CG	11.23	132.39	113.30
1	A	205	GLU	OE1-CD-OE2	-11.17	109.89	123.30
1	A	185	ARG	NE-CZ-NH2	10.64	125.62	120.30
1	A	214	ALA	CB-CA-C	-10.34	94.59	110.10
1	A	173	ARG	NE-CZ-NH2	-10.03	115.28	120.30
1	A	60	THR	C-N-CA	10.01	146.73	121.70
1	A	80	MET	CA-CB-CG	10.00	130.30	113.30
1	A	88	TYR	CB-CG-CD2	9.97	126.98	121.00
1	A	164	ASP	N-CA-CB	-9.73	93.09	110.60
1	A	207	ARG	CD-NE-CZ	-9.69	110.03	123.60
1	A	101	ARG	CB-CG-CD	9.58	136.52	111.60
1	A	148	ARG	NE-CZ-NH1	9.38	124.99	120.30
1	A	54	PRO	CA-C-N	8.97	136.94	117.20
1	A	163	SER	C-N-CA	8.94	144.04	121.70
1	A	154	ARG	CD-NE-CZ	-8.81	111.27	123.60
1	A	234	ARG	NE-CZ-NH2	-8.69	115.95	120.30
1	A	67	ARG	CD-NE-CZ	-8.54	111.64	123.60
1	A	133	ARG	NE-CZ-NH2	8.32	124.46	120.30
1	A	189	GLU	OE1-CD-OE2	8.32	133.28	123.30
1	A	164	ASP	CB-CA-C	-8.14	94.11	110.40
1	A	229	ARG	CD-NE-CZ	-8.08	112.28	123.60
1	A	121	ASN	CB-CA-C	8.02	126.43	110.40
1	A	208	VAL	CB-CA-C	7.97	126.53	111.40
1	A	152	ASP	CB-CG-OD1	-7.95	111.14	118.30
1	A	171	ARG	NH1-CZ-NH2	-7.86	110.75	119.40
1	A	88	TYR	CA-CB-CG	7.82	128.25	113.40
1	A	49	ASP	CB-CG-OD1	-7.79	111.29	118.30
1	A	123	LYS	CA-CB-CG	7.77	130.49	113.40
1	A	60	THR	CA-CB-CG2	7.75	123.25	112.40
1	A	211	LYS	N-CA-CB	7.57	124.22	110.60
1	A	116	ALA	C-N-CA	7.36	140.10	121.70
1	A	288	ALA	N-CA-CB	-7.33	99.84	110.10
1	A	15	GLU	CA-CB-CG	7.26	129.37	113.40
1	A	69	VAL	CA-CB-CG1	7.23	121.75	110.90
1	A	76	ARG	CD-NE-CZ	-7.05	113.73	123.60
1	A	52	GLU	CG-CD-OE1	-7.03	104.24	118.30
1	A	144	GLN	O-C-N	6.89	133.73	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	128	ASP	CB-CG-OD2	6.84	124.45	118.30
1	A	195	VAL	N-CA-CB	-6.83	96.47	111.50
1	A	76	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	A	202	THR	CA-CB-CG2	6.78	121.89	112.40
1	A	24	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	A	30	ILE	O-C-N	6.77	133.54	122.70
1	A	7	TYR	CB-CG-CD2	6.77	125.06	121.00
1	A	79	VAL	O-C-N	6.67	133.38	122.70
1	A	233	LEU	CA-CB-CG	6.66	130.62	115.30
1	A	245	VAL	CA-C-O	6.65	134.07	120.10
1	A	31	CYS	C-N-CA	6.62	136.20	122.30
1	A	268	ALA	N-CA-CB	6.58	119.31	110.10
1	A	178	TRP	CA-CB-CG	6.54	126.12	113.70
1	A	16	TRP	O-C-N	6.43	132.99	122.70
1	A	148	ARG	NH1-CZ-NH2	-6.42	112.34	119.40
1	A	154	ARG	CG-CD-NE	6.41	125.26	111.80
1	A	113	VAL	CA-CB-CG1	6.38	120.47	110.90
1	A	78	CYS	CA-CB-SG	6.38	125.48	114.00
1	A	155	PHE	C-N-CA	-6.24	109.20	122.30
1	A	104	HIS	CA-CB-CG	6.16	124.07	113.60
1	A	79	VAL	CB-CA-C	-6.05	99.90	111.40
1	A	253	GLU	CA-CB-CG	6.05	126.71	113.40
1	A	195	VAL	CA-CB-CG1	6.04	119.95	110.90
1	A	101	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	164	ASP	N-CA-C	5.99	127.19	111.00
1	A	130	MET	CA-CB-CG	-5.99	103.12	113.30
1	A	273	GLN	CA-CB-CG	5.99	126.57	113.40
1	A	222	VAL	CB-CA-C	5.98	122.77	111.40
1	A	157	ASP	N-CA-CB	-5.83	100.11	110.60
1	A	194	MET	C-N-CA	5.83	136.27	121.70
