Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:53 PM GMT

PDB ID	:	4DMU
Title	:	Crystal structure of the von Willebrand factor A3 domain in complex with a collagen III derived triple-helical peptide
Authors	:	Brondijk, T.H.C.; Huizinga, E.G.
Deposited on	:	2012-02-08
Resolution	:	2.80 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:

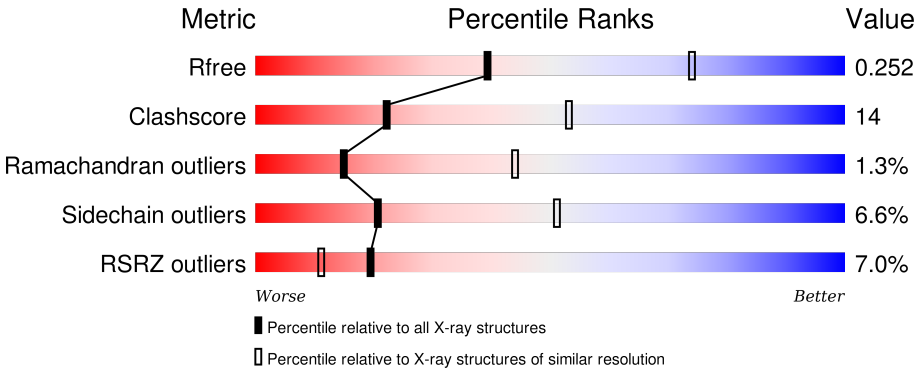
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	87	13% 80% 10% 9%
1	C	87	5% 82% 9% 9%
1	E	87	% 83% 7% • 9%
1	G	87	9% 78% 11% • 9%
1	I	87	2% 82% 9% 9%

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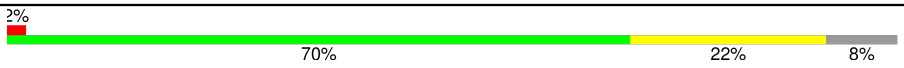
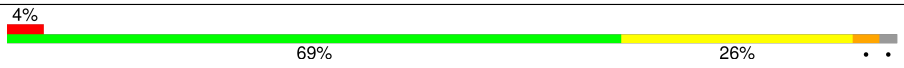
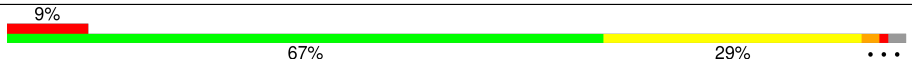
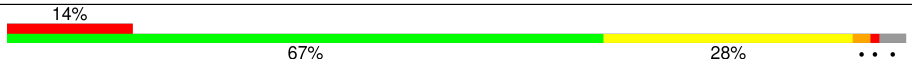
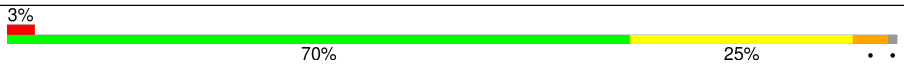
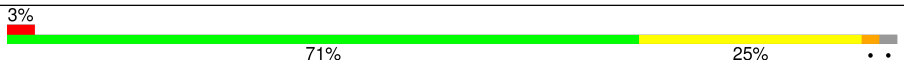
Mol	Chain	Length	Quality of chain
1	K	87	
2	B	192	
2	D	192	
2	F	192	
2	H	192	
2	J	192	
2	L	192	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11651 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.

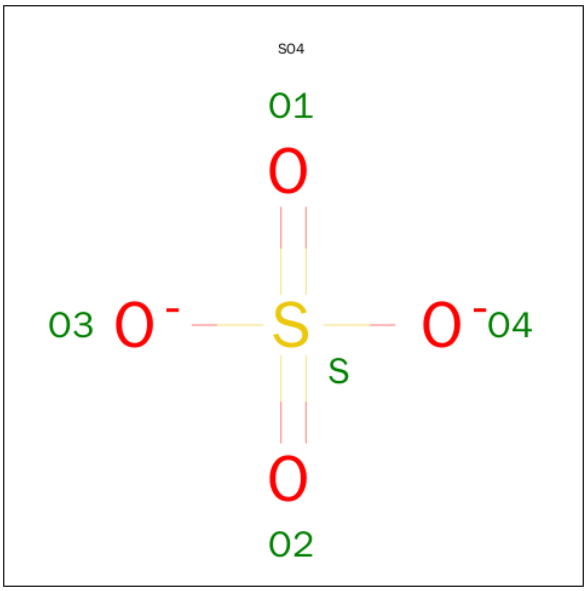
- Molecule 1 is a protein called Collagen III derived triple-helical peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	79	Total	C	N	O	S	0	0	0
			529	332	91	103	3			
1	C	79	Total	C	N	O	S	0	0	0
			529	332	91	103	3			
1	E	79	Total	C	N	O	S	0	0	0
			529	332	91	103	3			
1	G	79	Total	C	N	O	S	0	0	0
			529	332	91	103	3			
1	I	79	Total	C	N	O	S	0	0	0
			529	332	91	103	3			
1	K	80	Total	C	N	O	S	0	0	0
			536	337	92	104	3			

- Molecule 2 is a protein called von Willebrand factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	188	Total	C	N	O	S	0	0	0
			1406	890	241	269	6			
2	D	188	Total	C	N	O	S	0	0	0
			1406	890	241	269	6			
2	F	188	Total	C	N	O	S	0	0	0
			1406	890	241	269	6			
2	H	187	Total	C	N	O	S	0	0	0
			1400	887	240	268	5			
2	J	191	Total	C	N	O	S	0	0	0
			1426	902	244	274	6			
2	L	188	Total	C	N	O	S	0	0	0
			1406	890	241	269	6			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



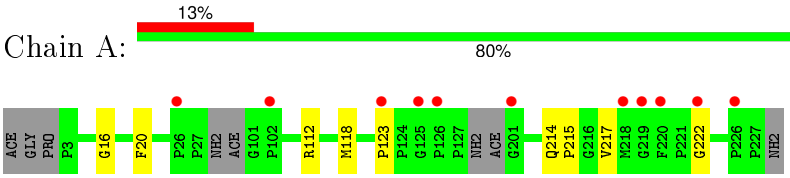
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	K	1	Total O S 5 4 1	0	0

3 Residue-property plots (i)

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

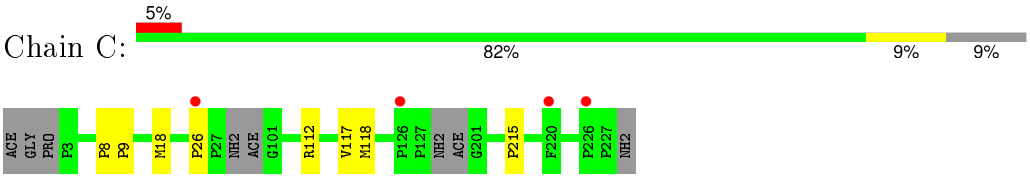
- Molecule 1: Collagen III derived triple-helical peptide

Chain A:



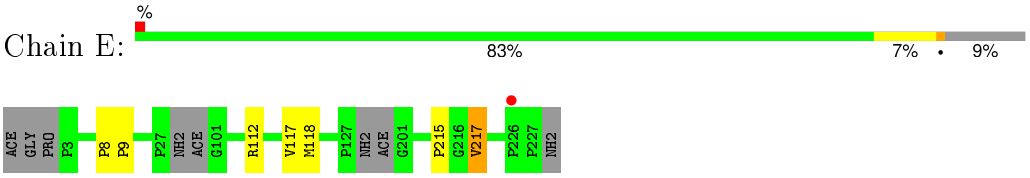
- Molecule 1: Collagen III derived triple-helical peptide

Chain C:



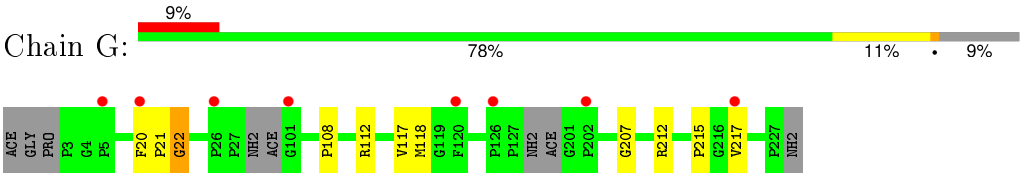
- Molecule 1: Collagen III derived triple-helical peptide

Chain E:



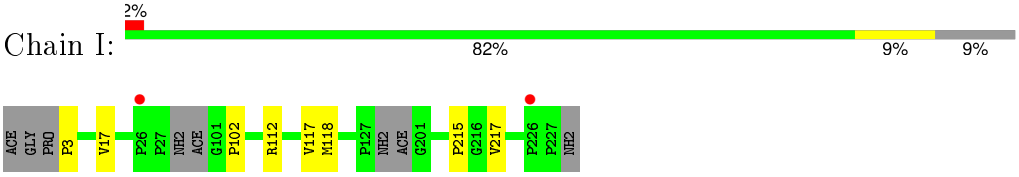
- Molecule 1: Collagen III derived triple-helical peptide

Chain G:



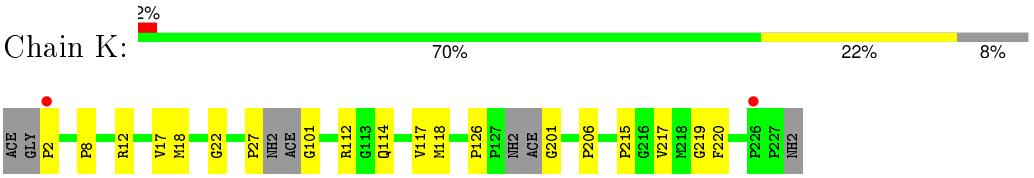
- Molecule 1: Collagen III derived triple-helical peptide

Chain I:



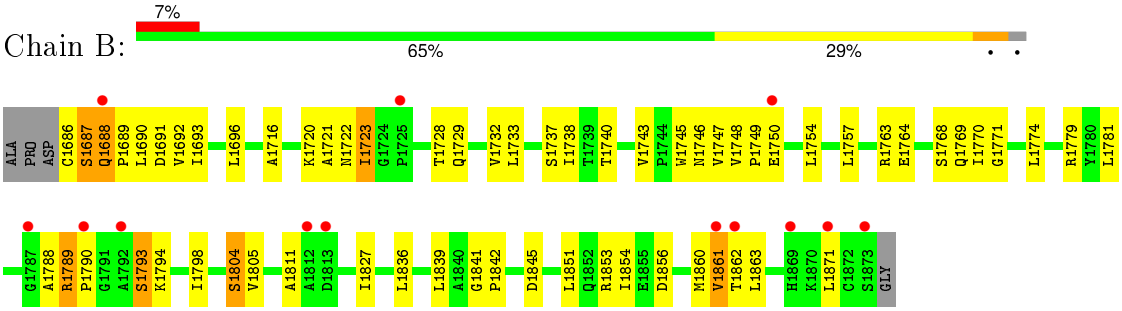
- Molecule 1: Collagen III derived triple-helical peptide

Chain K:



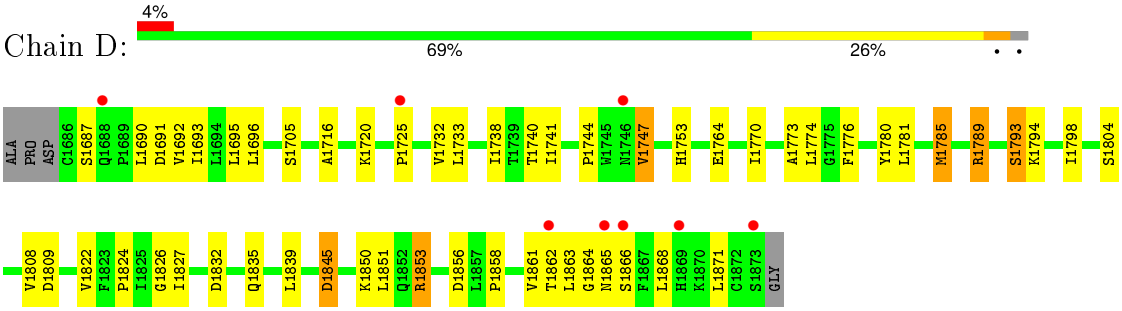
• Molecule 2: von Willebrand factor

Chain B:



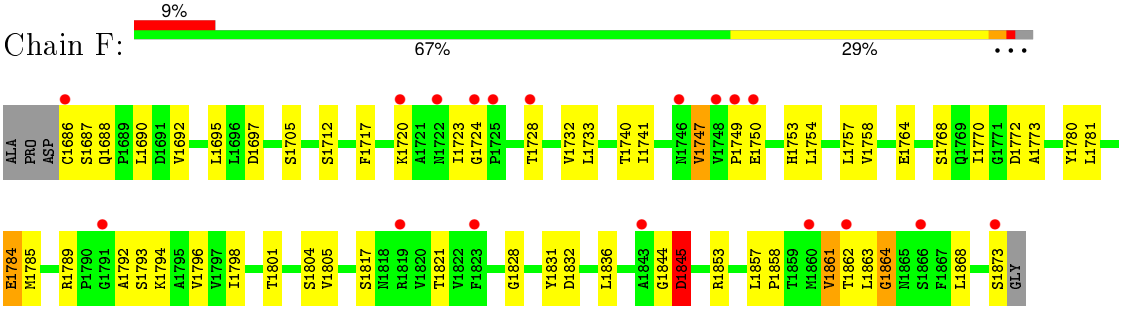
• Molecule 2: von Willebrand factor

Chain D:



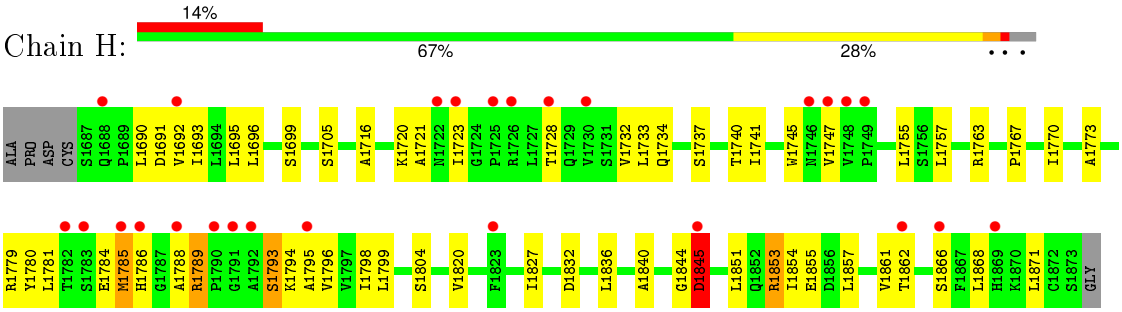
• Molecule 2: von Willebrand factor

Chain F:



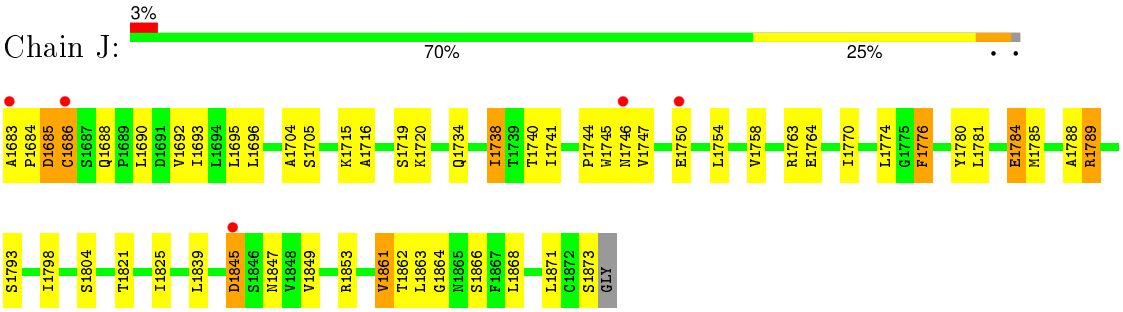
• Molecule 2: von Willebrand factor

Chain H:



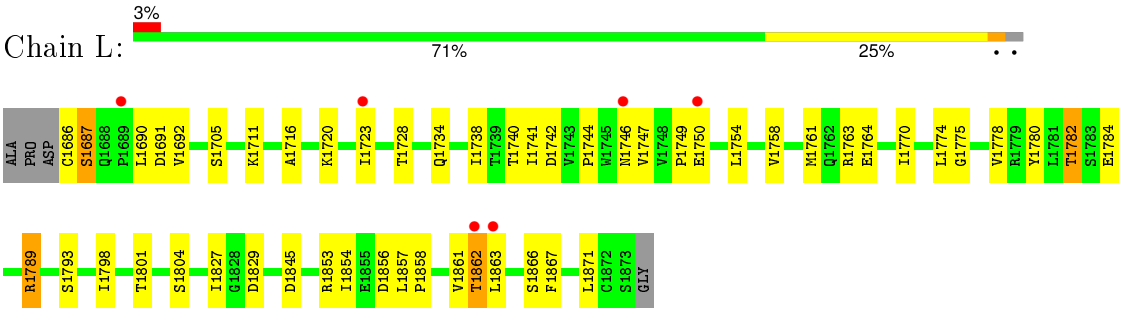
• Molecule 2: von Willebrand factor

Chain J:



- Molecule 2: von Willebrand factor

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, α, β, γ	187.61Å 187.61Å 89.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.32 – 2.80 46.32 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.2 (46.32-2.80) 92.4 (46.32-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.202 , 0.253 0.199 , 0.252	Depositor DCC
R_{free} test set	2097 reflections (5.39%)	DCC
Wilson B-factor (Å^2)	54.9	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 31.3	EDS
Estimated twinning fraction	0.518 for H, K, L 0.482 for H+K, -K, -L 0.477 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.518 for H, K, L 0.482 for H+K, -K, -L	Depositor
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Outliers	2 of 41013 reflections (0.005%)	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	11651	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.33 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.1368e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: HYP, 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	0.61	0/361	0.66	0/460
1	C	0.75	0/361	0.68	0/460
1	E	0.61	0/361	0.71	0/460
1	G	0.54	0/361	0.65	0/460
1	I	0.71	0/361	0.72	0/460
1	K	0.68	0/368	0.69	0/468
2	B	0.64	0/1431	0.73	0/1946
2	D	0.72	0/1431	0.79	1/1946 (0.1%)
2	F	0.64	0/1431	0.75	0/1946
2	H	0.57	0/1425	0.65	0/1938
2	J	0.88	0/1452	0.87	1/1976 (0.1%)
2	L	0.78	0/1431	0.80	0/1946
All	All	0.70	0/10774	0.75	2/14466 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	1789	ARG	NE-CZ-NH2	5.09	122.85	120.30
2	D	1692	VAL	CB-CA-C	-5.07	101.78	111.40

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	529	0	487	9	0
1	C	529	0	487	12	0
1	E	529	0	487	7	0
1	G	529	0	487	12	0
1	I	529	0	487	11	0
1	K	536	0	493	17	0
2	B	1406	0	1421	56	0
2	D	1406	0	1421	46	0
2	F	1406	0	1421	43	0
2	H	1400	0	1418	46	0
2	J	1426	0	1437	46	0
2	L	1406	0	1421	50	0
3	C	5	0	0	0	0
3	F	5	0	0	1	0
3	I	5	0	0	0	0
3	K	5	0	0	1	0
All	All	11651	0	11467	319	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 14.

