Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:38 PM GMT

PDB ID	:	4CX7
Title	:	Structure of human iNOS heme domain in complex with (R)-6-(3-AMINO-2-(5-(2-(6-AMINO-4- METHYLPYRIDIN-2-YL)ETHYL)PYRIDIN-3-YL)PROPYL)-4- METHYLPYRIDIN-2-AMINE
Authors	:	Li, H.; Poulos, T.L.
Deposited on	:	2014-04-03
Resolution	:	3.16 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

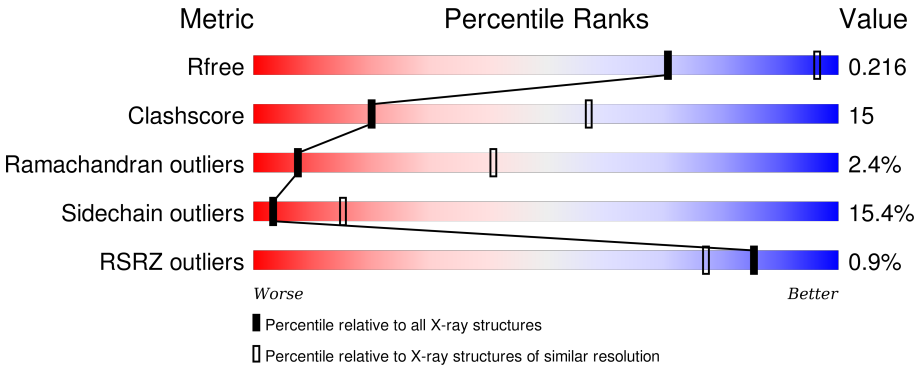
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.16 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	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)

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	431	64% 26% 6%
1	B	431	62% 25% 8%
1	C	431	54% 35% 7%
1	D	431	66% 22% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	B	880	-	-	-	X
6	SO4	D	920	-	-	-	X

2 Entry composition

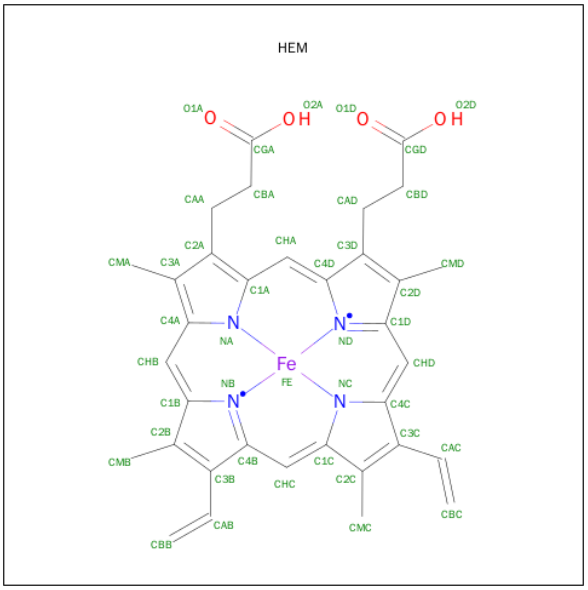
There are 6 unique types of molecules in this entry. The entry contains 13889 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NITRIC OXIDE SYNTHASE, INDUCIBLE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	0	1
			3367	2155	589	602	21			
1	B	414	Total	C	N	O	S	0	0	1
			3367	2155	589	602	21			
1	C	414	Total	C	N	O	S	0	0	1
			3367	2155	589	602	21			
1	D	414	Total	C	N	O	S	0	0	1
			3367	2155	589	602	21			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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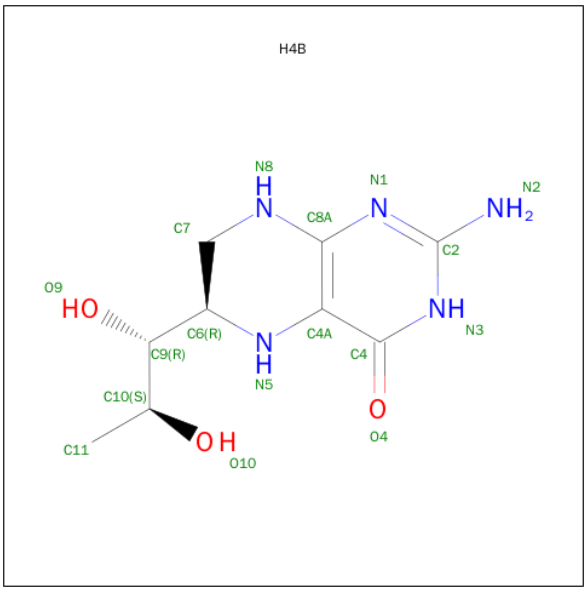
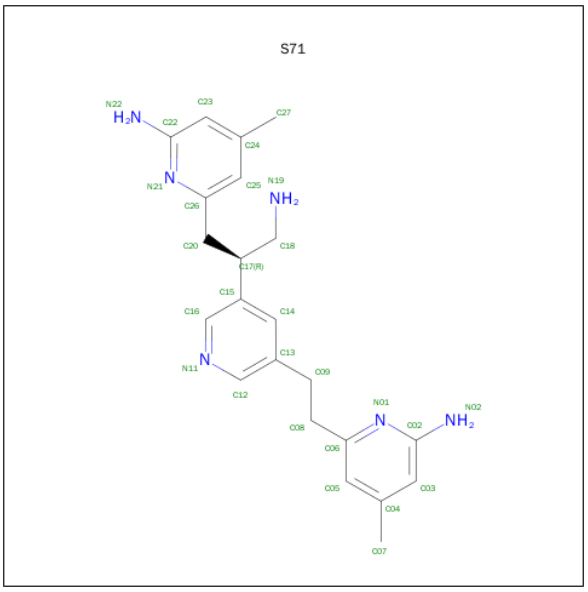
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).



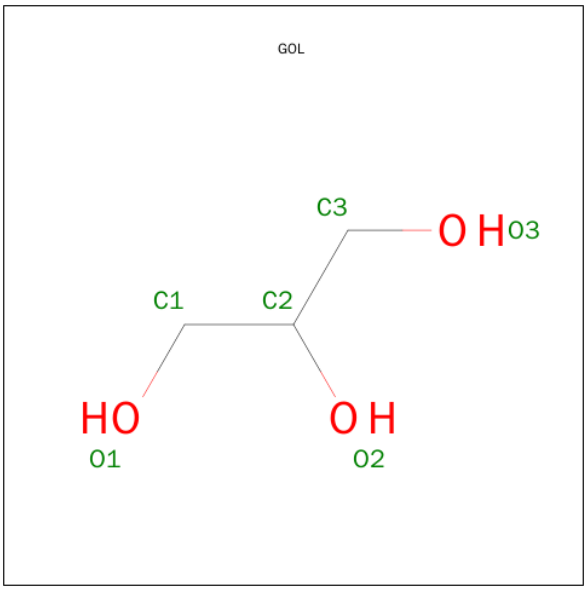
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		
3	C	1	Total	C	N	O	0	0
			17	9	5	3		
3	D	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is (R)-6-(3-AMINO-2-(5-(2-(6-AMINO-4-METHYLPYRIDIN-2-YL)ETHYL)PYRIDIN-3-YL)PROPYL)-4-METHYLPYRIDIN-2-AMINE (three-letter code: S71) (formula: $C_{22}H_{28}N_6$).