1	A	11	LYS	CA-CB-CG	5.81	126.18	113.40
1	A	185	ARG	CD-NE-CZ	-5.79	115.50	123.60
1	A	141	PHE	CA-CB-CG	5.78	127.78	113.90
1	A	79	VAL	N-CA-CB	5.74	124.14	111.50
1	A	168	ARG	NH1-CZ-NH2	-5.73	113.09	119.40
1	A	270	LYS	O-C-N	5.73	131.87	122.70
1	A	54	PRO	O-C-N	-5.71	113.56	122.70
1	A	233	LEU	CB-CA-C	5.70	121.03	110.20
1	A	118	GLY	C-N-CA	-5.69	110.35	122.30
1	A	263	ALA	C-N-CA	-5.67	110.39	122.30
1	A	34	GLY	O-C-N	5.65	131.74	122.70
1	A	236	PHE	CB-CA-C	5.65	121.70	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	153	GLU	CA-C-O	-5.64	108.25	120.10
1	A	118	GLY	CA-C-N	5.63	127.47	116.20
1	A	101	ARG	NH1-CZ-NH2	-5.63	113.21	119.40
1	A	86	HIS	CA-CB-CG	5.62	123.15	113.60
1	A	241	ILE	O-C-N	-5.61	113.73	122.70
1	A	84	ARG	CD-NE-CZ	-5.60	115.76	123.60
1	A	61	VAL	N-CA-C	5.59	126.11	111.00
1	A	106	LEU	CB-CA-C	5.59	120.83	110.20
1	A	204	ALA	CB-CA-C	5.59	118.48	110.10
1	A	189	GLU	CG-CD-OE2	-5.59	107.13	118.30
1	A	175	LEU	CB-CA-C	5.58	120.80	110.20
1	A	164	ASP	CA-CB-CG	-5.55	101.19	113.40
1	A	8	GLU	CB-CA-C	-5.53	99.33	110.40
1	A	148	ARG	CB-CG-CD	5.53	125.98	111.60
1	A	208	VAL	CA-CB-CG2	5.47	119.11	110.90
1	A	133	ARG	O-C-N	5.47	131.45	122.70
1	A	88	TYR	CG-CD1-CE1	5.46	125.67	121.30
1	A	79	VAL	CA-C-O	-5.44	108.68	120.10
1	A	153	GLU	CA-CB-CG	5.44	125.36	113.40
1	A	124	PHE	CB-CG-CD1	5.42	124.60	120.80
1	A	224	GLU	CB-CA-C	-5.39	99.62	110.40
1	A	206	CYS	CA-CB-SG	-5.39	104.31	114.00
1	A	201	GLU	CA-C-O	-5.37	108.81	120.10
1	A	277	ILE	CA-CB-CG2	5.37	121.64	110.90
1	A	96	VAL	C-N-CA	5.37	135.12	121.70
1	A	154	ARG	CA-C-O	5.37	131.37	120.10
1	A	137	ASN	O-C-N	-5.36	114.12	122.70
1	A	80	MET	CB-CA-C	5.35	121.11	110.40
1	A	81	MET	CG-SD-CE	-5.34	91.66	100.20
1	A	124	PHE	C-N-CA	-5.33	108.37	121.70
1	A	134	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	213	GLY	CA-C-O	-5.33	111.01	120.60
1	A	12	ASN	CB-CG-OD1	-5.31	110.97	121.60
1	A	52	GLU	OE1-CD-OE2	5.31	129.67	123.30
1	A	271	LEU	CB-CA-C	5.29	120.26	110.20
1	A	249	TYR	CB-CA-C	5.27	120.94	110.40
1	A	90	GLY	C-N-CA	5.24	134.81	121.70
1	A	8	GLU	N-CA-CB	5.21	119.99	110.60
1	A	40	ASP	CB-CA-C	5.20	120.80	110.40
1	A	96	VAL	CA-CB-CG2	5.18	118.68	110.90
1	A	170	MET	CA-CB-CG	5.18	122.10	113.30
1	A	3	ASN	CA-CB-CG	-5.15	102.07	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	154	ARG	NH1-CZ-NH2	-5.14	113.75	119.40
1	A	168	ARG	CG-CD-NE	5.12	122.56	111.80
1	A	245	VAL	CB-CA-C	5.12	121.13	111.40
1	A	101	ARG	CD-NE-CZ	5.12	130.77	123.60
1	A	95	LYS	CD-CE-NZ	-5.11	99.94	111.70
1	A	102	VAL	CA-CB-CG2	5.08	118.53	110.90
1	A	24	ARG	N-CA-CB	5.07	119.72	110.60
1	A	97	THR	N-CA-CB	-5.05	100.70	110.30
1	A	108	VAL	CB-CA-C	5.04	120.98	111.40
1	A	256	ASN	CA-C-O	5.03	130.67	120.10
1	A	138	LEU	CB-CA-C	5.01	119.71	110.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	207	ARG	Sidechain
1	A	229	ARG	Sidechain