All (319) 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:E:215:HYP:HD23	2:F:1740:THR:HG22	1.31	1.10
2:J:1770:ILE:HD12	2:J:1804:SER:HB2	1.38	1.06
1:C:215:HYP:HD23	2:D:1740:THR:HG22	1.37	1.02
1:K:215:HYP:HD23	2:L:1740:THR:HG22	1.41	0.98
2:B:1693:ILE:HG23	2:B:1733:LEU:HD13	1.49	0.91
2:H:1695:LEU:HD23	2:H:1798:ILE:HD12	1.52	0.88
2:B:1827:ILE:HD13	2:B:1854:ILE:HD12	1.57	0.87
2:D:1693:ILE:HG23	2:D:1733:LEU:HD13	1.57	0.84
2:L:1778:VAL:O	2:L:1782:THR:HG23	1.76	0.84
2:L:1716:ALA:CB	2:L:1861:VAL:HG21	2.09	0.83
1:G:118:MET:HG3	1:G:217:VAL:HG23	1.64	0.79
1:A:215:HYP:HD23	2:B:1740:THR:HG22	1.63	0.78
1:K:118:MET:HG3	1:K:217:VAL:HG23	1.65	0.76
2:H:1693:ILE:HB	2:H:1796:VAL:HG22	1.64	0.76
1:A:112:ARG:HH22	2:B:1740:THR:HG21	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:215:HYP:HD23	2:J:1740:THR:HG22	1.66	0.76
2:D:1781:LEU:O	2:D:1794:LYS:NZ	2.18	0.75
2:F:1864:GLY:HA2	2:F:1868:LEU:HD22	1.68	0.75
2:L:1716:ALA:HB1	2:L:1861:VAL:CG2	2.17	0.74
2:F:1770:ILE:HD12	2:F:1804:SER:HB2	1.69	0.74
2:F:1792:ALA:HB3	2:F:1794:LYS:HE2	1.71	0.73
2:J:1770:ILE:HG23	2:J:1798:ILE:HD11	1.71	0.73
2:H:1781:LEU:O	2:H:1794:LYS:NZ	2.22	0.72
2:L:1741:ILE:HD13	2:L:1780:TYR:CZ	2.23	0.72
2:L:1716:ALA:HB1	2:L:1861:VAL:HG21	1.69	0.72
2:J:1861:VAL:CG2	2:J:1862:THR:N	2.53	0.72
2:B:1781:LEU:O	2:B:1788:ALA:HB1	1.88	0.72
2:D:1716:ALA:HB3	2:D:1861:VAL:HG21	1.72	0.71
2:L:1723:ILE:HA	2:L:1728:THR:O	1.90	0.71
2:J:1744:PRO:O	2:J:1747:VAL:HG23	1.90	0.71
2:F:1741:ILE:HD13	2:F:1780:TYR:CZ	2.26	0.71
2:L:1871:LEU:N	2:L:1871:LEU:HD22	2.07	0.70
3:K:301:SO4:O3	2:L:1747:VAL:HG13	1.90	0.70
2:F:1690:LEU:HG	2:F:1692:VAL:HG23	1.73	0.70
1:A:112:ARG:NH1	2:B:1764:GLU:OE2	2.25	0.69
2:B:1696:LEU:HD23	2:B:1696:LEU:N	2.07	0.69
2:F:1686:CYS:C	2:F:1688:GLN:H	1.95	0.69
2:B:1743:VAL:HG22	2:B:1757:LEU:HB3	1.76	0.67
2:D:1774:LEU:HD23	2:D:1839:LEU:HD22	1.76	0.67
2:J:1861:VAL:HG23	2:J:1862:THR:N	2.09	0.67
2:L:1770:ILE:HD12	2:L:1804:SER:HB2	1.75	0.67
2:B:1750:GLU:O	2:B:1754:LEU:HD13	1.95	0.67
2:L:1716:ALA:HB3	2:L:1861:VAL:HG21	1.77	0.66
2:D:1861:VAL:HG23	2:D:1862:THR:N	2.11	0.66
2:D:1691:ASP:OD1	2:D:1789:ARG:NH2	2.29	0.65
2:F:1686:CYS:O	2:F:1688:GLN:N	2.30	0.65
2:F:1747:VAL:HG11	2:F:1757:LEU:HD11	1.78	0.65
2:F:1754:LEU:O	2:F:1758:VAL:HG23	1.96	0.65
1:E:215:HYP:CD	2:F:1740:THR:HG22	2.19	0.64
2:B:1768:SER:O	2:B:1805:VAL:HG22	1.97	0.64
2:H:1695:LEU:HD23	2:H:1798:ILE:CD1	2.25	0.64
2:H:1840:ALA:HB3	2:H:1844:GLY:HA2	1.77	0.64
2:B:1827:ILE:HD13	2:B:1854:ILE:CD1	2.28	0.64
2:L:1861:VAL:HG23	2:L:1862:THR:N	2.12	0.64
2:J:1684:PRO:HB2	2:J:1685:ASP:HB3	1.79	0.64
2:F:1781:LEU:O	2:F:1794:LYS:NZ	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1770:ILE:HD12	2:B:1804:SER:HB3	1.81	0.63
2:J:1690:LEU:HG	2:J:1692:VAL:HG23	1.81	0.63
2:H:1732:VAL:C	2:H:1733:LEU:HD12	2.19	0.63
2:F:1741:ILE:HD13	2:F:1780:TYR:CE1	2.34	0.63
1:C:117:VAL:HG12	1:C:118:MET:N	2.14	0.63
1:C:112:ARG:NH1	2:D:1764:GLU:OE2	2.31	0.63
2:F:1753:HIS:CE1	2:F:1757:LEU:HD11	2.34	0.62
2:B:1693:ILE:CG2	2:B:1733:LEU:HD13	2.27	0.62
2:L:1741:ILE:HD13	2:L:1780:TYR:CE1	2.34	0.62
2:D:1845:ASP:OD1	2:D:1845:ASP:N	2.28	0.62
2:L:1827:ILE:HG21	2:L:1854:ILE:CD1	2.29	0.62
2:J:1684:PRO:HB2	2:J:1685:ASP:CB	2.28	0.62
2:D:1732:VAL:C	2:D:1733:LEU:HD12	2.20	0.61
2:J:1683:ALA:HB3	2:J:1684:PRO:HD3	1.80	0.61
2:L:1861:VAL:CG2	2:L:1862:THR:N	2.64	0.61
2:B:1781:LEU:O	2:B:1794:LYS:NZ	2.34	0.61
2:B:1732:VAL:C	2:B:1733:LEU:HD12	2.21	0.61
2:B:1691:ASP:OD1	2:B:1789:ARG:NH2	2.31	0.61
1:E:117:VAL:HG21	1:K:18:MET:SD	2.40	0.61
2:B:1774:LEU:HB3	2:B:1811:ALA:HB1	1.82	0.60
1:I:17:VAL:HG21	2:J:1741:ILE:HG21	1.84	0.60
2:H:1690:LEU:HD12	2:H:1793:SER:O	2.01	0.60
2:B:1774:LEU:HD22	2:B:1839:LEU:CD2	2.32	0.60
2:F:1845:ASP:OD1	2:F:1845:ASP:N	2.34	0.60
2:L:1827:ILE:HG21	2:L:1854:ILE:HD13	1.83	0.60
2:B:1737:SER:HB3	2:D:1863:LEU:HD22	1.82	0.60
1:I:112:ARG:NH2	2:J:1764:GLU:OE2	2.35	0.59
1:A:20:PHE:CZ	2:B:1779:ARG:HB3	2.37	0.59
2:H:1798:ILE:O	2:H:1798:ILE:HG23	2.02	0.59
2:B:1738:ILE:HG23	2:B:1740:THR:HG23	1.83	0.59
2:B:1860:MET:CE	2:B:1860:MET:HA	2.32	0.59
2:B:1861:VAL:O	2:B:1863:LEU:N	2.35	0.59
2:F:1697:ASP:OD2	2:F:1801:THR:OG1	2.18	0.59
2:H:1716:ALA:HB1	2:H:1861:VAL:HG23	1.84	0.59
2:H:1770:ILE:HD12	2:H:1804:SER:HB2	1.85	0.59
2:B:1738:ILE:CG2	2:B:1740:THR:HG23	2.32	0.58
2:H:1693:ILE:HG23	2:H:1733:LEU:HD13	1.84	0.58
2:D:1716:ALA:CB	2:D:1861:VAL:HG21	2.32	0.58
1:K:117:VAL:HG12	1:K:118:MET:N	2.18	0.58
2:H:1690:LEU:HG	2:H:1692:VAL:HG23	1.84	0.58
2:B:1690:LEU:HD23	2:B:1728:THR:HG23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1686:CYS:C	2:J:1688:GLN:H	2.06	0.58
2:D:1690:LEU:HD12	2:D:1793:SER:O	2.03	0.58
2:L:1691:ASP:OD1	2:L:1789:ARG:NH2	2.37	0.57
1:C:18:MET:HE1	2:D:1785:MET:HE1	1.86	0.57
1:E:112:ARG:NH2	2:F:1764:GLU:OE2	2.37	0.57
2:F:1753:HIS:HE1	2:F:1757:LEU:HD11	1.68	0.56
2:B:1723:ILE:N	2:B:1723:ILE:CD1	2.68	0.56
1:K:17:VAL:HG21	2:L:1741:ILE:HG21	1.86	0.56
1:K:27:HYP:HA	1:K:126:PRO:O	2.05	0.56
2:D:1770:ILE:HD12	2:D:1804:SER:HB2	1.87	0.56
2:J:1750:GLU:O	2:J:1754:LEU:HD13	2.06	0.56
2:B:1861:VAL:CG2	2:B:1862:THR:N	2.68	0.56
2:H:1745:TRP:CD1	2:H:1780:TYR:CZ	2.94	0.56
2:F:1781:LEU:HD11	2:F:1796:VAL:HG22	1.87	0.56
2:B:1723:ILE:HD12	2:B:1723:ILE:N	2.19	0.56
2:D:1864:GLY:HA2	2:D:1868:LEU:HD22	1.88	0.56
2:J:1690:LEU:HD21	2:J:1692:VAL:HG21	1.86	0.56
2:L:1871:LEU:CD2	2:L:1871:LEU:N	2.68	0.55
2:F:1690:LEU:CG	2:F:1692:VAL:HG23	2.37	0.55
2:D:1695:LEU:HD21	2:D:1773:ALA:HB1	1.89	0.55
2:H:1716:ALA:HB1	2:H:1861:VAL:CG2	2.37	0.54
2:H:1716:ALA:CB	2:H:1861:VAL:CG2	2.86	0.54
1:A:112:ARG:NH2	2:B:1740:THR:HG21	2.18	0.54
2:J:1684:PRO:HD2	2:J:1821:THR:OG1	2.07	0.54
1:I:118:MET:HG3	1:I:217:VAL:HG23	1.88	0.54
2:L:1690:LEU:HG	2:L:1692:VAL:HG23	1.89	0.54
2:D:1781:LEU:HD13	2:D:1794:LYS:HB3	1.90	0.54
2:J:1690:LEU:HD11	2:J:1692:VAL:HG22	1.89	0.54
2:F:1864:GLY:HA2	2:F:1868:LEU:CD2	2.36	0.54
2:H:1716:ALA:HB3	2:H:1861:VAL:HG21	1.89	0.53
2:J:1770:ILE:HD12	2:J:1804:SER:CB	2.25	0.53
2:D:1744:PRO:O	2:D:1747:VAL:HG23	2.08	0.53
1:A:215:HYP:CD	2:B:1740:THR:HG22	2.38	0.53
2:B:1686:CYS:O	2:B:1687:SER:CB	2.57	0.53
2:F:1723:ILE:HA	2:F:1728:THR:O	2.09	0.53
2:F:1828:GLY:O	2:F:1831:TYR:CE2	2.62	0.53
2:L:1734:GLN:NE2	2:L:1742:ASP:OD2	2.38	0.53
2:F:1741:ILE:CD1	2:F:1780:TYR:CE1	2.91	0.52
2:B:1733:LEU:N	2:B:1733:LEU:HD12	2.24	0.52
2:L:1723:ILE:HG21	2:L:1749:PRO:O	2.09	0.52
2:J:1863:LEU:N	2:J:1863:LEU:HD12	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1745:TRP:O	2:J:1747:VAL:N	2.35	0.52
2:H:1784:GLU:OE2	2:H:1784:GLU:N	2.40	0.52
2:D:1716:ALA:CB	2:D:1861:VAL:CG2	2.88	0.52
2:J:1741:ILE:HD13	2:J:1780:TYR:CZ	2.44	0.52
2:D:1741:ILE:HD13	2:D:1780:TYR:CE1	2.44	0.51
1:K:112:ARG:NH1	2:L:1764:GLU:OE2	2.44	0.51
2:J:1862:THR:O	2:J:1862:THR:HG22	2.09	0.51
2:L:1862:THR:HG22	2:L:1862:THR:O	2.10	0.51
1:C:18:MET:SD	1:I:117:VAL:HG21	2.51	0.51
2:J:1776:PHE:CD1	2:J:1776:PHE:C	2.83	0.51
2:L:1686:CYS:O	2:L:1687:SER:HB3	2.09	0.51
2:J:1861:VAL:O	2:J:1863:LEU:N	2.44	0.51
2:L:1742:ASP:OD2	2:L:1761:MET:HE2	2.11	0.51
2:L:1686:CYS:O	2:L:1687:SER:CB	2.58	0.51
2:D:1774:LEU:CD2	2:D:1839:LEU:HD22	2.39	0.51
1:C:117:VAL:HG11	1:I:117:VAL:HG12	1.93	0.51
1:C:18:MET:CE	2:D:1785:MET:HE1	2.41	0.51
2:B:1745:TRP:CZ2	2:B:1781:LEU:HD23	2.46	0.50
2:B:1690:LEU:HD21	2:B:1692:VAL:CG2	2.41	0.50
2:J:1825:ILE:HG23	2:J:1849:VAL:HG12	1.93	0.50
2:D:1716:ALA:HB1	2:D:1861:VAL:HG23	1.93	0.50
2:B:1716:ALA:HB1	2:B:1861:VAL:CG2	2.42	0.50
2:H:1723:ILE:HD12	2:H:1723:ILE:N	2.27	0.50
2:J:1683:ALA:N	2:J:1847:ASN:HD21	2.09	0.50
2:F:1686:CYS:C	2:F:1688:GLN:N	2.64	0.50
2:J:1798:ILE:HG23	2:J:1798:ILE:O	2.13	0.49
2:F:1798:ILE:HG23	2:F:1798:ILE:O	2.11	0.49
2:B:1770:ILE:HD12	2:B:1804:SER:CB	2.42	0.49
2:H:1799:LEU:HD23	2:H:1799:LEU:N	2.27	0.49
2:H:1747:VAL:HG11	2:H:1757:LEU:HD11	1.95	0.49
2:J:1845:ASP:OD1	2:J:1845:ASP:N	2.36	0.49
2:H:1785:MET:HE2	2:H:1786:HIS:N	2.28	0.49
2:D:1861:VAL:CG2	2:D:1862:THR:N	2.75	0.49
2:H:1851:LEU:HD11	2:H:1857:LEU:HD12	1.94	0.49
2:F:1857:LEU:HB3	2:F:1858:PRO:HD3	1.94	0.49
2:J:1774:LEU:HD22	2:J:1839:LEU:CD2	2.43	0.48
1:A:118:MET:HG3	1:A:217:VAL:HG23	1.94	0.48
2:F:1747:VAL:HG13	3:F:1901:SO4:O2	2.14	0.48
2:D:1853:ARG:NH1	2:D:1856:ASP:OD2	2.46	0.48
1:G:21:HYP:O	1:G:22:GLY:O	2.31	0.48
2:H:1862:THR:HG22	2:H:1862:THR:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1696:LEU:HD23	2:D:1696:LEU:N	2.27	0.48
1:K:112:ARG:HH22	2:L:1740:THR:HG21	1.78	0.48
2:B:1690:LEU:CD2	2:B:1692:VAL:CG2	2.91	0.48
1:I:3:HYP:H	1:I:102:PRO:HD2	1.78	0.48
2:L:1744:PRO:HD2	2:L:1747:VAL:HG21	1.96	0.48
2:B:1688:GLN:HB3	2:B:1689:PRO:HA	1.95	0.47
2:L:1750:GLU:O	2:L:1754:LEU:HD13	2.14	0.47
2:L:1716:ALA:CB	2:L:1861:VAL:CG2	2.81	0.47
2:J:1774:LEU:HD22	2:J:1839:LEU:HD22	1.96	0.47
2:F:1844:GLY:O	2:F:1845:ASP:C	2.53	0.47
1:G:118:MET:HG3	1:G:217:VAL:CG2	2.41	0.47
1:C:117:VAL:HG11	1:I:118:MET:O	2.14	0.47
2:D:1798:ILE:HD13	2:D:1839:LEU:HD13	1.97	0.47
2:L:1867:PHE:O	2:L:1871:LEU:HD23	2.15	0.47
2:L:1741:ILE:CD1	2:L:1780:TYR:CE1	2.98	0.46
2:F:1862:THR:C	2:F:1863:LEU:HD12	2.36	0.46
2:B:1747:VAL:HG12	2:B:1748:VAL:N	2.30	0.46
2:L:1744:PRO:HD2	2:L:1747:VAL:CG2	2.46	0.46
2:B:1770:ILE:HG23	2:B:1798:ILE:HD11	1.97	0.46
1:A:123:PRO:O	1:A:222:GLY:HA3	2.15	0.46
2:D:1716:ALA:HB3	2:D:1861:VAL:CG2	2.45	0.46
2:J:1684:PRO:CB	2:J:1685:ASP:CB	2.93	0.46
2:L:1690:LEU:HD11	2:L:1692:VAL:HG22	1.96	0.46
2:D:1693:ILE:CG2	2:D:1733:LEU:HD13	2.39	0.46
1:K:17:VAL:HG21	2:L:1741:ILE:CG2	2.46	0.46
2:F:1784:GLU:OE2	2:F:1784:GLU:N	2.48	0.46
2:J:1770:ILE:CG2	2:J:1798:ILE:HD11	2.43	0.46
1:K:2:PRO:O	1:K:201:GLY:HA3	2.16	0.46
1:K:118:MET:HG3	1:K:217:VAL:CG2	2.42	0.46
2:H:1737:SER:HA	2:H:1767:PRO:HD2	1.98	0.46
2:J:1864:GLY:HA2	2:J:1868:LEU:HD22	1.98	0.46
2:H:1733:LEU:N	2:H:1733:LEU:HD12	2.30	0.46
2:L:1784:GLU:N	2:L:1784:GLU:OE2	2.49	0.46
2:H:1781:LEU:O	2:H:1788:ALA:HB1	2.16	0.45
1:G:108:PRO:O	1:G:207:GLY:HA3	2.16	0.45
1:G:212:ARG:HD2	2:H:1741:ILE:O	2.16	0.45
2:D:1741:ILE:HD13	2:D:1780:TYR:CZ	2.50	0.45
2:F:1863:LEU:N	2:F:1863:LEU:HD12	2.31	0.45
2:D:1716:ALA:HB1	2:D:1861:VAL:CG2	2.45	0.45
1:E:117:VAL:HG12	1:E:118:MET:O	2.17	0.45
1:G:215:HYP:HD23	2:H:1740:THR:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1695:LEU:HD23	2:J:1798:ILE:HD12	1.97	0.45
2:J:1716:ALA:CB	2:J:1861:VAL:HG21	2.46	0.45
2:B:1861:VAL:HG23	2:B:1862:THR:N	2.31	0.45
2:H:1716:ALA:CB	2:H:1861:VAL:HG21	2.45	0.45
2:B:1722:ASN:C	2:B:1723:ILE:HD12	2.37	0.45
2:H:1691:ASP:OD1	2:H:1789:ARG:NH2	2.44	0.45
2:F:1750:GLU:O	2:F:1754:LEU:HD13	2.17	0.45
1:I:117:VAL:HG12	1:I:118:MET:N	2.31	0.45
2:B:1769:GLN:OE1	2:D:1865:ASN:ND2	2.49	0.45
2:F:1832:ASP:O	2:F:1836:LEU:HD13	2.17	0.45
2:D:1770:ILE:HG21	2:D:1839:LEU:HD11	1.98	0.45
2:F:1723:ILE:CG2	2:F:1724:GLY:N	2.81	0.45
2:D:1695:LEU:HD23	2:D:1798:ILE:HG13	1.99	0.44
1:K:8:PRO:HD2	1:K:206:HYP:HA	1.99	0.44
1:G:20:PHE:CE2	2:H:1779:ARG:HB3	2.52	0.44
2:J:1704:ALA:O	2:J:1705:SER:C	2.56	0.44
2:J:1715:LYS:HG3	2:J:1758:VAL:HG11	1.98	0.44
2:H:1696:LEU:O	2:H:1734:GLN:HA	2.16	0.44
1:K:118:MET:HG2	1:K:219:GLY:HA2	1.99	0.44
2:D:1862:THR:HG22	2:D:1862:THR:O	2.17	0.44
1:G:21:HYP:C	1:G:22:GLY:O	2.66	0.44
2:J:1690:LEU:HD21	2:J:1692:VAL:CG2	2.48	0.44
2:L:1827:ILE:HG21	2:L:1854:ILE:HD12	1.99	0.44
2:F:1717:PHE:N	2:F:1861:VAL:HG21	2.32	0.44
1:G:117:VAL:HG12	1:G:118:MET:O	2.18	0.44
2:J:1738:ILE:CG2	2:J:1740:THR:HG23	2.47	0.44
2:B:1860:MET:HA	2:B:1860:MET:HE2	1.98	0.44
2:D:1822:VAL:O	2:D:1824:PRO:HD3	2.18	0.43
2:D:1861:VAL:HG23	2:D:1862:THR:H	1.82	0.43
2:D:1808:VAL:O	2:D:1809:ASP:C	2.56	0.43
1:K:22:GLY:HA3	1:K:220:PHE:O	2.18	0.43
1:G:117:VAL:CG1	1:G:118:MET:N	2.80	0.43
2:B:1729:GLN:NE2	2:B:1789:ARG:HD3	2.33	0.43
2:B:1721:ALA:HB3	2:B:1723:ILE:HD11	2.00	0.43
2:H:1723:ILE:N	2:H:1723:ILE:CD1	2.82	0.43
2:B:1836:LEU:HD12	2:B:1836:LEU:N	2.33	0.43
2:L:1858:PRO:O	2:L:1861:VAL:HG22	2.18	0.43
2:F:1770:ILE:HG23	2:F:1798:ILE:HD11	2.00	0.43
2:B:1805:VAL:HG12	2:D:1850:LYS:O	2.19	0.43
2:L:1798:ILE:O	2:L:1798:ILE:HG23	2.18	0.43
2:L:1770:ILE:CD1	2:L:1804:SER:HB2	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:112:ARG:NH2	2:H:1740:THR:HG21	2.34	0.43
2:J:1784:GLU:OE2	2:J:1784:GLU:N	2.51	0.43
2:J:1745:TRP:C	2:J:1747:VAL:H	2.20	0.43
2:H:1836:LEU:N	2:H:1836:LEU:CD1	2.82	0.43
1:C:8:PRO:O	1:C:9:HYP:C	2.67	0.43
2:H:1844:GLY:O	2:H:1845:ASP:C	2.57	0.43
2:H:1716:ALA:HB3	2:H:1861:VAL:CG2	2.49	0.43
1:K:2:PRO:CA	1:K:101:GLY:HA3	2.49	0.42
2:H:1827:ILE:HD13	2:H:1854:ILE:CD1	2.49	0.42
2:D:1776:PHE:C	2:D:1776:PHE:CD1	2.92	0.42
2:H:1695:LEU:HD21	2:H:1773:ALA:HB1	2.01	0.42
2:B:1770:ILE:O	2:B:1771:GLY:C	2.56	0.42
1:C:117:VAL:CG1	1:C:118:MET:N	2.81	0.42
2:F:1695:LEU:HD21	2:F:1773:ALA:HB1	2.01	0.42
1:E:118:MET:HG3	1:E:217:VAL:CG2	2.49	0.42
2:B:1836:LEU:CD1	2:B:1836:LEU:N	2.82	0.42
2:J:1741:ILE:HD13	2:J:1780:TYR:CE1	2.55	0.42
2:D:1747:VAL:CG1	2:D:1753:HIS:CE1	3.02	0.42
2:D:1858:PRO:O	2:D:1861:VAL:HG22	2.20	0.42
2:F:1772:ASP:O	2:F:1773:ALA:C	2.57	0.42
1:E:8:PRO:O	1:E:9:HYP:C	2.68	0.42
1:G:20:PHE:CZ	2:H:1779:ARG:HB3	2.54	0.42
2:L:1829:ASP:N	2:L:1829:ASP:OD2	2.53	0.42
2:F:1768:SER:O	2:F:1805:VAL:HG22	2.18	0.42
1:C:117:VAL:HG11	1:I:117:VAL:CG1	2.50	0.42
2:B:1716:ALA:CB	2:B:1861:VAL:HG21	2.49	0.42
2:D:1826:GLY:C	2:D:1827:ILE:HG13	2.40	0.42
1:K:112:ARG:NH2	2:L:1740:THR:HG21	2.35	0.42
2:L:1861:VAL:O	2:L:1863:LEU:N	2.53	0.41
2:H:1794:LYS:HB3	2:H:1820:VAL:HG22	2.02	0.41
2:B:1851:LEU:HD22	2:B:1856:ASP:HB2	2.01	0.41
2:H:1832:ASP:O	2:H:1836:LEU:HD13	2.20	0.41
2:H:1862:THR:O	2:H:1862:THR:CG2	2.68	0.41
2:B:1774:LEU:HD22	2:B:1839:LEU:HD22	2.03	0.41
2:B:1861:VAL:C	2:B:1863:LEU:N	2.74	0.41
2:F:1741:ILE:HD11	2:F:1780:TYR:CD1	2.55	0.41
2:L:1866:SER:OG	2:L:1867:PHE:N	2.54	0.41
2:L:1774:LEU:O	2:L:1775:GLY:C	2.59	0.41
2:F:1732:VAL:C	2:F:1733:LEU:HD12	2.40	0.41
1:A:16:GLY:HA3	1:A:214:GLN:O	2.20	0.41
2:J:1781:LEU:O	2:J:1788:ALA:HB1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1721:ALA:HB1	2:H:1728:THR:HG21	2.03	0.41
2:L:1861:VAL:CG2	2:L:1862:THR:H	2.33	0.41
2:H:1781:LEU:HD11	2:H:1795:ALA:O	2.21	0.41
2:D:1827:ILE:HG12	2:D:1851:LEU:HD12	2.02	0.41
1:K:12:ARG:NH2	1:K:114:GLN:HB3	2.36	0.41
2:D:1832:ASP:O	2:D:1835:GLN:N	2.54	0.41
2:J:1696:LEU:O	2:J:1734:GLN:HA	2.21	0.41
2:L:1801:THR:HG22	2:L:1827:ILE:HB	2.02	0.41
2:L:1856:ASP:O	2:L:1857:LEU:C	2.60	0.41
2:F:1732:VAL:O	2:F:1733:LEU:HD12	2.21	0.40
2:B:1793:SER:O	2:B:1794:LYS:HD3	2.22	0.40
1:C:117:VAL:HG12	1:C:118:MET:H	1.83	0.40
2:L:1711:LYS:HE3	2:L:1758:VAL:O	2.21	0.40
1:I:17:VAL:HG21	2:J:1741:ILE:CG2	2.50	0.40
2:H:1853:ARG:HB2	2:H:1855:GLU:OE1	2.20	0.40
2:B:1841:GLY:HA3	2:B:1842:PRO:HD3	1.97	0.40
2:J:1693:ILE:CD1	2:J:1781:LEU:HG	2.51	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	56/87 (64%)	52 (93%)	4 (7%)	0	100 100
1	C	56/87 (64%)	51 (91%)	4 (7%)	1 (2%)	11 34
1	E	56/87 (64%)	53 (95%)	3 (5%)	0	100 100
1	G	56/87 (64%)	51 (91%)	4 (7%)	1 (2%)	11 34
1	I	56/87 (64%)	54 (96%)	2 (4%)	0	100 100
1	K	56/87 (64%)	53 (95%)	3 (5%)	0	100 100
2	B	186/192 (97%)	172 (92%)	9 (5%)	5 (3%)	6 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	D	186/192 (97%)	163 (88%)	21 (11%)	2 (1%)	17 50
2	F	186/192 (97%)	168 (90%)	14 (8%)	4 (2%)	8 28
2	H	185/192 (96%)	169 (91%)	15 (8%)	1 (0%)	34 69
2	J	189/192 (98%)	168 (89%)	19 (10%)	2 (1%)	17 50
2	L	186/192 (97%)	169 (91%)	14 (8%)	3 (2%)	12 38
All	All	1454/1674 (87%)	1323 (91%)	112 (8%)	19 (1%)	15 44