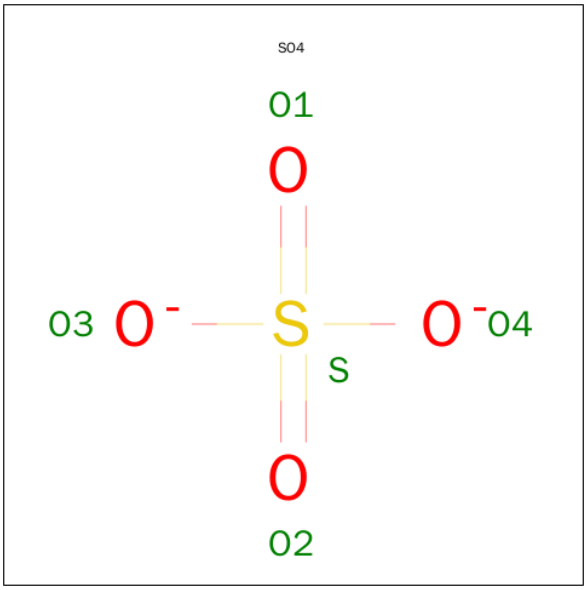
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N 28 22 6	0	0
4	B	1	Total C N 28 22 6	0	0
4	C	1	Total C N 28 22 6	0	0
4	D	1	Total C N 28 22 6	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0

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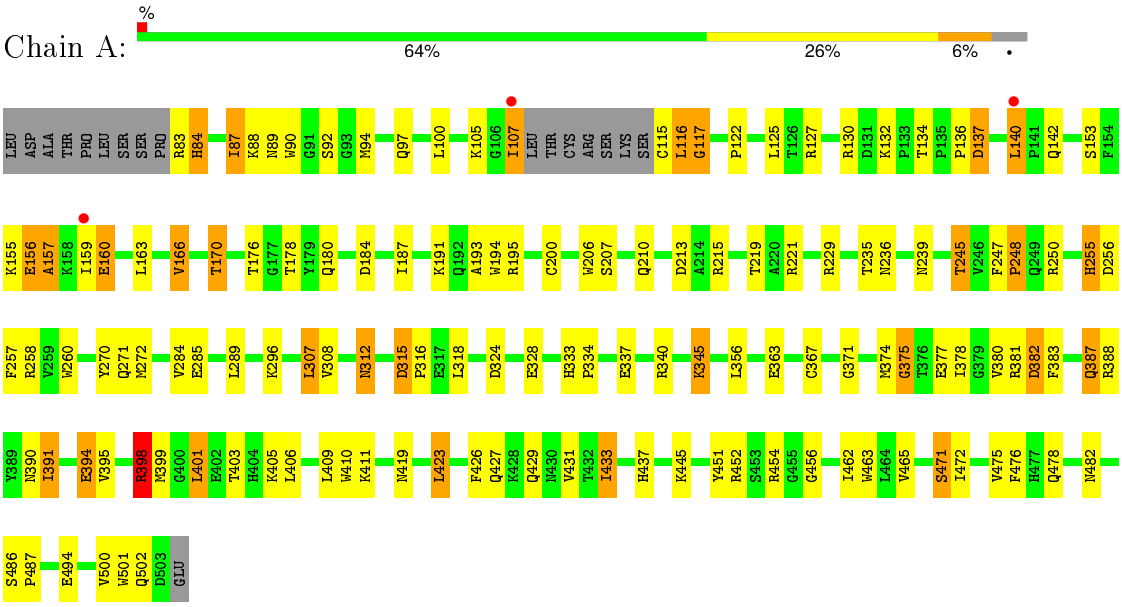
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total O S 5 4 1	0	0

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.

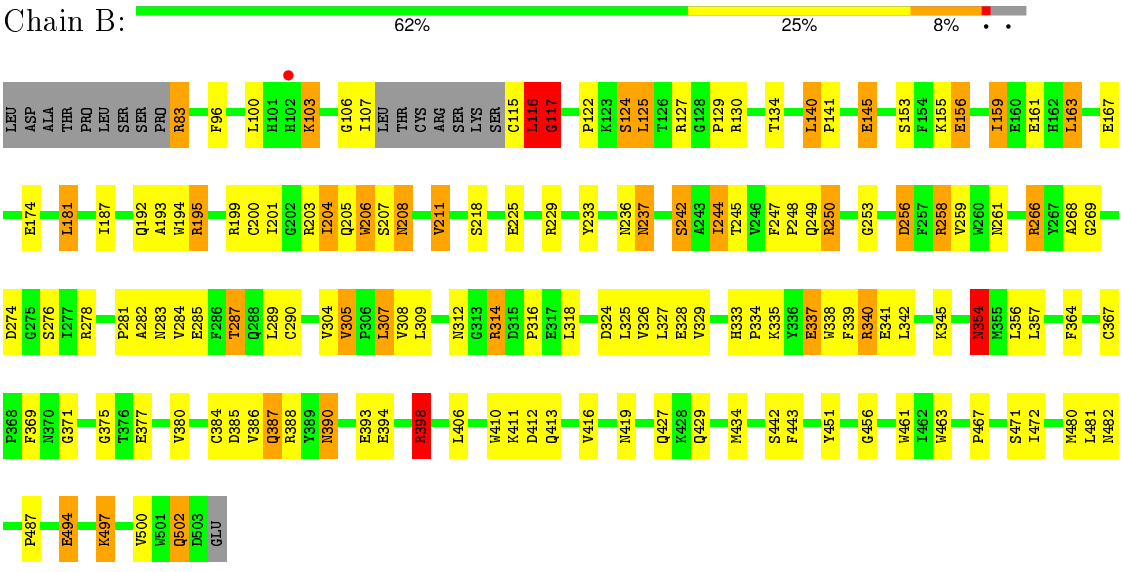
- Molecule 1: NITRIC OXIDE SYNTHASE, INDUCIBLE

Chain A:



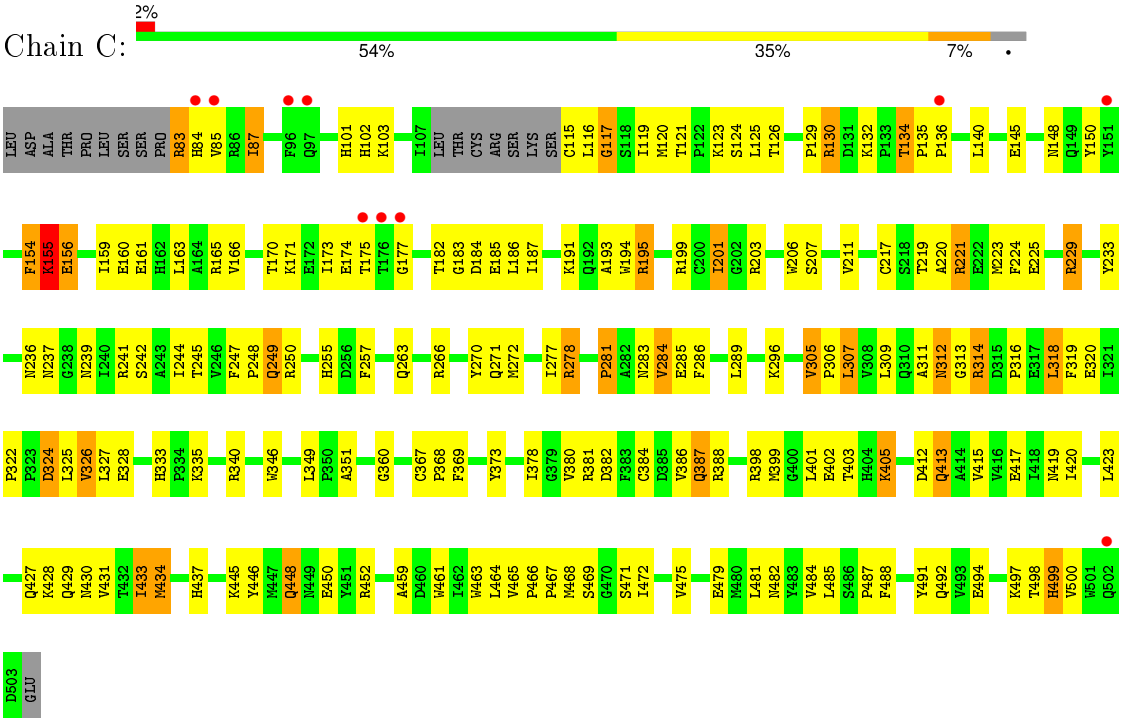
- Molecule 1: NITRIC OXIDE SYNTHASE, INDUCIBLE

Chain B:



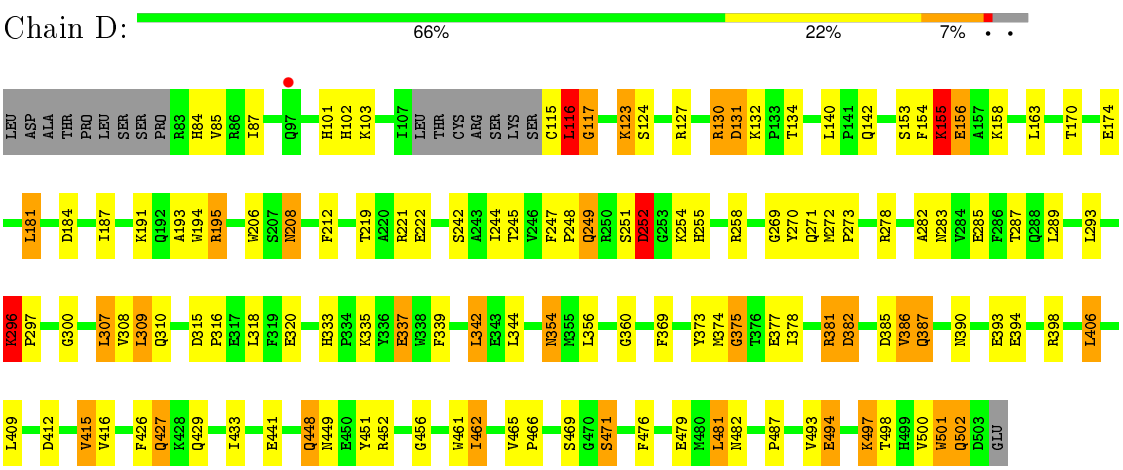
• Molecule 1: NITRIC OXIDE SYNTHASE, INDUCIBLE

Chain C:



• Molecule 1: NITRIC OXIDE SYNTHASE, INDUCIBLE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	189.22Å 189.22Å 232.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	146.83 – 3.16 39.50 – 3.16	Depositor EDS
% Data completeness (in resolution range)	99.5 (146.83-3.16) 99.5 (39.50-3.16)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.174 , 0.216 0.174 , 0.216	Depositor DCC
R_{free} test set	3675 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	81.0	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 37.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 72640 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13889	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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: S71, GOL, SO4, H4B, HEM

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	0.72	0/3465	0.97	6/4703 (0.1%)
1	B	0.71	1/3465 (0.0%)	0.98	9/4703 (0.2%)
1	C	0.61	0/3465	0.87	0/4703
1	D	0.71	0/3465	0.94	5/4703 (0.1%)
All	All	0.69	1/13860 (0.0%)	0.94	20/18812 (0.1%)

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	1
1	B	0	1
1	C	0	2
1	D	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	117	GLY	N-CA	5.37	1.54	1.46

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	116	LEU	CA-CB-CG	8.38	134.56	115.30
1	A	382	ASP	CB-CG-OD1	-8.36	110.78	118.30
1	D	163	LEU	CA-CB-CG	7.58	132.73	115.30
1	A	382	ASP	CB-CG-OD2	7.23	124.81	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	116	LEU	CA-CB-CG	6.51	130.26	115.30
1	B	250	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	D	406	LEU	CA-CB-CG	6.40	130.02	115.30
1	B	305	VAL	CG1-CB-CG2	6.33	121.03	110.90
1	B	266	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	A	87	ILE	CG1-CB-CG2	-6.14	97.89	111.40
1	B	266	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	B	398	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	B	163	LEU	CA-CB-CG	5.68	128.37	115.30
1	D	381	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	D	382	ASP	CB-CG-OD1	-5.49	113.36	118.30
1	A	398	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	D	296	LYS	CD-CE-NZ	5.22	123.71	111.70
1	B	116	LEU	CB-CG-CD1	5.15	119.75	111.00
1	A	140	LEU	CA-CB-CG	5.11	127.05	115.30
1	B	83	ARG	NE-CZ-NH1	5.03	122.82	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	284	VAL	Peptide
1	B	207	SER	Peptide
1	C	160	GLU	Peptide
1	C	284	VAL	Peptide
1	D	251	SER	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3367	0	3268	94	0
1	B	3367	0	3268	94	0
1	C	3367	0	3268	133	0
1	D	3367	0	3268	86	0
2	A	43	0	30	2	0
2	B	43	0	30	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	43	0	30	3	0
2	D	43	0	30	2	0
3	A	17	0	15	1	0
3	B	17	0	15	0	0
3	C	17	0	15	0	0
3	D	17	0	15	0	0
4	A	28	0	28	3	0
4	B	28	0	28	1	0
4	C	28	0	28	1	0
4	D	28	0	28	1	0
5	A	6	0	8	3	0
5	B	6	0	8	1	0
5	C	6	0	8	1	0
5	D	6	0	8	1	0
6	A	15	0	0	0	0
6	B	10	0	0	0	0
6	C	10	0	0	0	0
6	D	10	0	0	0	0
All	All	13889	0	13396	400	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 15.