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	A	2258	0	2230	168	1
2	A	10	0	0	2	0
All	All	2268	0	2230	168	1

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 37.

All (168) 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:210:GLN:CD	1:A:247:MET:HE3	1.49	1.33
1:A:210:GLN:NE2	1:A:247:MET:HE3	1.42	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:GLU:HG2	1:A:264:GLY:HA3	1.18	1.15
1:A:210:GLN:CD	1:A:247:MET:CE	2.25	1.04
1:A:258:GLU:CG	1:A:264:GLY:HA3	1.93	0.98
1:A:210:GLN:NE2	1:A:247:MET:CE	2.26	0.97
1:A:92:PRO:HD2	1:A:95:LYS:HD2	1.53	0.91
1:A:117:ALA:HB1	1:A:216:ALA:HB1	1.55	0.89
1:A:136:ILE:HB	1:A:193:VAL:HG23	1.57	0.85
1:A:34:GLY:HA3	1:A:258:GLU:CD	1.98	0.83
1:A:21:THR:HG23	1:A:48:PHE:HZ	1.44	0.81
1:A:60:THR:O	1:A:62:PRO:HD2	1.82	0.79
1:A:42:LEU:HD22	1:A:71:GLY:HA3	1.63	0.79
1:A:165:ALA:HA	1:A:229:ARG:HD2	1.64	0.79
1:A:60:THR:HB	1:A:61:VAL:HG23	1.65	0.79
1:A:39:THR:HG22	1:A:80:MET:HG2	1.66	0.78
1:A:35:LEU:HD21	1:A:271:LEU:HD22	1.66	0.77
1:A:42:LEU:HD11	1:A:80:MET:HE3	1.65	0.76
1:A:203:VAL:O	1:A:207:ARG:HG3	1.84	0.76
1:A:47:ILE:HD12	1:A:67:ARG:NH2	2.04	0.73
1:A:58:ARG:HH11	1:A:58:ARG:HG2	1.54	0.73
1:A:139:PRO:O	1:A:144:GLN:HB2	1.89	0.71
1:A:86:HIS:N	1:A:89:GLU:OE2	2.22	0.71
1:A:210:GLN:OE1	1:A:247:MET:CE	2.37	0.71
1:A:21:THR:HG23	1:A:48:PHE:CZ	2.24	0.71
1:A:179:LYS:HG3	1:A:180:GLN:N	2.04	0.71
1:A:221:THR:O	1:A:225:VAL:HG23	1.93	0.69
1:A:57:PRO:HG2	1:A:85:PHE:CE2	2.28	0.69
1:A:149:GLY:O	1:A:158:ARG:NH2	2.25	0.69
1:A:97:THR:HG23	1:A:227:VAL:HG21	1.74	0.69
1:A:132:ILE:HG23	1:A:192:TYR:HB2	1.74	0.69
1:A:236:PHE:HE1	1:A:238:PHE:CZ	2.10	0.69
1:A:97:THR:HG21	1:A:227:VAL:HG11	1.76	0.68
1:A:32:GLY:O	1:A:33:SER:C	2.32	0.68
1:A:35:LEU:HD21	1:A:271:LEU:CD2	2.24	0.68
1:A:206:CYS:SG	1:A:245:VAL:HG12	2.34	0.68
1:A:97:THR:CG2	1:A:227:VAL:HG21	2.24	0.67
1:A:225:VAL:HG13	1:A:235:VAL:HG11	1.77	0.67