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1687	SER
2	F	1687	SER
2	D	1687	SER
2	F	1864	GLY
1	G	22	GLY
2	J	1746	ASN
2	L	1687	SER
2	H	1845	ASP
2	B	1746	ASN
2	F	1845	ASP
2	J	1784	GLU
2	L	1746	ASN
2	B	1688	GLN
2	B	1790	PRO
2	L	1862	THR
1	C	26	PRO
2	D	1725	PRO
2	B	1749	PRO
2	F	1749	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	32/33 (97%)	32 (100%)	0	100 100
1	C	32/33 (97%)	32 (100%)	0	100 100
1	E	32/33 (97%)	31 (97%)	1 (3%)	47 81
1	G	32/33 (97%)	32 (100%)	0	100 100
1	I	32/33 (97%)	32 (100%)	0	100 100
1	K	33/33 (100%)	33 (100%)	0	100 100
2	B	155/157 (99%)	145 (94%)	10 (6%)	21 52
2	D	155/157 (99%)	144 (93%)	11 (7%)	18 46
2	F	155/157 (99%)	141 (91%)	14 (9%)	12 34
2	H	154/157 (98%)	141 (92%)	13 (8%)	14 37
2	J	157/157 (100%)	141 (90%)	16 (10%)	9 26
2	L	155/157 (99%)	146 (94%)	9 (6%)	25 57
All	All	1124/1140 (99%)	1050 (93%)	74 (7%)	21 51

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1720	LYS
2	B	1723	ILE
2	B	1763	ARG
2	B	1789	ARG
2	B	1793	SER
2	B	1804	SER
2	B	1845	ASP
2	B	1853	ARG
2	B	1861	VAL
2	B	1871	LEU
2	D	1705	SER
2	D	1720	LYS
2	D	1738	ILE
2	D	1747	VAL
2	D	1785	MET
2	D	1789	ARG
2	D	1793	SER
2	D	1845	ASP
2	D	1853	ARG
2	D	1866	SER
2	D	1871	LEU
1	E	217	VAL

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Mol	Chain	Res	Type
2	F	1705	SER
2	F	1712	SER
2	F	1720	LYS
2	F	1747	VAL
2	F	1784	GLU
2	F	1785	MET
2	F	1789	ARG
2	F	1793	SER
2	F	1817	SER
2	F	1821	THR
2	F	1845	ASP
2	F	1853	ARG
2	F	1861	VAL
2	F	1873	SER
2	H	1699	SER
2	H	1705	SER
2	H	1720	LYS
2	H	1755	LEU
2	H	1763	ARG
2	H	1785	MET
2	H	1789	ARG
2	H	1793	SER
2	H	1845	ASP
2	H	1853	ARG
2	H	1866	SER
2	H	1868	LEU
2	H	1871	LEU
2	J	1685	ASP
2	J	1686	CYS
2	J	1719	SER
2	J	1720	LYS
2	J	1738	ILE
2	J	1763	ARG
2	J	1776	PHE
2	J	1785	MET
2	J	1789	ARG
2	J	1793	SER
2	J	1845	ASP
2	J	1853	ARG
2	J	1861	VAL
2	J	1866	SER
2	J	1871	LEU

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Mol	Chain	Res	Type
2	J	1873	SER
2	L	1705	SER
2	L	1720	LYS
2	L	1738	ILE
2	L	1763	ARG
2	L	1782	THR
2	L	1789	ARG
2	L	1793	SER
2	L	1845	ASP
2	L	1853	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1729	GLN
2	D	1729	GLN
2	D	1753	HIS
2	D	1762	GLN
2	D	1769	GLN
2	D	1869	HIS
2	F	1753	HIS
2	H	1818	ASN
2	H	1852	GLN
2	H	1869	HIS
2	J	1762	GLN
2	L	1729	GLN
2	L	1753	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