All (400) 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:B:387:GLN:HE21	1:B:387:GLN:H	1.05	1.02
1:C:140:LEU:HD21	1:C:170:THR:HG22	1.42	1.00
1:C:130:ARG:HH21	1:C:134:THR:HG23	1.25	1.00
1:C:278:ARG:HG3	1:C:278:ARG:HH11	1.29	0.98
1:B:283:ASN:O	1:B:287:THR:HG23	1.66	0.95
1:C:387:GLN:HE21	1:C:387:GLN:H	1.01	0.93
1:C:130:ARG:HG2	1:C:130:ARG:HH11	1.33	0.92
1:C:130:ARG:NH2	1:C:134:THR:HG23	1.84	0.92
1:A:387:GLN:HE21	1:A:387:GLN:H	0.94	0.91
1:D:448:GLN:NE2	1:D:452:ARG:HH12	1.69	0.90
1:B:181:LEU:HD23	1:B:181:LEU:H	1.38	0.87
1:D:269:GLY:H	1:D:287:THR:HG21	1.39	0.87
1:D:181:LEU:HD23	1:D:181:LEU:H	1.39	0.86
1:A:387:GLN:NE2	1:A:387:GLN:H	1.74	0.85
1:C:236:ASN:HB3	1:C:239:ASN:O	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:ALA:HB3	1:C:314:ARG:HH12	1.40	0.85
1:C:387:GLN:NE2	1:C:387:GLN:H	1.74	0.85
1:B:269:GLY:H	1:B:287:THR:HG21	1.39	0.85
1:A:387:GLN:HE21	1:A:387:GLN:N	1.74	0.83
1:A:247:PHE:HB3	1:A:248:PRO:HD2	1.62	0.82
1:B:181:LEU:HD23	1:B:181:LEU:N	1.94	0.81
1:C:182:THR:O	1:C:184:ASP:N	2.13	0.80
1:C:278:ARG:CG	1:C:278:ARG:HH11	1.96	0.78
1:C:221:ARG:HB2	1:C:221:ARG:CZ	2.14	0.77
1:C:459:ALA:HB1	1:C:464:LEU:CD1	2.14	0.77
1:B:387:GLN:NE2	1:B:387:GLN:H	1.84	0.76
1:C:201:ILE:HG13	1:C:201:ILE:O	1.85	0.75
1:C:130:ARG:CG	1:C:130:ARG:HH11	1.99	0.75
1:A:160:GLU:CD	1:A:160:GLU:H	1.91	0.74
1:C:387:GLN:N	1:C:387:GLN:HE21	1.83	0.74
1:B:369:PHE:CD2	2:B:550:HEM:HAC	2.23	0.73
1:C:278:ARG:HG3	1:C:278:ARG:NH1	1.96	0.73
1:A:100:LEU:HD22	1:A:454:ARG:HD2	1.71	0.73
1:C:130:ARG:HH21	1:C:134:THR:CG2	1.99	0.72
1:A:84:HIS:HB2	1:A:97:GLN:NE2	2.04	0.72
1:D:181:LEU:HD23	1:D:181:LEU:N	2.05	0.72
1:C:322:PRO:HD2	1:C:325:LEU:HD12	1.71	0.72
1:C:459:ALA:HB1	1:C:464:LEU:HD11	1.70	0.72
1:A:270:TYR:HB2	1:A:272:MET:CE	2.20	0.72
1:C:173:ILE:O	1:C:177:GLY:HA2	1.90	0.72
1:D:448:GLN:HE22	1:D:452:ARG:HH12	1.36	0.72
1:C:266:ARG:HH22	5:C:880:GOL:H2	1.55	0.71
1:D:116:LEU:HD13	1:D:123:LYS:HE3	1.73	0.71
1:A:213:ASP:OD1	1:A:215:ARG:HG3	1.91	0.71
1:D:252:ASP:HB3	1:D:254:LYS:H	1.56	0.70
1:D:181:LEU:CD2	1:D:181:LEU:N	2.54	0.70
1:A:257:PHE:CE1	1:A:312:ASN:HB3	2.27	0.70
1:B:145:GLU:HA	1:B:145:GLU:OE1	1.91	0.69
1:B:187:ILE:HG12	1:B:211:VAL:HG21	1.74	0.69
1:B:129:PRO:HA	1:B:250:ARG:NH2	2.07	0.69
1:C:130:ARG:NH1	1:C:130:ARG:HG2	2.08	0.69
1:B:247:PHE:HB3	1:B:248:PRO:HD2	1.76	0.68
1:C:429:GLN:O	1:C:431:VAL:HG23	1.93	0.68
1:C:247:PHE:HB3	1:C:248:PRO:HD2	1.75	0.68
1:D:115:CYS:O	1:D:117:GLY:N	2.26	0.68
1:D:116:LEU:CD1	1:D:123:LYS:HE3	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:PRO:HA	1:C:250:ARG:HH22	1.59	0.68
1:D:181:LEU:CD2	1:D:181:LEU:H	2.07	0.67
1:B:266:ARG:NH2	1:B:388:ARG:NH2	2.42	0.67
1:B:181:LEU:CD2	1:B:181:LEU:N	2.58	0.67
1:A:122:PRO:HD2	1:A:125:LEU:HD12	1.76	0.67
1:B:380:VAL:HG11	1:B:467:PRO:HB2	1.75	0.67
1:B:398:ARG:CG	1:B:398:ARG:HH11	2.07	0.67
1:A:394:GLU:OE2	1:A:398:ARG:NH1	2.27	0.67
1:C:437:HIS:HB2	1:D:406:LEU:HD11	1.77	0.67
1:C:484:VAL:HG12	1:C:488:PHE:CE2	2.31	0.66
1:A:260:TRP:CZ2	1:A:316:PRO:HG3	2.30	0.66
1:D:412:ASP:O	1:D:416:VAL:HG23	1.96	0.66
1:B:115:CYS:O	1:B:117:GLY:N	2.29	0.66
1:C:182:THR:C	1:C:184:ASP:H	1.99	0.65
1:B:333:HIS:ND1	1:B:334:PRO:HD2	2.10	0.65
1:D:116:LEU:HD13	1:D:123:LYS:CE	2.26	0.65
1:C:129:PRO:HA	1:C:250:ARG:NH2	2.11	0.64
1:A:378:ILE:HA	1:A:382:ASP:HB2	1.77	0.64
1:B:307:LEU:HB3	1:B:309:LEU:HD13	1.79	0.64
1:A:180:GLN:NE2	1:A:180:GLN:HA	2.11	0.64
1:A:451:TYR:CE1	1:A:456:GLY:HA2	2.32	0.64
1:B:380:VAL:O	1:B:384:CYS:HB2	1.97	0.64
1:D:155:LYS:HG3	1:D:156:GLU:OE2	1.98	0.64
1:A:250:ARG:NH2	1:A:256:ASP:OD2	2.31	0.63
1:B:107:ILE:HD12	1:B:124:SER:O	1.98	0.63
1:B:451:TYR:CE1	1:B:456:GLY:HA2	2.33	0.63
1:B:281:PRO:O	1:B:284:VAL:HG23	1.99	0.63
1:A:140:LEU:HD21	1:A:170:THR:HG23	1.80	0.63
1:A:127:ARG:NH1	1:A:363:GLU:OE2	2.32	0.62
1:D:448:GLN:NE2	1:D:452:ARG:NH1	2.45	0.62
1:A:115:CYS:O	1:A:117:GLY:N	2.25	0.62
1:D:356:LEU:HD23	1:D:356:LEU:C	2.19	0.62
1:B:129:PRO:HA	1:B:250:ARG:HH22	1.62	0.62
4:A:800:S71:H271	5:A:880:GOL:H11	1.82	0.62
1:D:283:ASN:O	1:D:287:THR:HG23	2.00	0.61
1:C:327:LEU:HD12	1:C:328:GLU:H	1.64	0.61
1:C:244:ILE:HD11	1:C:367:CYS:HB2	1.82	0.61
1:B:357:LEU:HB3	1:B:364:PHE:HB2	1.83	0.61
1:C:140:LEU:CD2	1:C:170:THR:HG22	2.25	0.61
1:D:369:PHE:CD1	2:D:550:HEM:HAC	2.36	0.61
1:B:253:GLY:HA2	1:B:256:ASP:OD1	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:800:S71:H25	5:A:880:GOL:H11	1.84	0.60
1:C:263:GLN:HB3	1:C:351:ALA:O	2.00	0.60
1:A:328:GLU:OE1	1:A:345:LYS:HE2	2.00	0.60
1:C:184:ASP:HA	1:C:187:ILE:HD12	1.83	0.60
1:A:395:VAL:O	1:A:399:MET:HG3	2.02	0.60
1:C:193:ALA:HB2	1:C:487:PRO:HB2	1.83	0.60
1:D:308:VAL:HG22	1:D:318:LEU:HD22	1.84	0.59
1:D:116:LEU:HD13	1:D:123:LYS:HZ1	1.66	0.59
1:C:420:ILE:HG13	1:D:409:LEU:HD12	1.84	0.59
1:C:257:PHE:CE2	1:C:312:ASN:HB3	2.38	0.59
1:A:377:GLU:O	1:A:381:ARG:HB2	2.02	0.59
1:D:244:ILE:HD12	1:D:369:PHE:HB3	1.84	0.59
1:B:100:LEU:HB3	1:B:456:GLY:HA3	1.85	0.59
1:B:337:GLU:O	1:B:340:ARG:HG3	2.03	0.59
1:A:308:VAL:HG22	1:A:318:LEU:HD22	1.85	0.58
1:B:494:GLU:OE2	1:B:497:LYS:HE2	2.04	0.58
1:C:381:ARG:NH1	1:C:381:ARG:HG3	2.19	0.58
1:A:100:LEU:HB3	1:A:456:GLY:HA3	1.84	0.58
1:C:171:LYS:O	1:C:174:GLU:HB3	2.02	0.58
1:C:187:ILE:HA	1:C:211:VAL:HG21	1.85	0.57
1:A:84:HIS:HB2	1:A:97:GLN:HE21	1.67	0.57
1:D:387:GLN:H	1:D:387:GLN:NE2	2.01	0.57
1:A:156:GLU:O	1:A:157:ALA:CB	2.52	0.57
1:A:308:VAL:HG22	1:A:318:LEU:CD2	2.34	0.57
1:C:150:TYR:CE2	1:C:185:GLU:HA	2.39	0.57
1:C:324:ASP:N	1:C:324:ASP:OD1	2.37	0.57
1:C:309:LEU:O	1:C:316:PRO:HA	2.04	0.57
1:C:484:VAL:HG12	1:C:488:PHE:CZ	2.40	0.57
1:A:100:LEU:CD2	1:A:454:ARG:HD2	2.35	0.56
1:C:220:ALA:O	1:C:223:MET:HB2	2.04	0.56
1:A:155:LYS:HG3	1:A:156:GLU:H	1.69	0.56
1:B:369:PHE:CD2	2:B:550:HEM:CAC	2.88	0.56
1:C:437:HIS:CB	1:D:406:LEU:HD11	2.36	0.56
1:A:328:GLU:CD	1:A:345:LYS:HE2	2.26	0.56
1:C:327:LEU:HD12	1:C:328:GLU:N	2.21	0.56
1:A:383:PHE:HB3	1:A:391:ILE:HD13	1.88	0.56
1:C:333:HIS:NE2	1:C:417:GLU:OE1	2.37	0.56
1:C:119:ILE:HA	1:D:479:GLU:HG2	1.88	0.56
1:D:252:ASP:HB3	1:D:254:LYS:N	2.21	0.56
1:A:193:ALA:HB2	1:A:487:PRO:HB2	1.87	0.56
1:B:205:GLN:O	1:B:208:ASN:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:PHE:HB3	1:A:248:PRO:CD	2.34	0.55
1:B:116:LEU:HD12	1:B:124:SER:OG	2.06	0.55
1:C:182:THR:C	1:C:184:ASP:N	2.58	0.55
1:C:380:VAL:O	1:C:384:CYS:HB2	2.07	0.55
1:D:195:ARG:HD2	1:D:206:TRP:CE2	2.42	0.55
1:D:427:GLN:C	1:D:429:GLN:H	2.10	0.55
1:C:307:LEU:HB3	1:C:309:LEU:HD21	1.89	0.55
4:D:800:S71:H271	5:D:880:GOL:H12	1.87	0.55
1:C:326:VAL:CG1	1:C:326:VAL:O	2.55	0.55
1:A:410:TRP:CZ2	1:A:411:LYS:HG3	2.42	0.54
1:A:229:ARG:NH1	1:A:229:ARG:HB3	2.22	0.54
1:B:194:TRP:CE3	1:B:206:TRP:HA	2.43	0.54
1:A:398:ARG:CG	1:A:398:ARG:HH11	2.21	0.54
1:B:140:LEU:N	1:B:141:PRO:HD2	2.21	0.54
1:C:380:VAL:HG21	1:C:468:MET:HB3	1.90	0.54
1:D:87:ILE:HG21	1:D:481:LEU:HD13	1.90	0.54
1:B:282:ALA:HB1	5:B:880:GOL:H2	1.90	0.54
1:C:314:ARG:NH1	1:C:314:ARG:HB2	2.23	0.54
1:B:327:LEU:HD12	1:B:328:GLU:N	2.23	0.54
1:C:417:GLU:HA	1:C:420:ILE:HD12	1.89	0.54
1:C:498:THR:O	1:C:499:HIS:C	2.46	0.54
1:C:437:HIS:HB2	1:D:406:LEU:CD1	2.37	0.54
1:B:274:ASP:OD1	1:B:276:SER:OG	2.26	0.54
1:B:333:HIS:CE1	1:B:335:LYS:HB2	2.43	0.53
1:C:381:ARG:HG3	1:C:381:ARG:HH11	1.72	0.53
1:C:461:TRP:CE3	1:D:462:ILE:HD13	2.44	0.53
1:A:388:ARG:HG3	1:A:388:ARG:HH11	1.73	0.53
1:C:378:ILE:HA	1:C:382:ASP:HB2	1.90	0.53
1:B:398:ARG:HH11	1:B:398:ARG:HG2	1.72	0.53
1:B:259:VAL:HG12	1:B:261:ASN:HB2	1.90	0.53
1:A:463:TRP:HA	3:A:600:H4B:N1	2.23	0.53
1:B:314:ARG:HG2	1:B:502:GLN:HE22	1.74	0.53
1:A:215:ARG:O	1:A:248:PRO:HG3	2.08	0.53
1:A:255:HIS:HB3	1:A:312:ASN:HB2	1.91	0.52
1:A:388:ARG:HG3	1:A:388:ARG:NH1	2.24	0.52
1:D:194:TRP:CE3	1:D:206:TRP:HA	2.44	0.52
1:A:245:THR:O	1:A:367:CYS:HA	2.09	0.52
1:C:255:HIS:HB3	1:C:312:ASN:HB2	1.91	0.52
1:D:354:ASN:HD22	1:D:354:ASN:C	2.12	0.52
1:D:426:PHE:CG	1:D:433:ILE:HD12	2.44	0.52
1:D:374:MET:O	1:D:375:GLY:C	2.47	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:THR:HA	1:C:491:TYR:O	2.10	0.52
1:C:221:ARG:CB	1:C:221:ARG:CZ	2.86	0.52
1:C:412:ASP:O	1:C:415:VAL:HG12	2.10	0.52
1:C:461:TRP:CZ3	1:D:462:ILE:HG23	2.44	0.52
1:C:314:ARG:HH11	1:C:314:ARG:HB2	1.75	0.52
1:B:195:ARG:HD2	1:B:206:TRP:CE2	2.45	0.52
1:C:233:TYR:CE1	1:C:241:ARG:CZ	2.93	0.52
1:B:387:GLN:HE21	1:B:387:GLN:N	1.90	0.52
1:C:369:PHE:CD2	2:C:550:HEM:HAC	2.45	0.52
1:A:236:ASN:HB3	1:A:239:ASN:O	2.10	0.51
1:B:269:GLY:N	1:B:287:THR:HG21	2.18	0.51
1:C:87:ILE:HD12	1:C:479:GLU:HB3	1.91	0.51
1:D:101:HIS:C	1:D:103:LYS:H	2.14	0.51
1:C:311:ALA:HB3	1:C:314:ARG:NH1	2.18	0.51
1:B:200:CYS:HB2	2:B:550:HEM:ND	2.24	0.51
1:C:145:GLU:HA	1:C:145:GLU:OE1	2.11	0.51
1:C:472:ILE:O	1:C:472:ILE:HG22	2.11	0.51
1:A:472:ILE:O	1:A:472:ILE:HG22	2.11	0.51
1:C:115:CYS:O	1:C:117:GLY:N	2.44	0.51
1:C:305:VAL:HG22	1:C:306:PRO:HD2	1.92	0.51
1:D:116:LEU:HD13	1:D:123:LYS:NZ	2.26	0.51
1:A:356:LEU:HD23	1:A:356:LEU:C	2.31	0.51
1:A:270:TYR:HB2	1:A:272:MET:HE3	1.92	0.51