1:A:34:GLY:HA2	2:A:291:SO4:O4	1.95	0.66
1:A:81:MET:HG3	1:A:103:PHE:HZ	1.61	0.65
1:A:206:CYS:SG	1:A:245:VAL:CG1	2.85	0.64
1:A:129:ILE:HD13	1:A:271:LEU:HB2	1.79	0.64
1:A:285:PRO:O	1:A:287:LYS:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:LYS:CG	1:A:180:GLN:N	2.61	0.64
1:A:179:LYS:O	1:A:182:GLY:N	2.30	0.63
1:A:28:ALA:HB3	1:A:111:LEU:HD12	1.80	0.63
1:A:271:LEU:C	1:A:271:LEU:HD23	2.21	0.61
1:A:60:THR:C	1:A:62:PRO:HD2	2.22	0.60
1:A:66:GLY:HA2	1:A:82:GLN:O	2.00	0.60
1:A:268:ALA:O	1:A:272:GLU:HG3	2.02	0.59
1:A:34:GLY:HA3	1:A:258:GLU:OE2	2.01	0.59
1:A:135:HIS:HA	1:A:192:TYR:O	2.03	0.59
1:A:18:LEU:HD13	1:A:106:LEU:HD12	1.85	0.59
1:A:93:LEU:HA	1:A:96:VAL:HG13	1.85	0.58
1:A:127:GLY:HA2	1:A:267:ALA:HB2	1.85	0.58
1:A:31:CYS:HB2	1:A:81:MET:O	2.03	0.58
1:A:57:PRO:HG2	1:A:85:PHE:HE2	1.68	0.58
1:A:34:GLY:HA3	1:A:258:GLU:OE1	2.04	0.57
1:A:117:ALA:CB	1:A:216:ALA:HB1	2.33	0.57
1:A:51:SER:HA	1:A:58:ARG:HD3	1.86	0.57
1:A:176:SER:O	1:A:179:LYS:N	2.34	0.56
1:A:99:PRO:O	1:A:100:VAL:C	2.44	0.56
1:A:28:ALA:HB1	1:A:103:PHE:CE2	2.41	0.56
1:A:114:THR:O	1:A:115:ASN:HB3	2.06	0.55
1:A:26:GLN:HG2	1:A:26:GLN:O	2.05	0.55
1:A:97:THR:HG23	1:A:227:VAL:CG2	2.37	0.55
1:A:42:LEU:HD22	1:A:71:GLY:CA	2.36	0.54
1:A:43:THR:O	1:A:44:GLN:HB2	2.07	0.54
1:A:135:HIS:CE1	1:A:222:VAL:HG13	2.43	0.54
1:A:183:GLU:OE2	1:A:270:LYS:HD2	2.08	0.54
1:A:97:THR:CG2	1:A:227:VAL:HG11	2.37	0.53
1:A:285:PRO:O	1:A:287:LYS:HG3	2.08	0.53
1:A:211:LYS:C	1:A:213:GLY:H	2.11	0.53
1:A:252:LEU:O	1:A:252:LEU:HD12	2.09	0.53
1:A:204:ALA:O	1:A:207:ARG:N	2.41	0.53
1:A:246:ILE:HD12	1:A:250:GLU:CD	2.30	0.53
1:A:115:ASN:HB2	2:A:290:SO4:O3	2.09	0.53
1:A:162:MET:O	1:A:163:SER:C	2.44	0.53
1:A:102:VAL:O	1:A:103:PHE:C	2.48	0.53
1:A:93:LEU:HD22	1:A:223:PRO:HG3	1.91	0.52
1:A:274:PHE:O	1:A:278:LEU:HD12	2.08	0.52
1:A:30:ILE:O	1:A:114:THR:OG1	2.23	0.52