126 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	HYP	A	103	1	7,8,9	0.50	0	5,10,12	2.44	3 (60%)
1	HYP	A	106	1	7,8,9	0.76	0	5,10,12	1.76	2 (40%)
1	HYP	A	109	1	7,8,9	0.39	0	5,10,12	1.65	1 (20%)
1	HYP	A	115	1	7,8,9	0.83	0	5,10,12	1.94	2 (40%)
1	HYP	A	121	1	7,8,9	0.81	0	5,10,12	0.98	1 (20%)
1	HYP	A	124	1	7,8,9	0.56	0	5,10,12	1.99	3 (60%)
1	HYP	A	127	1	7,8,9	0.47	0	5,10,12	2.17	2 (40%)
1	HYP	A	15	1	7,8,9	1.10	0	5,10,12	1.81	2 (40%)
1	HYP	A	203	1	7,8,9	0.63	0	5,10,12	1.59	1 (20%)
1	HYP	A	206	1	7,8,9	0.69	0	5,10,12	0.98	0
1	HYP	A	209	1	7,8,9	0.78	0	5,10,12	1.60	2 (40%)
1	HYP	A	21	1	7,8,9	0.61	0	5,10,12	1.71	2 (40%)
1	HYP	A	215	1	7,8,9	0.76	0	5,10,12	1.73	1 (20%)
1	HYP	A	221	1	7,8,9	0.49	0	5,10,12	1.70	2 (40%)
1	HYP	A	224	1	7,8,9	0.75	0	5,10,12	1.51	0
1	HYP	A	227	1	7,8,9	0.72	0	5,10,12	2.08	2 (40%)
1	HYP	A	24	1	7,8,9	0.57	0	5,10,12	1.91	3 (60%)
1	HYP	A	27	1	7,8,9	0.49	0	5,10,12	1.79	3 (60%)
1	HYP	A	3	1	7,8,9	0.44	0	5,10,12	2.21	3 (60%)
1	HYP	A	6	1	7,8,9	0.84	0	5,10,12	1.48	1 (20%)
1	HYP	A	9	1	7,8,9	0.49	0	5,10,12	1.49	1 (20%)
1	HYP	C	103	1	7,8,9	1.02	0	5,10,12	1.57	2 (40%)
1	HYP	C	106	1	7,8,9	0.70	0	5,10,12	1.51	2 (40%)
1	HYP	C	109	1	7,8,9	0.67	0	5,10,12	1.40	1 (20%)
1	HYP	C	115	1	7,8,9	1.00	0	5,10,12	1.70	1 (20%)
1	HYP	C	121	1	7,8,9	0.48	0	5,10,12	1.44	2 (40%)
1	HYP	C	124	1	7,8,9	0.51	0	5,10,12	2.27	3 (60%)
1	HYP	C	127	1	7,8,9	0.54	0	5,10,12	2.35	3 (60%)
1	HYP	C	15	1	7,8,9	1.20	1 (14%)	5,10,12	1.70	2 (40%)
1	HYP	C	203	1	7,8,9	0.77	0	5,10,12	1.53	2 (40%)
1	HYP	C	206	1	7,8,9	0.78	0	5,10,12	1.98	2 (40%)
1	HYP	C	209	1	7,8,9	1.06	0	5,10,12	2.27	3 (60%)
1	HYP	C	21	1	7,8,9	0.79	0	5,10,12	1.77	3 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	HYP	C	215	1	7,8,9	0.48	0	5,10,12	1.28	1 (20%)
1	HYP	C	221	1	7,8,9	0.75	0	5,10,12	1.54	1 (20%)
1	HYP	C	224	1	7,8,9	0.75	0	5,10,12	1.57	1 (20%)
1	HYP	C	227	1	7,8,9	0.52	0	5,10,12	1.33	1 (20%)
1	HYP	C	24	1	7,8,9	0.58	0	5,10,12	1.73	1 (20%)
1	HYP	C	27	1	7,8,9	0.70	0	5,10,12	1.43	1 (20%)
1	HYP	C	3	1	7,8,9	0.73	0	5,10,12	2.32	3 (60%)
1	HYP	C	6	1	7,8,9	0.95	0	5,10,12	1.84	1 (20%)
1	HYP	C	9	1	7,8,9	0.45	0	5,10,12	1.18	0
1	HYP	E	103	1	7,8,9	0.89	0	5,10,12	1.53	0
1	HYP	E	106	1	7,8,9	0.97	0	5,10,12	1.28	0
1	HYP	E	109	1	7,8,9	0.71	0	5,10,12	1.52	2 (40%)
1	HYP	E	115	1	7,8,9	1.00	0	5,10,12	1.62	1 (20%)
1	HYP	E	121	1	7,8,9	1.03	0	5,10,12	1.69	1 (20%)
1	HYP	E	124	1	7,8,9	0.79	0	5,10,12	2.00	3 (60%)
1	HYP	E	127	1	7,8,9	0.59	0	5,10,12	2.25	3 (60%)
1	HYP	E	15	1	7,8,9	0.82	0	5,10,12	2.43	4 (80%)
1	HYP	E	203	1	7,8,9	0.62	0	5,10,12	1.28	1 (20%)
1	HYP	E	206	1	7,8,9	0.52	0	5,10,12	1.52	2 (40%)
1	HYP	E	209	1	7,8,9	0.69	0	5,10,12	2.03	3 (60%)
1	HYP	E	21	1	7,8,9	1.08	0	5,10,12	1.54	1 (20%)
1	HYP	E	215	1	7,8,9	1.14	1 (14%)	5,10,12	1.36	1 (20%)
1	HYP	E	221	1	7,8,9	0.58	0	5,10,12	1.24	1 (20%)
1	HYP	E	224	1	7,8,9	0.86	0	5,10,12	1.17	1 (20%)
1	HYP	E	227	1	7,8,9	0.54	0	5,10,12	1.68	1 (20%)
1	HYP	E	24	1	7,8,9	0.47	0	5,10,12	1.57	1 (20%)
1	HYP	E	27	1	7,8,9	1.05	1 (14%)	5,10,12	1.69	2 (40%)
1	HYP	E	3	1	7,8,9	0.59	0	5,10,12	1.90	2 (40%)
1	HYP	E	6	1	7,8,9	0.77	0	5,10,12	1.85	1 (20%)
1	HYP	E	9	1	7,8,9	0.68	0	5,10,12	1.26	1 (20%)
1	HYP	G	103	1	7,8,9	0.72	0	5,10,12	1.97	2 (40%)
1	HYP	G	106	1	7,8,9	0.73	0	5,10,12	1.28	0
1	HYP	G	109	1	7,8,9	0.84	0	5,10,12	0.97	0
1	HYP	G	115	1	7,8,9	0.55	0	5,10,12	1.76	1 (20%)
1	HYP	G	121	1	7,8,9	0.59	0	5,10,12	1.91	1 (20%)
1	HYP	G	124	1	7,8,9	0.59	0	5,10,12	2.31	3 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	HYP	G	127	1	7,8,9	0.83	0	5,10,12	2.26	3 (60%)
1	HYP	G	15	1	7,8,9	0.80	0	5,10,12	2.14	2 (40%)
1	HYP	G	203	1	7,8,9	0.49	0	5,10,12	1.41	2 (40%)
1	HYP	G	206	1	7,8,9	0.69	0	5,10,12	1.23	0
1	HYP	G	209	1	7,8,9	0.78	0	5,10,12	1.49	0
1	HYP	G	21	1	7,8,9	0.83	0	5,10,12	1.92	2 (40%)
1	HYP	G	215	1	7,8,9	1.11	1 (14%)	5,10,12	1.51	1 (20%)
1	HYP	G	221	1	7,8,9	0.67	0	5,10,12	1.99	2 (40%)
1	HYP	G	224	1	7,8,9	0.48	0	5,10,12	1.72	3 (60%)
1	HYP	G	227	1	7,8,9	0.49	0	5,10,12	2.26	3 (60%)
1	HYP	G	24	1	7,8,9	0.54	0	5,10,12	2.00	1 (20%)
1	HYP	G	27	1	7,8,9	0.47	0	5,10,12	1.96	2 (40%)
1	HYP	G	3	1	7,8,9	0.64	0	5,10,12	1.98	3 (60%)
1	HYP	G	6	1	7,8,9	0.59	0	5,10,12	2.03	2 (40%)
1	HYP	G	9	1	7,8,9	0.75	0	5,10,12	1.66	2 (40%)
1	HYP	I	103	1	7,8,9	0.70	0	5,10,12	2.16	2 (40%)
1	HYP	I	106	1	7,8,9	0.53	0	5,10,12	1.25	1 (20%)
1	HYP	I	109	1	7,8,9	0.69	0	5,10,12	1.36	1 (20%)
1	HYP	I	115	1	7,8,9	1.13	0	5,10,12	2.01	1 (20%)
1	HYP	I	121	1	7,8,9	0.91	0	5,10,12	1.25	1 (20%)
1	HYP	I	124	1	7,8,9	0.54	0	5,10,12	1.63	2 (40%)
1	HYP	I	127	1	7,8,9	0.57	0	5,10,12	2.32	3 (60%)
1	HYP	I	15	1	7,8,9	1.26	1 (14%)	5,10,12	2.07	2 (40%)
1	HYP	I	203	1	7,8,9	0.72	0	5,10,12	1.85	1 (20%)
1	HYP	I	206	1	7,8,9	0.93	0	5,10,12	1.55	1 (20%)
1	HYP	I	209	1	7,8,9	0.84	0	5,10,12	2.12	2 (40%)
1	HYP	I	21	1	7,8,9	1.06	0	5,10,12	1.74	2 (40%)
1	HYP	I	215	1	7,8,9	1.13	1 (14%)	5,10,12	1.22	0
1	HYP	I	221	1	7,8,9	0.70	0	5,10,12	1.05	0
1	HYP	I	224	1	7,8,9	0.51	0	5,10,12	2.02	1 (20%)
1	HYP	I	227	1	7,8,9	0.47	0	5,10,12	1.54	2 (40%)
1	HYP	I	24	1	7,8,9	0.58	0	5,10,12	2.13	1 (20%)
1	HYP	I	27	1	7,8,9	0.80	0	5,10,12	1.62	2 (40%)
1	HYP	I	3	1	7,8,9	0.55	0	5,10,12	2.03	1 (20%)
1	HYP	I	6	1	7,8,9	0.86	0	5,10,12	1.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	HYP	I	9	1	7,8,9	0.48	0	5,10,12	1.38	1 (20%)
1	HYP	K	103	1	7,8,9	0.92	0	5,10,12	1.92	3 (60%)
1	HYP	K	106	1	7,8,9	0.57	0	5,10,12	1.39	0
1	HYP	K	109	1	7,8,9	0.50	0	5,10,12	1.07	0
1	HYP	K	115	1	7,8,9	0.82	0	5,10,12	2.12	1 (20%)
1	HYP	K	121	1	7,8,9	1.01	0	5,10,12	1.71	1 (20%)
1	HYP	K	124	1	7,8,9	0.71	0	5,10,12	2.15	3 (60%)
1	HYP	K	127	1	7,8,9	0.53	0	5,10,12	2.00	3 (60%)
1	HYP	K	15	1	7,8,9	0.73	0	5,10,12	1.62	2 (40%)
1	HYP	K	203	1	7,8,9	0.77	0	5,10,12	1.71	3 (60%)
1	HYP	K	206	1	7,8,9	0.76	0	5,10,12	1.48	0
1	HYP	K	209	1	7,8,9	1.34	2 (28%)	5,10,12	1.73	1 (20%)
1	HYP	K	21	1	7,8,9	0.98	0	5,10,12	1.01	0
1	HYP	K	215	1	7,8,9	1.50	1 (14%)	5,10,12	0.79	0
1	HYP	K	221	1	7,8,9	0.57	0	5,10,12	1.33	0
1	HYP	K	224	1	7,8,9	0.76	0	5,10,12	1.50	0
1	HYP	K	227	1	7,8,9	0.59	0	5,10,12	1.31	1 (20%)
1	HYP	K	24	1	7,8,9	0.56	0	5,10,12	2.09	2 (40%)
1	HYP	K	27	1	7,8,9	0.89	1 (14%)	5,10,12	2.08	2 (40%)
1	HYP	K	3	1	7,8,9	0.88	0	5,10,12	1.88	2 (40%)
1	HYP	K	6	1	7,8,9	0.76	0	5,10,12	1.33	0
1	HYP	K	9	1	7,8,9	0.74	0	5,10,12	2.29	2 (40%)