1:B:247:PHE:CB	1:B:248:PRO:HD2	2.37	0.51
1:B:380:VAL:HG23	1:B:419:ASN:HD21	1.77	0.50
1:A:92:SER:OG	1:A:94:MET:HB3	2.12	0.50
1:B:122:PRO:HG2	1:B:125:LEU:HD22	1.93	0.50
1:B:266:ARG:HH22	1:B:388:ARG:NH2	2.08	0.50
1:D:289:LEU:HD23	1:D:293:LEU:HD12	1.94	0.50
1:D:289:LEU:HD21	1:D:293:LEU:HD11	1.93	0.50
1:A:380:VAL:HG23	1:A:419:ASN:HD21	1.75	0.50
1:A:229:ARG:HB3	1:A:229:ARG:HH11	1.77	0.50
1:A:88:LYS:HD3	1:A:90:TRP:CE2	2.47	0.50
1:D:377:GLU:O	1:D:381:ARG:HB2	2.12	0.50
1:C:225:GLU:O	1:C:229:ARG:HG3	2.11	0.50
1:A:462:ILE:HG23	1:B:461:TRP:CZ3	2.47	0.50
1:A:429:GLN:O	1:A:431:VAL:HG23	2.12	0.50
1:B:309:LEU:O	1:B:316:PRO:HA	2.12	0.49
1:C:247:PHE:HB3	1:C:248:PRO:CD	2.40	0.49
1:A:180:GLN:NE2	1:A:180:GLN:CA	2.72	0.49
1:D:354:ASN:C	1:D:354:ASN:ND2	2.65	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ASN:HB2	1:A:478:GLN:OE1	2.12	0.49
1:A:380:VAL:CG2	1:A:419:ASN:HD21	2.26	0.49
1:D:342:LEU:HB3	1:D:344:LEU:HG	1.94	0.49
1:B:385:ASP:HB3	1:B:387:GLN:NE2	2.28	0.49
1:B:244:ILE:HD12	1:B:369:PHE:HB3	1.94	0.49
1:A:195:ARG:HD2	1:A:206:TRP:CE2	2.47	0.49
1:A:180:GLN:HE21	1:A:180:GLN:CA	2.26	0.49
1:C:150:TYR:CE1	1:C:154:PHE:HE2	2.30	0.49
1:B:390:ASN:HD22	1:B:390:ASN:C	2.15	0.49
1:B:308:VAL:HG22	1:B:318:LEU:CD2	2.43	0.49
1:B:204:ILE:HG21	1:B:442:SER:OG	2.13	0.49
1:C:277:ILE:HG21	1:C:281:PRO:HB3	1.93	0.49
1:B:338:TRP:O	1:B:341:GLU:HB2	2.13	0.48
1:D:154:PHE:CD2	1:D:158:LYS:HD2	2.47	0.48
1:A:210:GLN:HA	1:A:210:GLN:NE2	2.28	0.48
1:B:304:VAL:HG21	1:B:326:VAL:HG11	1.94	0.48
1:A:333:HIS:CE1	1:A:334:PRO:HD2	2.48	0.48
1:A:471:SER:HB3	1:B:467:PRO:HB3	1.94	0.48
1:A:156:GLU:O	1:A:157:ALA:HB3	2.13	0.48
1:C:369:PHE:CD2	2:C:550:HEM:CAC	2.97	0.48
1:C:399:MET:O	1:C:401:LEU:HD23	2.14	0.48
2:B:550:HEM:O1A	4:B:800:S71:N19	2.47	0.48
1:D:208:ASN:HD22	1:D:208:ASN:C	2.17	0.48
1:A:187:ILE:HG22	1:A:191:LYS:HD2	1.95	0.48
1:C:223:MET:HG2	1:C:247:PHE:CZ	2.49	0.48
1:A:184:ASP:HA	1:A:187:ILE:HD12	1.96	0.48
1:C:245:THR:O	1:C:367:CYS:HA	2.13	0.47
1:D:123:LYS:HE2	1:D:124:SER:H	1.78	0.47
1:A:195:ARG:HD2	1:A:206:TRP:CZ2	2.48	0.47
1:C:191:LYS:HE2	1:C:207:SER:O	2.14	0.47
1:A:471:SER:HA	1:A:476:PHE:CG	2.49	0.47
1:A:315:ASP:OD2	1:A:501:TRP:HE3	1.96	0.47
1:C:326:VAL:O	1:C:326:VAL:HG12	2.14	0.47
1:B:308:VAL:HG22	1:B:318:LEU:HD22	1.95	0.47
1:B:159:ILE:H	1:B:159:ILE:HG12	1.44	0.47
1:C:244:ILE:HG13	1:C:368:PRO:O	2.14	0.47
1:B:205:GLN:HG3	2:B:550:HEM:CBB	2.44	0.47
1:A:388:ARG:HD2	1:A:388:ARG:HA	1.70	0.47
1:D:296:LYS:HE3	1:D:297:PRO:O	2.14	0.47
1:B:187:ILE:HG12	1:B:211:VAL:CG2	2.42	0.47
1:D:212:PHE:HB2	1:D:245:THR:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:GLU:CD	1:C:156:GLU:N	2.68	0.47
1:C:307:LEU:O	1:C:318:LEU:HA	2.15	0.46
1:D:85:VAL:HG11	1:D:481:LEU:HD21	1.98	0.46
1:D:465:VAL:HA	1:D:466:PRO:HD3	1.76	0.46
1:C:249:GLN:HG2	1:C:249:GLN:H	1.59	0.46
1:A:194:TRP:CZ3	1:A:206:TRP:HA	2.50	0.46
1:C:161:GLU:O	1:C:165:ARG:N	2.47	0.46
1:C:314:ARG:HH11	1:C:314:ARG:CB	2.28	0.46
1:B:333:HIS:CG	1:B:334:PRO:HD2	2.50	0.46
1:A:423:LEU:HD12	1:A:433:ILE:CG2	2.46	0.46
1:B:472:ILE:HG22	1:B:472:ILE:O	2.14	0.46
1:D:206:TRP:C	1:D:208:ASN:H	2.18	0.46
1:C:472:ILE:HD11	1:D:415:VAL:HG21	1.98	0.46
1:C:145:GLU:O	1:C:148:ASN:HB2	2.16	0.46
1:C:281:PRO:HD2	1:C:388:ARG:HA	1.98	0.46
1:D:272:MET:HB3	1:D:273:PRO:CD	2.47	0.45
1:C:380:VAL:N	1:C:419:ASN:HD21	2.15	0.45
1:B:193:ALA:HB2	1:B:487:PRO:HB2	1.97	0.45
1:C:173:ILE:O	1:C:177:GLY:CA	2.61	0.45
1:A:260:TRP:CE2	1:A:316:PRO:HG3	2.51	0.45
1:A:229:ARG:CB	1:A:229:ARG:HH11	2.30	0.45
1:B:337:GLU:O	1:B:339:PHE:N	2.49	0.45
1:C:448:GLN:HE21	1:C:448:GLN:HB3	1.37	0.45
1:C:380:VAL:HG11	1:C:467:PRO:HB2	1.99	0.45
1:B:390:ASN:ND2	1:B:390:ASN:C	2.68	0.45
1:C:156:GLU:H	1:C:156:GLU:CD	2.19	0.45
1:C:101:HIS:NE2	1:C:102:HIS:HD2	2.15	0.45
1:B:242:SER:HB3	1:B:371:GLY:HA2	1.98	0.45
1:C:313:GLY:O	1:C:314:ARG:O	2.35	0.44
1:D:385:ASP:HB3	1:D:387:GLN:OE1	2.17	0.44
1:B:199:ARG:HD3	1:B:463:TRP:CD2	2.52	0.44
1:A:401:LEU:O	1:A:403:THR:HG23	2.17	0.44
1:C:224:PHE:CD1	1:C:319:PHE:HB2	2.52	0.44
1:C:283:ASN:OD1	1:C:286:PHE:HB3	2.18	0.44
1:C:120:MET:HG2	4:C:800:S71:H273	1.99	0.44
1:B:233:TYR:O	1:B:236:ASN:HB2	2.17	0.44
1:C:469:SER:H	1:D:469:SER:H	1.66	0.44
1:D:170:THR:O	1:D:174:GLU:HG2	2.17	0.44
1:A:84:HIS:ND1	1:A:84:HIS:N	2.66	0.44
1:A:465:VAL:HG22	1:A:475:VAL:HG23	2.00	0.44
1:B:356:LEU:HD23	1:B:356:LEU:C	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:ARG:HD3	1:C:132:LYS:O	2.18	0.44
1:A:194:TRP:CE3	1:A:206:TRP:HA	2.53	0.44
1:B:434:MET:HE2	1:B:434:MET:HB2	1.74	0.44
1:C:140:LEU:HD21	1:C:170:THR:CG2	2.30	0.44
1:B:244:ILE:HD11	1:B:367:CYS:HB2	1.99	0.44
1:B:192:GLN:NE2	1:B:192:GLN:HA	2.32	0.44
1:D:378:ILE:HA	1:D:382:ASP:HB2	1.99	0.44
1:B:388:ARG:HD2	1:B:388:ARG:HA	1.81	0.43
1:C:163:LEU:HA	1:C:166:VAL:HG12	1.99	0.43
1:B:245:THR:O	1:B:367:CYS:HA	2.18	0.43
1:D:247:PHE:HB3	1:D:248:PRO:HD2	2.00	0.43
1:C:402:GLU:OE2	1:C:405:LYS:HD3	2.19	0.43
1:B:266:ARG:NH2	1:B:388:ARG:HH22	2.16	0.43
1:D:315:ASP:H	1:D:502:GLN:NE2	2.17	0.43
1:C:195:ARG:HD2	1:C:206:TRP:CE2	2.53	0.43
1:A:423:LEU:HD12	1:A:433:ILE:HG21	1.99	0.43
1:B:237:ASN:HD22	1:B:237:ASN:HA	1.60	0.43
1:B:354:ASN:HD22	1:B:354:ASN:N	2.15	0.43
1:A:127:ARG:HB2	1:A:356:LEU:HD13	2.00	0.43
1:D:307:LEU:HB3	1:D:309:LEU:HD13	2.01	0.43
1:A:163:LEU:O	1:A:166:VAL:HG12	2.18	0.43
1:D:494:GLU:HG3	1:D:497:LYS:HE3	2.00	0.43
1:A:176:THR:OG1	1:A:178:THR:O	2.36	0.43
1:C:335:LYS:HE3	1:C:335:LYS:HB3	1.61	0.43
1:B:329:VAL:HA	1:B:429:GLN:OE1	2.19	0.43
1:C:433:ILE:HD13	1:C:434:MET:H	1.84	0.43
1:D:270:TYR:HE2	1:D:300:GLY:H	1.65	0.43
1:D:451:TYR:CE1	1:D:456:GLY:HA2	2.53	0.43
1:A:437:HIS:CB	1:B:406:LEU:HD22	2.49	0.43
1:C:485:LEU:O	1:C:488:PHE:HB2	2.18	0.42
1:D:316:PRO:HD2	1:D:501:TRP:HZ3	1.84	0.42
1:C:412:ASP:OD2	1:D:469:SER:HB2	2.19	0.42
1:B:194:TRP:CZ3	1:B:206:TRP:HA	2.54	0.42
1:D:142:GLN:HE21	1:D:142:GLN:HB3	1.54	0.42
1:C:465:VAL:HA	1:C:466:PRO:HD3	1.84	0.42
1:C:221:ARG:NH1	1:C:221:ARG:CB	2.83	0.42
1:A:200:CYS:HB2	2:A:550:HEM:ND	2.35	0.42
1:C:85:VAL:HG11	1:C:481:LEU:HD11	2.02	0.42
1:D:333:HIS:CE1	1:D:335:LYS:HB2	2.54	0.42
1:B:256:ASP:HB3	1:B:258:ARG:HD3	2.01	0.42
1:C:307:LEU:HB3	1:C:309:LEU:CD2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:GLU:H	1:B:156:GLU:CD	2.23	0.42
1:C:194:TRP:O	1:C:203:ARG:HD3	2.19	0.42
1:A:398:ARG:HG3	1:A:398:ARG:HH11	1.83	0.42
1:D:194:TRP:CZ3	1:D:206:TRP:HA	2.54	0.42
1:D:448:GLN:HE22	1:D:452:ARG:NH1	2.07	0.41
1:C:154:PHE:O	1:C:155:LYS:C	2.58	0.41
1:D:123:LYS:N	1:D:123:LYS:HE2	2.34	0.41
1:D:187:ILE:CG2	1:D:191:LYS:HE2	2.50	0.41
1:A:142:GLN:HB3	1:A:142:GLN:HE21	1.52	0.41
1:D:471:SER:HA	1:D:476:PHE:CG	2.54	0.41
1:B:410:TRP:CG	1:B:411:LYS:N	2.88	0.41
1:B:100:LEU:CB	1:B:456:GLY:HA3	2.49	0.41
1:A:307:LEU:O	1:A:318:LEU:HA	2.19	0.41
1:D:85:VAL:CG1	1:D:481:LEU:HD21	2.50	0.41
1:C:87:ILE:HA	1:C:87:ILE:HD13	1.53	0.41
1:D:337:GLU:O	1:D:339:PHE:N	2.53	0.41
1:D:386:VAL:HG23	1:D:387:GLN:NE2	2.34	0.41
1:C:199:ARG:HG2	1:C:463:TRP:CG	2.55	0.41
1:A:374:MET:O	1:A:375:GLY:C	2.59	0.41
1:C:249:GLN:HB2	1:C:250:ARG:H	1.62	0.41
1:D:130:ARG:O	1:D:131:ASP:HB3	2.20	0.41
1:B:268:ALA:HA	1:B:287:THR:HG21	2.02	0.41
1:D:369:PHE:CG	2:D:550:HEM:HAC	2.55	0.41
1:C:346:TRP:CD1	1:C:378:ILE:HG12	2.55	0.41
1:A:406:LEU:HA	1:A:406:LEU:HD12	1.92	0.41
1:C:186:LEU:O	1:C:187:ILE:C	2.59	0.41
1:B:259:VAL:CG1	1:B:261:ASN:HB2	2.50	0.41
1:D:426:PHE:CD2	1:D:433:ILE:HD12	2.55	0.41
1:A:371:GLY:CA	2:A:550:HEM:HAB	2.50	0.41
2:C:550:HEM:HBC2	2:C:550:HEM:CMC	2.51	0.41
1:B:204:ILE:O	1:B:204:ILE:HG13	2.18	0.41
1:D:296:LYS:HG2	1:D:297:PRO:HD2	2.03	0.41
1:A:163:LEU:HD23	1:A:163:LEU:HA	1.83	0.41
1:D:193:ALA:HB2	1:D:487:PRO:HB2	2.01	0.41
1:A:409:LEU:HA	1:A:409:LEU:HD23	1.80	0.41
1:A:107:ILE:H	1:A:107:ILE:HG13	1.70	0.41
1:D:116:LEU:HD11	1:D:123:LYS:HE3	2.01	0.41
1:D:155:LYS:H	1:D:155:LYS:HG2	1.57	0.41
1:C:83:ARG:HH11	1:C:83:ARG:HB2	1.85	0.41
1:C:413:GLN:HE21	1:C:413:GLN:HB2	1.42	0.41
1:A:235:THR:O	1:A:236:ASN:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:ILE:HD13	1:C:284:VAL:HG21	2.03	0.40
1:C:446:TYR:CZ	1:C:450:GLU:HG3	2.56	0.40
1:C:270:TYR:HB2	1:C:272:MET:CE	2.52	0.40
1:C:135:PRO:O	1:C:136:PRO:C	2.57	0.40
1:D:315:ASP:OD1	1:D:502:GLN:HG3	2.21	0.40
1:B:201:ILE:HG13	1:B:443:PHE:HB2	2.02	0.40
1:B:96:PHE:CD2	1:B:451:TYR:CG	3.10	0.40
4:A:800:S71:H25	5:A:880:GOL:C1	2.50	0.40
1:C:281:PRO:O	1:C:284:VAL:HG23	2.22	0.40
1:B:266:ARG:HG2	1:B:283:ASN:ND2	2.36	0.40
1:D:461:TRP:CE2	1:D:465:VAL:HG21	2.57	0.40
1:A:426:PHE:CG	1:A:433:ILE:HG13	2.57	0.40
1:D:493:VAL:O	1:D:494:GLU:C	2.59	0.40
1:A:105:LYS:NZ	1:A:486:SER:HB2	2.36	0.40
1:B:103:LYS:HD3	1:B:103:LYS:HA	1.63	0.40
1:B:412:ASP:O	1:B:416:VAL:HG23	2.21	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	410/431 (95%)	368 (90%)	32 (8%)	10 (2%)	7 41
1	B	410/431 (95%)	367 (90%)	35 (8%)	8 (2%)	9 46
1	C	410/431 (95%)	351 (86%)	47 (12%)	12 (3%)	6 35
1	D	410/431 (95%)	351 (86%)	49 (12%)	10 (2%)	7 41
All	All	1640/1724 (95%)	1437 (88%)	163 (10%)	40 (2%)	7 41