1:A:258:GLU:HA	1:A:264:GLY:H	1.75	0.52
1:A:56:PHE:O	1:A:57:PRO:C	2.49	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:LEU:N	1:A:139:PRO:CD	2.73	0.51
1:A:179:LYS:CG	1:A:180:GLN:H	2.22	0.51
1:A:124:PHE:O	1:A:244:LYS:HD2	2.10	0.51
1:A:284:LEU:HD23	1:A:284:LEU:C	2.31	0.51
1:A:32:GLY:O	1:A:35:LEU:HB2	2.11	0.51
1:A:207:ARG:O	1:A:211:LYS:HG2	2.12	0.50
1:A:284:LEU:O	1:A:287:LYS:HG3	2.11	0.50
1:A:42:LEU:HD11	1:A:80:MET:CE	2.37	0.50
1:A:29:ILE:HG12	1:A:112:VAL:HG13	1.94	0.49
1:A:101:ARG:O	1:A:104:HIS:HB3	2.12	0.49
1:A:131:LEU:HD11	1:A:171:ARG:HG2	1.94	0.49
1:A:177:THR:HA	1:A:180:GLN:HB2	1.95	0.48
1:A:50:TYR:O	1:A:52:GLU:N	2.47	0.48
1:A:187:LEU:HD13	1:A:274:PHE:CE2	2.48	0.48
1:A:264:GLY:O	1:A:268:ALA:CB	2.62	0.48
1:A:123:LYS:O	1:A:124:PHE:CD1	2.67	0.48
1:A:25:PRO:HG3	1:A:79:VAL:HG22	1.95	0.48
1:A:22:LYS:HE2	1:A:23:HIS:CD2	2.49	0.47
1:A:169:THR:O	1:A:173:ARG:HB2	2.14	0.47
1:A:138:LEU:O	1:A:139:PRO:C	2.53	0.47
1:A:170:MET:CE	1:A:282:ILE:HG13	2.44	0.47
1:A:201:GLU:HB2	1:A:206:CYS:SG	2.54	0.47
1:A:138:LEU:HB2	1:A:139:PRO:HD3	1.96	0.47
1:A:262:ALA:O	1:A:266:GLN:N	2.48	0.47
1:A:236:PHE:HE1	1:A:238:PHE:HZ	1.59	0.46
1:A:211:LYS:C	1:A:213:GLY:N	2.69	0.46
1:A:14:ALA:O	1:A:17:LEU:N	2.48	0.46
1:A:132:ILE:CG2	1:A:192:TYR:HB2	2.42	0.46
1:A:222:VAL:O	1:A:226:ILE:HG13	2.15	0.46
1:A:228:ALA:O	1:A:231:CYS:HB2	2.16	0.46
1:A:39:THR:HB	1:A:69:VAL:HG11	1.98	0.46
1:A:3:ASN:C	1:A:5:TYR:H	2.18	0.46
1:A:21:THR:HG22	1:A:46:GLN:CD	2.36	0.46
1:A:236:PHE:CE1	1:A:238:PHE:CZ	2.97	0.46
1:A:252:LEU:HD12	1:A:252:LEU:C	2.37	0.46
1:A:43:THR:O	1:A:44:GLN:CB	2.63	0.45
1:A:42:LEU:CD2	1:A:71:GLY:HA3	2.40	0.45
1:A:57:PRO:HB3	1:A:95:LYS:HG2	1.99	0.45
1:A:112:VAL:HA	1:A:236:PHE:O	2.16	0.45
1:A:147:LEU:HD22	1:A:226:ILE:CG2	2.46	0.45
1:A:98:PHE:N	1:A:99:PRO:CD	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:LEU:C	1:A:37:GLY:N	2.68	0.45