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
1	HYP	A	103	1	-	0/0/11/13	0/1/1/1
1	HYP	A	106	1	-	0/0/11/13	0/1/1/1
1	HYP	A	109	1	-	0/0/11/13	0/1/1/1
1	HYP	A	115	1	-	0/0/11/13	0/1/1/1
1	HYP	A	121	1	-	0/0/11/13	0/1/1/1
1	HYP	A	124	1	-	0/0/11/13	0/1/1/1
1	HYP	A	127	1	-	0/0/11/13	0/1/1/1
1	HYP	A	15	1	-	0/0/11/13	0/1/1/1
1	HYP	A	203	1	-	0/0/11/13	0/1/1/1
1	HYP	A	206	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	A	209	1	-	0/0/11/13	0/1/1/1
1	HYP	A	21	1	-	0/0/11/13	0/1/1/1
1	HYP	A	215	1	-	0/0/11/13	0/1/1/1
1	HYP	A	221	1	-	0/0/11/13	0/1/1/1
1	HYP	A	224	1	-	0/0/11/13	0/1/1/1
1	HYP	A	227	1	-	0/0/11/13	0/1/1/1
1	HYP	A	24	1	-	0/0/11/13	0/1/1/1
1	HYP	A	27	1	-	0/0/11/13	0/1/1/1
1	HYP	A	3	1	-	0/0/11/13	0/1/1/1
1	HYP	A	6	1	-	0/0/11/13	0/1/1/1
1	HYP	A	9	1	-	0/0/11/13	0/1/1/1
1	HYP	C	103	1	-	0/0/11/13	0/1/1/1
1	HYP	C	106	1	-	0/0/11/13	0/1/1/1
1	HYP	C	109	1	-	0/0/11/13	0/1/1/1
1	HYP	C	115	1	-	0/0/11/13	0/1/1/1
1	HYP	C	121	1	-	0/0/11/13	0/1/1/1
1	HYP	C	124	1	-	0/0/11/13	0/1/1/1
1	HYP	C	127	1	-	0/0/11/13	0/1/1/1
1	HYP	C	15	1	-	0/0/11/13	0/1/1/1
1	HYP	C	203	1	-	0/0/11/13	0/1/1/1
1	HYP	C	206	1	-	0/0/11/13	0/1/1/1
1	HYP	C	209	1	-	0/0/11/13	0/1/1/1
1	HYP	C	21	1	-	0/0/11/13	0/1/1/1
1	HYP	C	215	1	-	0/0/11/13	0/1/1/1
1	HYP	C	221	1	-	0/0/11/13	0/1/1/1
1	HYP	C	224	1	-	0/0/11/13	0/1/1/1
1	HYP	C	227	1	-	0/0/11/13	0/1/1/1
1	HYP	C	24	1	-	0/0/11/13	0/1/1/1
1	HYP	C	27	1	-	0/0/11/13	0/1/1/1
1	HYP	C	3	1	-	0/0/11/13	0/1/1/1
1	HYP	C	6	1	-	0/0/11/13	0/1/1/1
1	HYP	C	9	1	-	0/0/11/13	0/1/1/1
1	HYP	E	103	1	-	0/0/11/13	0/1/1/1
1	HYP	E	106	1	-	0/0/11/13	0/1/1/1
1	HYP	E	109	1	-	0/0/11/13	0/1/1/1
1	HYP	E	115	1	-	0/0/11/13	0/1/1/1
1	HYP	E	121	1	-	0/0/11/13	0/1/1/1
1	HYP	E	124	1	-	0/0/11/13	0/1/1/1
1	HYP	E	127	1	-	0/0/11/13	0/1/1/1
1	HYP	E	15	1	-	0/0/11/13	0/1/1/1
1	HYP	E	203	1	-	0/0/11/13	0/1/1/1
1	HYP	E	206	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	E	209	1	-	0/0/11/13	0/1/1/1
1	HYP	E	21	1	-	0/0/11/13	0/1/1/1
1	HYP	E	215	1	-	0/0/11/13	0/1/1/1
1	HYP	E	221	1	-	0/0/11/13	0/1/1/1
1	HYP	E	224	1	-	0/0/11/13	0/1/1/1
1	HYP	E	227	1	-	0/0/11/13	0/1/1/1
1	HYP	E	24	1	-	0/0/11/13	0/1/1/1
1	HYP	E	27	1	-	0/0/11/13	0/1/1/1
1	HYP	E	3	1	-	0/0/11/13	0/1/1/1
1	HYP	E	6	1	-	0/0/11/13	0/1/1/1
1	HYP	E	9	1	-	0/0/11/13	0/1/1/1
1	HYP	G	103	1	-	0/0/11/13	0/1/1/1
1	HYP	G	106	1	-	0/0/11/13	0/1/1/1
1	HYP	G	109	1	-	0/0/11/13	0/1/1/1
1	HYP	G	115	1	-	0/0/11/13	0/1/1/1
1	HYP	G	121	1	-	0/0/11/13	0/1/1/1
1	HYP	G	124	1	-	0/0/11/13	0/1/1/1
1	HYP	G	127	1	-	0/0/11/13	0/1/1/1
1	HYP	G	15	1	-	0/0/11/13	0/1/1/1
1	HYP	G	203	1	-	0/0/11/13	0/1/1/1
1	HYP	G	206	1	-	0/0/11/13	0/1/1/1
1	HYP	G	209	1	-	0/0/11/13	0/1/1/1
1	HYP	G	21	1	-	0/0/11/13	0/1/1/1
1	HYP	G	215	1	-	0/0/11/13	0/1/1/1
1	HYP	G	221	1	-	0/0/11/13	0/1/1/1
1	HYP	G	224	1	-	0/0/11/13	0/1/1/1
1	HYP	G	227	1	-	0/0/11/13	0/1/1/1
1	HYP	G	24	1	-	0/0/11/13	0/1/1/1
1	HYP	G	27	1	-	0/0/11/13	0/1/1/1
1	HYP	G	3	1	-	0/0/11/13	0/1/1/1
1	HYP	G	6	1	-	0/0/11/13	0/1/1/1
1	HYP	G	9	1	-	0/0/11/13	0/1/1/1
1	HYP	I	103	1	-	0/0/11/13	0/1/1/1
1	HYP	I	106	1	-	0/0/11/13	0/1/1/1
1	HYP	I	109	1	-	0/0/11/13	0/1/1/1
1	HYP	I	115	1	-	0/0/11/13	0/1/1/1
1	HYP	I	121	1	-	0/0/11/13	0/1/1/1
1	HYP	I	124	1	-	0/0/11/13	0/1/1/1
1	HYP	I	127	1	-	0/0/11/13	0/1/1/1
1	HYP	I	15	1	-	0/0/11/13	0/1/1/1
1	HYP	I	203	1	-	0/0/11/13	0/1/1/1
1	HYP	I	206	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	I	209	1	-	0/0/11/13	0/1/1/1
1	HYP	I	21	1	-	0/0/11/13	0/1/1/1
1	HYP	I	215	1	-	0/0/11/13	0/1/1/1
1	HYP	I	221	1	-	0/0/11/13	0/1/1/1
1	HYP	I	224	1	-	0/0/11/13	0/1/1/1
1	HYP	I	227	1	-	0/0/11/13	0/1/1/1
1	HYP	I	24	1	-	0/0/11/13	0/1/1/1
1	HYP	I	27	1	-	0/0/11/13	0/1/1/1
1	HYP	I	3	1	-	0/0/11/13	0/1/1/1
1	HYP	I	6	1	-	0/0/11/13	0/1/1/1
1	HYP	I	9	1	-	0/0/11/13	0/1/1/1
1	HYP	K	103	1	-	0/0/11/13	0/1/1/1
1	HYP	K	106	1	-	0/0/11/13	0/1/1/1
1	HYP	K	109	1	-	0/0/11/13	0/1/1/1
1	HYP	K	115	1	-	0/0/11/13	0/1/1/1
1	HYP	K	121	1	-	0/0/11/13	0/1/1/1
1	HYP	K	124	1	-	0/0/11/13	0/1/1/1
1	HYP	K	127	1	-	0/0/11/13	0/1/1/1
1	HYP	K	15	1	-	0/0/11/13	0/1/1/1
1	HYP	K	203	1	-	0/0/11/13	0/1/1/1
1	HYP	K	206	1	-	0/0/11/13	0/1/1/1
1	HYP	K	209	1	-	0/0/11/13	0/1/1/1
1	HYP	K	21	1	-	0/0/11/13	0/1/1/1
1	HYP	K	215	1	-	0/0/11/13	0/1/1/1
1	HYP	K	221	1	-	0/0/11/13	0/1/1/1
1	HYP	K	224	1	-	0/0/11/13	0/1/1/1
1	HYP	K	227	1	-	0/0/11/13	0/1/1/1
1	HYP	K	24	1	-	0/0/11/13	0/1/1/1
1	HYP	K	27	1	-	0/0/11/13	0/1/1/1
1	HYP	K	3	1	-	0/0/11/13	0/1/1/1
1	HYP	K	6	1	-	0/0/11/13	0/1/1/1
1	HYP	K	9	1	-	0/0/11/13	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	215	HYP	CA-N	-3.00	1.43	1.47
1	G	215	HYP	CA-N	-2.42	1.44	1.47
1	E	27	HYP	CA-N	-2.37	1.44	1.47
1	C	15	HYP	CB-CA	-2.37	1.48	1.54
1	K	209	HYP	CB-CA	-2.27	1.49	1.54
1	K	209	HYP	CA-N	-2.13	1.44	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	215	HYP	CA-N	-2.10	1.44	1.47
1	K	27	HYP	CA-N	-2.08	1.44	1.47
1	I	15	HYP	CB-CA	-2.04	1.49	1.54
1	I	215	HYP	CA-N	-2.03	1.45	1.47