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	LEU
1	A	156	GLU
1	A	157	ALA
1	A	285	GLU
1	A	312	ASN
1	B	116	LEU
1	C	116	LEU
1	C	217	CYS
1	C	249	GLN
1	C	285	GLU
1	C	312	ASN
1	D	116	LEU
1	D	249	GLN
1	D	252	ASP
1	D	375	GLY
1	A	117	GLY
1	A	137	ASP
1	A	375	GLY
1	B	106	GLY
1	B	203	ARG
1	B	206	TRP
1	B	314	ARG
1	C	117	GLY
1	C	155	LYS
1	C	183	GLY
1	C	314	ARG
1	C	430	ASN
1	D	117	GLY
1	D	131	ASP
1	D	282	ALA
1	B	354	ASN
1	C	499	HIS
1	D	360	GLY
1	B	375	GLY
1	D	155	LYS
1	A	136	PRO
1	B	117	GLY
1	D	501	TRP
1	C	360	GLY
1	A	248	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	359/376 (96%)	314 (88%)	45 (12%)	6 25
1	B	359/376 (96%)	296 (82%)	63 (18%)	2 11
1	C	359/376 (96%)	302 (84%)	57 (16%)	3 14
1	D	359/376 (96%)	303 (84%)	56 (16%)	3 14
All	All	1436/1504 (96%)	1215 (85%)	221 (15%)	3 15