1:A:277:ILE:CG2	1:A:277:ILE:O	2.65	0.45
1:A:284:LEU:O	1:A:285:PRO:C	2.56	0.44
1:A:151:ASN:ND2	1:A:157:ASP:O	2.51	0.44
1:A:224:GLU:O	1:A:228:ALA:HB2	2.16	0.44
1:A:193:VAL:O	1:A:193:VAL:HG13	2.18	0.44
1:A:32:GLY:O	1:A:33:SER:O	2.36	0.44
1:A:222:VAL:O	1:A:223:PRO:C	2.55	0.44
1:A:206:CYS:SG	1:A:245:VAL:HG11	2.58	0.44
1:A:94:TRP:CZ3	1:A:95:LYS:HE2	2.53	0.44
1:A:152:ASP:O	1:A:155:PHE:N	2.36	0.44
1:A:11:LYS:O	1:A:12:ASN:C	2.55	0.44
1:A:116:ALA:HB1	1:A:242:THR:CG2	2.48	0.44
1:A:103:PHE:O	1:A:104:HIS:C	2.55	0.43
1:A:246:ILE:HG22	1:A:248:ASP:H	1.82	0.43
1:A:117:ALA:HB3	1:A:241:ILE:HD12	2.00	0.43
1:A:284:LEU:HD23	1:A:285:PRO:N	2.34	0.43
1:A:149:GLY:O	1:A:158:ARG:NH1	2.47	0.43
1:A:25:PRO:CG	1:A:79:VAL:HG22	2.48	0.43
1:A:180:GLN:HE21	1:A:180:GLN:HB3	1.42	0.43
1:A:133:ARG:CG	1:A:133:ARG:O	2.66	0.43
1:A:133:ARG:O	1:A:133:ARG:HG2	2.18	0.42
1:A:265:LYS:O	1:A:266:GLN:C	2.57	0.42
1:A:209:LEU:HD12	1:A:209:LEU:HA	1.91	0.42
1:A:129:ILE:HG12	1:A:240:LEU:HD12	2.02	0.42
1:A:3:ASN:C	1:A:5:TYR:N	2.73	0.42
1:A:58:ARG:NH1	1:A:58:ARG:HG2	2.27	0.42
1:A:46:GLN:N	1:A:70:PHE:O	2.49	0.42
1:A:109:ASP:OD1	1:A:234:ARG:NH2	2.52	0.42
1:A:93:LEU:CD2	1:A:223:PRO:HG3	2.50	0.41
1:A:10:TYR:O	1:A:11:LYS:C	2.58	0.41
1:A:10:TYR:CD2	1:A:155:PHE:HZ	2.38	0.41
1:A:144:GLN:OE1	1:A:144:GLN:HA	2.21	0.41
1:A:28:ALA:CB	1:A:103:PHE:CD2	3.03	0.41
1:A:152:ASP:OD1	1:A:152:ASP:C	2.58	0.41
1:A:115:ASN:ND2	1:A:239:SER:OG	2.52	0.41
1:A:70:PHE:N	1:A:70:PHE:CD1	2.89	0.41
1:A:258:GLU:HA	1:A:264:GLY:N	2.36	0.41
1:A:211:LYS:O	1:A:213:GLY:N	2.54	0.40
1:A:10:TYR:O	1:A:13:THR:N	2.54	0.40
1:A:67:ARG:HG3	1:A:67:ARG:NH1	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ASP:HB3	1:A:155:PHE:HD2	1.87	0.40
1:A:135:HIS:ND1	1:A:222:VAL:HG13	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:GLY:O	1:A:180:GLN:OE1[12_555]	2.06	0.14