All (193) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	206	HYP	CB-CG-CD	-3.67	98.59	103.14
1	E	15	HYP	OD1-CG-CB	-2.81	102.47	110.00
1	E	227	HYP	O-C-CA	-2.75	118.18	125.44
1	K	3	HYP	O-C-CA	-2.71	118.29	125.44
1	K	9	HYP	CG-CB-CA	-2.60	100.18	103.90
1	E	127	HYP	O-C-CA	-2.53	118.76	125.44
1	I	21	HYP	OD1-CG-CD	-2.43	105.19	110.47
1	C	3	HYP	O-C-CA	-2.43	119.02	125.44
1	C	21	HYP	O-C-CA	-2.42	119.05	125.44
1	E	206	HYP	CB-CG-CD	-2.41	100.15	103.14
1	I	127	HYP	O-C-CA	-2.41	119.07	125.44
1	I	227	HYP	O-C-CA	-2.41	119.07	125.44
1	K	121	HYP	OD1-CG-CB	-2.40	103.56	110.00
1	I	106	HYP	O-C-CA	-2.37	119.17	125.44
1	I	206	HYP	OD1-CG-CB	-2.36	103.68	110.00
1	C	109	HYP	OD1-CG-CD	-2.35	105.36	110.47
1	I	21	HYP	O-C-CA	-2.33	119.28	125.44
1	A	103	HYP	O-C-CA	-2.31	119.34	125.44
1	C	127	HYP	O-C-CA	-2.31	119.34	125.44
1	E	215	HYP	OD1-CG-CD	-2.26	105.55	110.47
1	E	109	HYP	OD1-CG-CB	-2.26	103.94	110.00
1	C	27	HYP	O-C-CA	-2.26	119.48	125.44
1	E	15	HYP	O-C-CA	-2.25	119.50	125.44
1	E	9	HYP	O-C-CA	-2.25	119.50	125.44
1	I	27	HYP	O-C-CA	-2.25	119.50	125.44
1	G	127	HYP	O-C-CA	-2.24	119.51	125.44
1	C	227	HYP	O-C-CA	-2.24	119.52	125.44
1	K	227	HYP	O-C-CA	-2.22	119.59	125.44
1	C	106	HYP	O-C-CA	-2.21	119.59	125.44
1	G	3	HYP	O-C-CA	-2.20	119.62	125.44
1	E	221	HYP	O-C-CA	-2.19	119.66	125.44
1	G	9	HYP	O-C-CA	-2.19	119.67	125.44
1	K	203	HYP	O-C-CA	-2.18	119.69	125.44
1	C	206	HYP	O-C-CA	-2.17	119.70	125.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	209	HYP	O-C-CA	-2.17	119.72	125.44
1	E	27	HYP	OD1-CG-CD	-2.16	105.79	110.47
1	C	209	HYP	OD1-CG-CB	-2.15	104.24	110.00
1	I	124	HYP	O-C-CA	-2.14	119.78	125.44
1	K	127	HYP	O-C-CA	-2.13	119.80	125.44
1	I	27	HYP	OD1-CG-CD	-2.12	105.87	110.47
1	C	215	HYP	O-C-CA	-2.12	119.85	125.44
1	A	24	HYP	O-C-CA	-2.12	119.85	125.44
1	E	224	HYP	O-C-CA	-2.11	119.86	125.44
1	C	106	HYP	OD1-CG-CD	-2.11	105.89	110.47
1	C	124	HYP	O-C-CA	-2.11	119.86	125.44
1	E	27	HYP	O-C-CA	-2.09	119.92	125.44
1	E	21	HYP	OD1-CG-CD	-2.09	105.94	110.47
1	A	27	HYP	O-C-CA	-2.08	119.94	125.44
1	C	203	HYP	O-C-CA	-2.07	119.96	125.44
1	A	121	HYP	O-C-CA	-2.07	119.96	125.44
1	G	203	HYP	O-C-CA	-2.07	119.97	125.44
1	I	15	HYP	OD1-CG-CB	-2.07	104.45	110.00
1	E	206	HYP	O-C-CA	-2.07	119.97	125.44
1	G	227	HYP	O-C-CA	-2.06	119.99	125.44
1	K	103	HYP	O-C-CA	-2.06	119.99	125.44
1	E	124	HYP	O-C-CA	-2.06	120.00	125.44
1	A	124	HYP	O-C-CA	-2.05	120.02	125.44
1	I	227	HYP	OD1-CG-CD	-2.05	106.01	110.47
1	K	203	HYP	OD1-CG-CB	-2.05	104.51	110.00
1	A	106	HYP	O-C-CA	-2.05	120.04	125.44
1	E	203	HYP	O-C-CA	-2.04	120.04	125.44
1	G	124	HYP	O-C-CA	-2.04	120.04	125.44
1	A	221	HYP	O-C-CA	-2.04	120.04	125.44
1	G	15	HYP	O-C-CA	-2.04	120.06	125.44
1	E	109	HYP	O-C-CA	-2.03	120.07	125.44
1	K	15	HYP	O-C-CA	-2.03	120.07	125.44
1	K	124	HYP	O-C-CA	-2.03	120.09	125.44
1	C	121	HYP	O-C-CA	-2.03	120.09	125.44
1	K	24	HYP	O-C-CA	-2.02	120.09	125.44
1	C	103	HYP	O-C-CA	-2.02	120.09	125.44
1	C	203	HYP	OD1-CG-CD	-2.02	106.08	110.47
1	C	15	HYP	O-C-CA	-2.01	120.12	125.44
1	A	3	HYP	O-C-CA	-2.01	120.13	125.44
1	G	224	HYP	O-C-CA	-2.01	120.13	125.44
1	K	203	HYP	CB-CG-CD	2.02	105.63	103.14
1	A	3	HYP	CG-CB-CA	2.02	106.79	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	224	HYP	CB-CG-CD	2.06	105.69	103.14
1	G	21	HYP	CB-CG-CD	2.07	105.70	103.14
1	A	115	HYP	CG-CB-CA	2.08	106.88	103.90
1	A	209	HYP	CG-CB-CA	2.11	106.92	103.90
1	K	103	HYP	CB-CG-CD	2.12	105.76	103.14
1	A	21	HYP	CG-CB-CA	2.13	106.95	103.90
1	C	21	HYP	CG-CB-CA	2.15	106.98	103.90
1	E	3	HYP	OD1-CG-CB	2.17	115.80	110.00
1	G	3	HYP	CG-CB-CA	2.17	107.01	103.90
1	K	15	HYP	CB-CG-CD	2.17	105.82	103.14
1	C	21	HYP	CB-CG-CD	2.19	105.84	103.14
1	A	15	HYP	CB-CG-CD	2.19	105.85	103.14
1	G	6	HYP	CG-CB-CA	2.19	107.04	103.90
1	G	224	HYP	CG-CB-CA	2.21	107.06	103.90
1	G	203	HYP	CB-CG-CD	2.21	105.87	103.14
1	G	9	HYP	CB-CG-CD	2.23	105.90	103.14
1	A	27	HYP	CB-CG-CD	2.23	105.90	103.14
1	E	209	HYP	CB-CG-CD	2.25	105.92	103.14
1	A	9	HYP	CB-CG-CD	2.26	105.93	103.14
1	I	9	HYP	CB-CG-CD	2.27	105.94	103.14
1	A	227	HYP	CG-CB-CA	2.27	107.14	103.90
1	I	109	HYP	CB-CG-CD	2.29	105.97	103.14
1	C	103	HYP	CB-CG-CD	2.31	106.00	103.14
1	A	6	HYP	CG-CB-CA	2.33	107.23	103.90
1	G	215	HYP	CG-CB-CA	2.34	107.25	103.90
1	E	124	HYP	CG-CB-CA	2.34	107.25	103.90
1	I	121	HYP	CB-CG-CD	2.35	106.05	103.14
1	K	127	HYP	CB-CG-CD	2.36	106.06	103.14
1	C	15	HYP	CB-CG-CD	2.37	106.07	103.14
1	I	124	HYP	CB-CG-CD	2.38	106.08	103.14
1	G	224	HYP	CB-CG-CD	2.39	106.09	103.14
1	A	21	HYP	CB-CG-CD	2.40	106.10	103.14
1	C	121	HYP	CG-CB-CA	2.40	107.33	103.90
1	A	209	HYP	CB-CG-CD	2.42	106.13	103.14
1	C	221	HYP	CG-CB-CA	2.43	107.38	103.90
1	G	221	HYP	CB-CG-CD	2.45	106.17	103.14
1	E	15	HYP	OD1-CG-CD	2.46	115.81	110.47
1	E	127	HYP	CG-CB-CA	2.50	107.49	103.90
1	I	103	HYP	CG-CB-CA	2.51	107.50	103.90
1	A	24	HYP	CG-CB-CA	2.53	107.52	103.90
1	A	27	HYP	CG-CB-CA	2.54	107.54	103.90
1	C	3	HYP	CB-CG-CD	2.55	106.29	103.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	115	HYP	CG-CB-CA	2.56	107.56	103.90
1	A	124	HYP	CG-CB-CA	2.57	107.58	103.90
1	E	24	HYP	CB-CG-CD	2.57	106.31	103.14
1	G	103	HYP	CG-CB-CA	2.62	107.65	103.90
1	E	121	HYP	CB-CG-CD	2.64	106.40	103.14
1	A	24	HYP	CB-CG-CD	2.64	106.40	103.14
1	E	3	HYP	CG-CB-CA	2.66	107.70	103.90
1	A	106	HYP	CB-CG-CD	2.66	106.42	103.14
1	G	27	HYP	CG-CB-CA	2.68	107.73	103.90
1	I	203	HYP	CB-CG-CD	2.70	106.47	103.14
1	K	3	HYP	CB-CG-CD	2.71	106.49	103.14
1	E	6	HYP	CB-CG-CD	2.74	106.52	103.14
1	G	3	HYP	CB-CG-CD	2.75	106.54	103.14
1	G	27	HYP	CB-CG-CD	2.77	106.57	103.14
1	K	27	HYP	CB-CG-CD	2.80	106.60	103.14
1	G	227	HYP	CG-CB-CA	2.81	107.92	103.90
1	I	127	HYP	CG-CB-CA	2.82	107.93	103.90
1	A	15	HYP	CG-CB-CA	2.82	107.94	103.90
1	G	103	HYP	CB-CG-CD	2.83	106.64	103.14
1	K	124	HYP	CG-CB-CA	2.84	107.96	103.90
1	C	6	HYP	CB-CG-CD	2.84	106.65	103.14
1	G	21	HYP	CG-CB-CA	2.84	107.97	103.90
1	E	15	HYP	CG-CB-CA	2.88	108.03	103.90
1	K	103	HYP	CG-CB-CA	2.88	108.03	103.90
1	A	221	HYP	CB-CG-CD	2.90	106.72	103.14
1	A	203	HYP	CB-CG-CD	2.90	106.73	103.14
1	C	209	HYP	CB-CG-CD	2.91	106.73	103.14
1	C	24	HYP	CB-CG-CD	2.92	106.75	103.14
1	K	209	HYP	CB-CG-CD	2.93	106.76	103.14
1	I	209	HYP	CB-CG-CD	2.95	106.78	103.14
1	E	124	HYP	CB-CG-CD	2.95	106.79	103.14
1	C	127	HYP	CG-CB-CA	2.96	108.13	103.90
1	A	124	HYP	CB-CG-CD	2.98	106.82	103.14
1	G	221	HYP	CG-CB-CA	2.99	108.19	103.90
1	G	6	HYP	CB-CG-CD	2.99	106.84	103.14
1	A	127	HYP	CG-CB-CA	3.01	108.21	103.90
1	I	15	HYP	CG-CB-CA	3.01	108.21	103.90
1	A	109	HYP	CB-CG-CD	3.05	106.91	103.14
1	K	27	HYP	CG-CB-CA	3.05	108.26	103.90
1	C	209	HYP	CG-CB-CA	3.07	108.30	103.90
1	K	127	HYP	CG-CB-CA	3.09	108.32	103.90
1	C	124	HYP	CB-CG-CD	3.09	106.96	103.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	215	HYP	CB-CG-CD	3.09	106.97	103.14
1	G	127	HYP	CB-CG-CD	3.12	107.00	103.14
1	C	115	HYP	CB-CG-CD	3.12	107.00	103.14
1	E	209	HYP	CG-CB-CA	3.15	108.41	103.90
1	I	103	HYP	CB-CG-CD	3.15	107.03	103.14
1	I	209	HYP	CG-CB-CA	3.16	108.43	103.90
1	A	115	HYP	CB-CG-CD	3.18	107.08	103.14
1	A	103	HYP	CG-CB-CA	3.19	108.46	103.90
1	I	3	HYP	CB-CG-CD	3.22	107.12	103.14
1	G	115	HYP	CB-CG-CD	3.23	107.13	103.14
1	G	121	HYP	CB-CG-CD	3.23	107.13	103.14
1	G	127	HYP	CG-CB-CA	3.25	108.55	103.90
1	A	127	HYP	CB-CG-CD	3.28	107.19	103.14
1	G	124	HYP	CB-CG-CD	3.28	107.20	103.14
1	I	115	HYP	CB-CG-CD	3.30	107.22	103.14
1	K	124	HYP	CB-CG-CD	3.30	107.22	103.14
1	C	3	HYP	CG-CB-CA	3.34	108.68	103.90
1	C	124	HYP	CG-CB-CA	3.37	108.72	103.90
1	K	9	HYP	CB-CG-CD	3.41	107.35	103.14
1	C	127	HYP	CB-CG-CD	3.42	107.37	103.14
1	G	124	HYP	CG-CB-CA	3.43	108.81	103.90
1	G	15	HYP	CB-CG-CD	3.45	107.40	103.14
1	E	127	HYP	CB-CG-CD	3.54	107.51	103.14
1	A	227	HYP	CB-CG-CD	3.55	107.53	103.14
1	I	224	HYP	CB-CG-CD	3.57	107.55	103.14
1	G	227	HYP	CB-CG-CD	3.60	107.59	103.14
1	I	127	HYP	CB-CG-CD	3.62	107.62	103.14
1	A	103	HYP	CB-CG-CD	3.63	107.62	103.14
1	A	3	HYP	CB-CG-CD	3.81	107.85	103.14
1	I	24	HYP	CB-CG-CD	3.82	107.87	103.14
1	G	24	HYP	CB-CG-CD	3.83	107.87	103.14
1	K	24	HYP	CB-CG-CD	3.84	107.89	103.14
1	K	115	HYP	CB-CG-CD	3.86	107.91	103.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	215	HYP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	215	HYP	1	0
1	C	9	HYP	1	0
1	E	215	HYP	2	0
1	E	9	HYP	1	0
1	G	21	HYP	2	0
1	G	215	HYP	1	0
1	I	215	HYP	1	0
1	I	3	HYP	1	0
1	K	206	HYP	1	0
1	K	215	HYP	1	0
1	K	27	HYP	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

4 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	$\#\|Z\| > 2$
3	SO4	C	301	-	4,4,4	0.30	0	6,6,6	0.67	0
3	SO4	F	1901	-	4,4,4	0.34	0	6,6,6	0.59	0
3	SO4	I	301	-	4,4,4	0.45	0	6,6,6	0.41	0
3	SO4	K	301	-	4,4,4	0.29	0	6,6,6	0.45	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
3	SO4	C	301	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	F	1901	-	-	0/0/0/0	0/0/0/0
3	SO4	I	301	-	-	0/0/0/0	0/0/0/0
3	SO4	K	301	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

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
3	F	1901	SO4	1	0
3	K	301	SO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	58/87 (66%)	1.35	11 (18%) 2 1	42, 61, 124, 149	0
1	C	58/87 (66%)	0.23	4 (6%) 20 11	23, 43, 89, 98	0
1	E	58/87 (66%)	-0.08	1 (1%) 73 63	31, 41, 74, 87	0
1	G	58/87 (66%)	0.86	8 (13%) 4 2	53, 67, 119, 134	0
1	I	58/87 (66%)	0.19	2 (3%) 49 36	19, 36, 78, 85	0
1	K	59/87 (67%)	0.18	2 (3%) 49 36	25, 42, 85, 94	0
2	B	188/192 (97%)	0.44	13 (6%) 20 11	36, 55, 84, 103	0
2	D	188/192 (97%)	0.12	8 (4%) 39 27	27, 45, 64, 79	0
2	F	188/192 (97%)	0.65	18 (9%) 10 5	35, 55, 78, 89	0
2	H	187/192 (97%)	0.91	26 (13%) 4 2	54, 67, 98, 116	0
2	J	191/192 (99%)	0.17	5 (2%) 59 47	20, 34, 56, 73	0
2	L	188/192 (97%)	0.20	6 (3%) 51 39	21, 42, 76, 99	0
All	All	1479/1674 (88%)	0.42	104 (7%) 19 11	19, 51, 86, 149	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	126	PRO	11.3
2	D	1873	SER	8.7
1	A	26	PRO	7.3
1	A	219	GLY	6.1
2	F	1862	THR	5.5
2	F	1725	PRO	5.3
1	A	123	PRO	5.2
2	F	1686	CYS	4.8
2	F	1873	SER	4.7
2	B	1873	SER	4.7
2	B	1862	THR	4.7