All (221) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ARG
1	A	84	HIS
1	A	87	ILE
1	A	107	ILE
1	A	130	ARG
1	A	132	LYS
1	A	134	THR
1	A	137	ASP
1	A	153	SER
1	A	159	ILE
1	A	160	GLU
1	A	166	VAL
1	A	170	THR
1	A	207	SER
1	A	219	THR
1	A	221	ARG
1	A	245	THR
1	A	255	HIS
1	A	258	ARG
1	A	271	GLN
1	A	289	LEU
1	A	296	LYS
1	A	307	LEU
1	A	315	ASP

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Mol	Chain	Res	Type
1	A	324	ASP
1	A	337	GLU
1	A	340	ARG
1	A	345	LYS
1	A	387	GLN
1	A	390	ASN
1	A	391	ILE
1	A	394	GLU
1	A	398	ARG
1	A	401	LEU
1	A	405	LYS
1	A	423	LEU
1	A	427	GLN
1	A	433	ILE
1	A	445	LYS
1	A	452	ARG
1	A	471	SER
1	A	482	ASN
1	A	494	GLU
1	A	500	VAL
1	A	502	GLN
1	B	83	ARG
1	B	103	LYS
1	B	124	SER
1	B	125	LEU
1	B	127	ARG
1	B	130	ARG
1	B	134	THR
1	B	140	LEU
1	B	145	GLU
1	B	153	SER
1	B	155	LYS
1	B	156	GLU
1	B	159	ILE
1	B	161	GLU
1	B	163	LEU
1	B	167	GLU
1	B	174	GLU
1	B	181	LEU
1	B	195	ARG
1	B	204	ILE
1	B	208	ASN