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	287/289 (99%)	223 (78%)	44 (15%)	20 (7%)	1 3

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	SER
1	A	54	PRO
1	A	196	ALA
1	A	197	GLY
1	A	254	LYS
1	A	184	GLN
1	A	260	VAL
1	A	286	ASP
1	A	61	VAL
1	A	104	HIS
1	A	164	ASP
1	A	266	GLN
1	A	50	TYR
1	A	202	THR

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Mol	Chain	Res	Type
1	A	105	LEU
1	A	167	ASP
1	A	255	ALA
1	A	223	PRO
1	A	4	GLY
1	A	283	PRO

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	240/240 (100%)	171 (71%)	69 (29%)	0 1

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	THR
1	A	15	GLU
1	A	22	LYS
1	A	24	ARG
1	A	25	PRO
1	A	35	LEU
1	A	38	LEU
1	A	47	ILE
1	A	49	ASP
1	A	51	SER
1	A	56	PHE
1	A	58	ARG
1	A	59	SER
1	A	67	ARG
1	A	69	VAL
1	A	70	PHE
1	A	78	CYS
1	A	79	VAL
1	A	86	HIS
1	A	96	VAL

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Mol	Chain	Res	Type
1	A	99	PRO
1	A	102	VAL
1	A	106	LEU
1	A	112	VAL
1	A	115	ASN
1	A	124	PHE
1	A	126	VAL
1	A	130	MET
1	A	131	LEU
1	A	135	HIS
1	A	137	ASN
1	A	139	PRO
1	A	141	PHE
1	A	142	SER
1	A	147	LEU
1	A	158	ARG
1	A	163	SER
1	A	164	ASP
1	A	167	ASP
1	A	168	ARG
1	A	172	GLN
1	A	177	THR
1	A	179	LYS
1	A	180	GLN
1	A	185	ARG
1	A	187	LEU
1	A	195	VAL
1	A	201	GLU
1	A	208	VAL
1	A	209	LEU
1	A	211	LYS
1	A	212	LEU
1	A	229	ARG
1	A	236	PHE
1	A	239	SER
1	A	241	ILE
1	A	243	ASN
1	A	244	LYS
1	A	247	MET
1	A	254	LYS
1	A	257	HIS
1	A	258	GLU

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Mol	Chain	Res	Type
1	A	259	GLU
1	A	270	LYS
1	A	271	LEU
1	A	276	SER
1	A	278	LEU
1	A	283	PRO
1	A	286	ASP

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

Mol	Chain	Res	Type
1	A	74	ASN
1	A	115	ASN
1	A	137	ASN
1	A	180	GLN
1	A	210	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 carbohydrates in this entry.

5.6 Ligand geometry

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	SO4	A	290	-	4,4,4	1.92	2 (50%)	6,6,6	1.14	0
2	SO4	A	291	-	4,4,4	0.93	0	6,6,6	0.41	0

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	SO4	A	290	-	-	0/0/0/0	0/0/0/0
2	SO4	A	291	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	290	SO4	O4-S	2.36	1.55	1.47
2	A	290	SO4	O1-S	2.44	1.55	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	290	SO4	1	0
2	A	291	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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	289/289 (100%)	0.88	45 (15%) 3 2	8, 25, 54, 59	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	260	VAL	13.2
1	A	261	LEU	9.9
1	A	64	HIS	9.0
1	A	258	GLU	8.1
1	A	259	GLU	7.4
1	A	287	LYS	6.9
1	A	1	MET	6.5
1	A	65	ALA	6.2
1	A	253	GLU	6.1
1	A	252	LEU	6.0
1	A	288	ALA	5.8
1	A	61	VAL	5.8
1	A	286	ASP	5.6
1	A	256	ASN	5.5
1	A	3	ASN	5.4
1	A	254	LYS	5.4
1	A	263	ALA	5.3
1	A	255	ALA	5.2
1	A	257	HIS	5.1
1	A	2	GLU	4.8
1	A	185	ARG	4.5
1	A	289	SER	4.5
1	A	262	ALA	3.5
1	A	285	PRO	3.3
1	A	113	VAL	3.0
1	A	266	GLN	3.0
1	A	180	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	250	GLU	2.8
1	A	179	LYS	2.7
1	A	184	GLN	2.6
1	A	62	PRO	2.6
1	A	267	ALA	2.6
1	A	248	ASP	2.6
1	A	251	SER	2.5
1	A	112	VAL	2.5
1	A	249	TYR	2.4
1	A	156	GLY	2.2
1	A	181	MET	2.2
1	A	221	THR	2.2
1	A	239	SER	2.2
1	A	63	GLY	2.1
1	A	8	GLU	2.1
1	A	114	THR	2.1
1	A	278	LEU	2.0
1	A	237	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	A	291	5/5	0.96	0.17	-0.55	50,51,51,51	0
2	SO4	A	290	5/5	0.99	0.15	-1.00	16,16,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.