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Mol	Chain	Res	Type	RSRZ
2	L	1746	ASN	4.2
1	A	218	MET	4.0
2	H	1823	PHE	4.0
2	F	1866	SER	3.9
2	H	1748	VAL	3.9
1	A	220	PHE	3.9
1	K	226	PRO	3.8
1	A	226	PRO	3.8
2	H	1725	PRO	3.7
2	J	1686	CYS	3.7
2	F	1750	GLU	3.6
2	H	1791	GLY	3.6
2	H	1722	ASN	3.6
2	F	1722	ASN	3.6
2	H	1749	PRO	3.5
2	H	1747	VAL	3.4
2	J	1746	ASN	3.4
2	H	1862	THR	3.3
1	G	120	PHE	3.3
2	D	1869	HIS	3.3
2	J	1683	ALA	3.3
1	C	126	PRO	3.3
2	B	1790	PRO	3.2
2	F	1819	ARG	3.1
2	H	1792	ALA	3.1
2	F	1748	VAL	3.1
1	C	226	PRO	3.1
2	H	1730	VAL	3.0
2	F	1749	PRO	3.0
2	H	1723	ILE	3.0
2	H	1786	HIS	3.0
1	G	26	PRO	2.9
2	F	1823	PHE	2.9
1	A	102	PRO	2.9
2	H	1746	ASN	2.9
2	F	1791	GLY	2.8
2	H	1785	MET	2.8
2	B	1792	ALA	2.8
2	B	1869	HIS	2.8
2	H	1726	ARG	2.8
1	A	222	GLY	2.8
1	G	101	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	201	GLY	2.7
1	K	2	PRO	2.7
2	D	1725	PRO	2.7
2	L	1862	THR	2.7
1	G	202	PRO	2.6
2	H	1866	SER	2.6
1	I	226	PRO	2.6
2	F	1860	MET	2.6
2	B	1688	GLN	2.5
1	G	5	PRO	2.5
2	H	1869	HIS	2.5
2	H	1782	THR	2.5
2	F	1724	GLY	2.5
2	H	1688	GLN	2.5
2	H	1692	VAL	2.5
2	B	1812	ALA	2.5
2	L	1723	ILE	2.5
2	D	1746	ASN	2.4
2	D	1862	THR	2.4
2	F	1728	THR	2.4
1	C	26	PRO	2.4
2	F	1746	ASN	2.4
2	H	1728	THR	2.4
2	L	1863	LEU	2.3
2	H	1788	ALA	2.3
1	A	125	GLY	2.3
2	B	1787	GLY	2.3
2	B	1871	LEU	2.3
2	H	1783	SER	2.3
2	D	1688	GLN	2.3
2	H	1790	PRO	2.3
2	B	1750	GLU	2.2
2	L	1689	PRO	2.2
1	G	20	PHE	2.2
2	B	1813	ASP	2.2
2	D	1865	ASN	2.2
2	H	1845	ASP	2.2
2	D	1866	SER	2.1
2	J	1845	ASP	2.1
1	G	217	VAL	2.1
2	B	1861	VAL	2.1
2	F	1720	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	26	PRO	2.1
1	E	226	PRO	2.1
1	C	220	PHE	2.0
2	F	1843	ALA	2.0
2	H	1795	ALA	2.0
1	G	126	PRO	2.0
2	B	1725	PRO	2.0
2	L	1750	GLU	2.0
2	J	1750	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	HYP	G	215	8/9	0.89	0.27	-	61,63,65,65	0
1	HYP	A	215	8/9	0.89	0.25	-	51,53,56,58	0
1	HYP	I	24	8/9	0.80	0.23	-	55,59,61,62	0
1	HYP	C	15	8/9	0.95	0.15	-	21,22,23,25	0
1	HYP	I	209	8/9	0.95	0.18	-	22,25,28,33	0
1	HYP	E	9	8/9	0.96	0.19	-	35,38,42,43	0
1	HYP	C	227	8/9	0.72	0.29	-	108,114,116,118	0
1	HYP	A	227	8/9	0.44	0.76	-	157,165,167,170	0
1	HYP	I	206	8/9	0.96	0.12	-	33,37,42,47	0
1	HYP	K	215	8/9	0.95	0.18	-	28,29,32,34	0
1	HYP	G	121	8/9	0.79	0.29	-	88,90,97,100	0
1	HYP	E	206	8/9	0.93	0.21	-	34,36,38,39	0
1	HYP	C	27	8/9	0.68	0.33	-	98,102,107,109	0
1	HYP	E	24	8/9	0.86	0.24	-	66,68,73,74	0
1	HYP	I	224	8/9	0.89	0.27	-	70,73,82,86	0
1	HYP	E	27	8/9	0.83	0.28	-	78,81,89,90	0
1	HYP	I	227	8/9	0.68	0.44	-	94,100,104,104	0
1	HYP	A	206	8/9	0.89	0.20	-	49,50,52,53	0
1	HYP	I	15	8/9	0.94	0.17	-	19,21,25,29	0
1	HYP	C	215	8/9	0.93	0.15	-	32,35,38,38	0
1	HYP	K	6	8/9	0.92	0.21	-	49,51,55,56	0
1	HYP	G	103	8/9	0.80	0.19	-	65,66,71,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	HYP	A	3	8/9	0.69	0.26	-	81,87,93,97	0
1	HYP	E	15	8/9	0.92	0.19	-	31,32,33,34	0
1	HYP	G	9	8/9	0.87	0.20	-	55,58,62,63	0
1	HYP	A	21	8/9	0.73	0.33	-	75,78,81,81	0
1	HYP	E	127	8/9	0.64	0.35	-	91,95,97,97	0
1	HYP	I	106	8/9	0.96	0.15	-	36,38,43,44	0
1	HYP	I	27	8/9	0.86	0.37	-	84,88,92,95	0
1	HYP	K	9	8/9	0.96	0.17	-	36,38,40,41	0
1	HYP	I	9	8/9	0.94	0.15	-	31,34,40,40	0
1	HYP	C	206	8/9	0.97	0.14	-	35,36,39,41	0
1	HYP	E	221	8/9	0.91	0.24	-	51,53,56,57	0
1	HYP	E	224	8/9	0.93	0.15	-	63,66,67,68	0
1	HYP	I	221	8/9	0.84	0.22	-	53,55,62,63	0
1	HYP	A	109	8/9	0.91	0.18	-	45,48,51,54	0
1	HYP	G	106	8/9	0.93	0.16	-	57,59,62,63	0
1	HYP	K	27	8/9	0.87	0.18	-	88,90,99,102	0
1	HYP	E	21	8/9	0.88	0.23	-	49,52,53,54	0
1	HYP	E	209	8/9	0.95	0.15	-	30,31,33,34	0
1	HYP	C	209	8/9	0.95	0.15	-	25,27,29,29	0
1	HYP	G	221	8/9	0.65	0.24	-	96,100,104,104	0
1	HYP	K	224	8/9	0.88	0.25	-	77,80,87,88	0
1	HYP	G	27	8/9	0.55	0.35	-	126,130,132,133	0
1	HYP	A	209	8/9	0.89	0.22	-	43,44,46,47	0
1	HYP	K	127	8/9	0.86	0.16	-	90,95,97,102	0
1	HYP	G	3	8/9	0.65	0.39	-	71,73,78,80	0
1	HYP	E	227	8/9	0.70	0.29	-	85,87,93,94	0
1	HYP	G	21	8/9	0.71	0.32	-	78,81,82,83	0
1	HYP	A	9	8/9	0.89	0.25	-	45,47,50,53	0
1	HYP	K	227	8/9	0.62	0.45	-	103,107,113,114	0
1	HYP	G	224	8/9	0.66	0.30	-	119,122,129,130	0
1	HYP	E	6	8/9	0.96	0.13	-	43,45,49,50	0
1	HYP	K	206	8/9	0.93	0.15	-	45,48,55,55	0
1	HYP	A	6	8/9	0.88	0.23	-	58,61,67,67	0
1	HYP	I	121	8/9	0.91	0.25	-	40,41,46,48	0
1	HYP	E	215	8/9	0.97	0.15	-	37,38,43,43	0
1	HYP	G	206	8/9	0.88	0.20	-	55,57,60,62	0
1	HYP	G	24	8/9	0.69	0.24	-	97,100,102,103	0
1	HYP	K	209	8/9	0.93	0.22	-	32,36,42,45	0
1	HYP	G	227	8/9	0.70	0.38	-	143,146,153,157	0
1	HYP	E	106	8/9	0.94	0.15	-	36,37,38,39	0
1	HYP	I	215	8/9	0.93	0.17	-	22,25,27,28	0
1	HYP	K	103	8/9	0.88	0.22	-	69,75,84,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	HYP	G	109	8/9	0.90	0.22	-	54,55,58,59	0
1	HYP	I	124	8/9	0.94	0.24	-	56,61,62,62	0
1	HYP	K	115	8/9	0.94	0.17	-	27,29,31,33	0
1	HYP	G	6	8/9	0.88	0.18	-	60,63,67,68	0
1	HYP	I	115	8/9	0.96	0.14	-	22,24,31,34	0
1	HYP	E	203	8/9	0.86	0.22	-	44,47,52,54	0
1	HYP	A	103	8/9	0.88	0.28	-	70,72,75,76	0
1	HYP	G	209	8/9	0.78	0.25	-	51,53,56,60	0
1	HYP	C	6	8/9	0.91	0.21	-	53,58,66,69	0
1	HYP	A	224	8/9	0.35	0.61	-	116,121,124,125	0
1	HYP	G	15	8/9	0.94	0.22	-	57,58,62,63	0
1	HYP	A	127	8/9	0.39	1.04	-	148,156,161,161	0
1	HYP	C	9	8/9	0.94	0.15	-	34,41,46,49	0
1	HYP	C	124	8/9	0.89	0.31	-	66,70,72,73	0
1	HYP	E	115	8/9	0.97	0.15	-	32,33,36,38	0
1	HYP	A	115	8/9	0.87	0.27	-	45,46,48,51	0
1	HYP	E	121	8/9	0.91	0.16	-	46,47,50,51	0
1	HYP	C	121	8/9	0.92	0.18	-	45,47,50,50	0
1	HYP	I	103	8/9	0.83	0.25	-	55,59,67,69	0
1	HYP	I	127	8/9	0.86	0.27	-	85,89,94,98	0
1	HYP	A	15	8/9	0.92	0.21	-	44,46,46,47	0
1	HYP	K	124	8/9	0.89	0.22	-	64,67,71,73	0
1	HYP	A	106	8/9	0.94	0.19	-	55,56,59,61	0
1	HYP	G	124	8/9	0.71	0.43	-	105,107,113,116	0
1	HYP	E	124	8/9	0.92	0.40	-	65,67,69,72	0
1	HYP	A	27	8/9	0.49	0.85	-	132,137,143,145	0
1	HYP	I	3	8/9	0.84	0.26	-	66,70,75,77	0
1	HYP	E	3	8/9	0.79	0.35	-	55,58,62,64	0
1	HYP	K	21	8/9	0.92	0.19	-	41,44,45,45	0
1	HYP	K	109	8/9	0.94	0.19	-	31,35,39,42	0
1	HYP	A	24	8/9	0.53	0.46	-	101,105,110,110	0
1	HYP	G	203	8/9	0.84	0.19	-	62,65,70,71	0
1	HYP	C	203	8/9	0.85	0.29	-	52,55,61,63	0
1	HYP	A	121	8/9	0.75	0.32	-	80,82,86,86	0
1	HYP	K	3	8/9	0.56	0.27	-	74,79,85,86	0
1	HYP	E	109	8/9	0.96	0.11	-	35,37,39,41	0
1	HYP	C	106	8/9	0.95	0.16	-	46,49,51,54	0
1	HYP	A	124	8/9	0.70	0.40	-	111,117,119,119	0
1	HYP	C	221	8/9	0.90	0.19	-	61,62,70,72	0
1	HYP	K	221	8/9	0.91	0.28	-	54,57,62,62	0
1	HYP	C	224	8/9	0.84	0.33	-	80,84,90,93	0
1	HYP	C	127	8/9	0.67	0.37	-	99,106,108,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	HYP	G	127	8/9	0.15	0.64	-	126,133,134,135	0
1	HYP	I	21	8/9	0.95	0.18	-	34,36,37,39	0
1	HYP	K	121	8/9	0.96	0.22	-	48,49,55,56	0
1	HYP	C	115	8/9	0.96	0.14	-	27,30,37,39	0
1	HYP	A	221	8/9	0.83	0.51	-	86,91,92,93	0
1	HYP	C	24	8/9	0.87	0.28	-	67,70,73,74	0
1	HYP	C	21	8/9	0.90	0.23	-	42,44,46,49	0
1	HYP	I	203	8/9	0.90	0.17	-	52,57,66,67	0
1	HYP	C	109	8/9	0.92	0.17	-	36,39,47,47	0
1	HYP	K	203	8/9	0.92	0.28	-	60,63,67,70	0
1	HYP	G	115	8/9	0.83	0.22	-	62,64,68,69	0
1	HYP	K	15	8/9	0.93	0.19	-	28,30,35,36	0
1	HYP	K	24	8/9	0.70	0.22	-	59,63,64,64	0
1	HYP	I	6	8/9	0.92	0.17	-	44,47,50,52	0
1	HYP	I	109	8/9	0.96	0.17	-	26,28,31,32	0
1	HYP	C	3	8/9	0.71	0.23	-	78,83,91,95	0
1	HYP	K	106	8/9	0.90	0.20	-	46,51,58,59	0
1	HYP	E	103	8/9	0.88	0.21	-	44,45,47,48	0
1	HYP	C	103	8/9	0.97	0.16	-	59,63,66,66	0
1	HYP	A	203	8/9	0.82	0.28	-	61,63,67,67	0

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, 95th 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
3	SO4	F	1901	5/5	0.88	0.30	1.10	70,73,74,74	0
3	SO4	C	301	5/5	0.88	0.24	0.43	43,49,49,49	0
3	SO4	K	301	5/5	0.85	0.31	0.28	53,56,59,59	0
3	SO4	I	301	5/5	0.90	0.23	-0.21	44,50,50,52	0

6.5 Other polymers (i)

There are no such residues in this entry.