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Mol	Chain	Res	Type
1	B	211	VAL
1	B	218	SER
1	B	225	GLU
1	B	229	ARG
1	B	237	ASN
1	B	242	SER
1	B	244	ILE
1	B	249	GLN
1	B	256	ASP
1	B	258	ARG
1	B	278	ARG
1	B	285	GLU
1	B	287	THR
1	B	289	LEU
1	B	290	CYS
1	B	305	VAL
1	B	307	LEU
1	B	312	ASN
1	B	324	ASP
1	B	325	LEU
1	B	337	GLU
1	B	340	ARG
1	B	342	LEU
1	B	345	LYS
1	B	354	ASN
1	B	377	GLU
1	B	386	VAL
1	B	387	GLN
1	B	390	ASN
1	B	393	GLU
1	B	394	GLU
1	B	398	ARG
1	B	413	GLN
1	B	427	GLN
1	B	471	SER
1	B	480	MET
1	B	481	LEU
1	B	482	ASN
1	B	494	GLU
1	B	497	LYS
1	B	500	VAL
1	B	502	GLN

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Mol	Chain	Res	Type
1	C	83	ARG
1	C	84	HIS
1	C	87	ILE
1	C	103	LYS
1	C	121	THR
1	C	123	LYS
1	C	124	SER
1	C	125	LEU
1	C	130	ARG
1	C	134	THR
1	C	154	PHE
1	C	155	LYS
1	C	156	GLU
1	C	159	ILE
1	C	175	THR
1	C	195	ARG
1	C	201	ILE
1	C	219	THR
1	C	221	ARG
1	C	229	ARG
1	C	237	ASN
1	C	242	SER
1	C	271	GLN
1	C	278	ARG
1	C	281	PRO
1	C	289	LEU
1	C	296	LYS
1	C	305	VAL
1	C	307	LEU
1	C	318	LEU
1	C	320	GLU
1	C	324	ASP
1	C	326	VAL
1	C	340	ARG
1	C	349	LEU
1	C	373	TYR
1	C	386	VAL
1	C	387	GLN
1	C	398	ARG
1	C	403	THR
1	C	405	LYS
1	C	413	GLN

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Mol	Chain	Res	Type
1	C	423	LEU
1	C	427	GLN
1	C	428	LYS
1	C	433	ILE
1	C	434	MET
1	C	445	LYS
1	C	448	GLN
1	C	452	ARG
1	C	471	SER
1	C	475	VAL
1	C	482	ASN
1	C	492	GLN
1	C	494	GLU
1	C	497	LYS
1	C	500	VAL
1	D	84	HIS
1	D	102	HIS
1	D	116	LEU
1	D	123	LYS
1	D	127	ARG
1	D	130	ARG
1	D	132	LYS
1	D	134	THR
1	D	140	LEU
1	D	153	SER
1	D	155	LYS
1	D	156	GLU
1	D	181	LEU
1	D	184	ASP
1	D	195	ARG
1	D	208	ASN
1	D	219	THR
1	D	221	ARG
1	D	222	GLU
1	D	242	SER
1	D	249	GLN
1	D	252	ASP
1	D	255	HIS
1	D	258	ARG
1	D	271	GLN
1	D	278	ARG
1	D	285	GLU

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Mol	Chain	Res	Type
1	D	296	LYS
1	D	307	LEU
1	D	309	LEU
1	D	310	GLN
1	D	320	GLU
1	D	337	GLU
1	D	342	LEU
1	D	354	ASN
1	D	373	TYR
1	D	386	VAL
1	D	387	GLN
1	D	390	ASN
1	D	393	GLU
1	D	394	GLU
1	D	398	ARG
1	D	415	VAL
1	D	427	GLN
1	D	441	GLU
1	D	448	GLN
1	D	449	ASN
1	D	462	ILE
1	D	471	SER
1	D	481	LEU
1	D	482	ASN
1	D	494	GLU
1	D	497	LYS
1	D	498	THR
1	D	500	VAL
1	D	502	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	GLN
1	A	142	GLN
1	A	180	GLN
1	A	192	GLN
1	A	205	GLN
1	A	210	GLN
1	A	226	HIS
1	A	237	ASN
1	A	271	GLN

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Mol	Chain	Res	Type
1	A	387	GLN
1	A	390	ASN
1	A	419	ASN
1	A	482	ASN
1	B	192	GLN
1	B	208	ASN
1	B	237	ASN
1	B	271	GLN
1	B	312	ASN
1	B	354	ASN
1	B	387	GLN
1	B	390	ASN
1	B	419	ASN
1	B	424	HIS
1	B	427	GLN
1	B	482	ASN
1	B	492	GLN
1	C	89	ASN
1	C	97	GLN
1	C	102	HIS
1	C	148	ASN
1	C	162	HIS
1	C	205	GLN
1	C	210	GLN
1	C	239	ASN
1	C	249	GLN
1	C	271	GLN
1	C	387	GLN
1	C	390	ASN
1	C	413	GLN
1	C	419	ASN
1	C	448	GLN
1	C	482	ASN
1	D	142	GLN
1	D	192	GLN
1	D	205	GLN
1	D	208	ASN
1	D	237	ASN
1	D	249	GLN
1	D	271	GLN
1	D	312	ASN
1	D	354	ASN

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Mol	Chain	Res	Type
1	D	387	GLN
1	D	390	ASN
1	D	419	ASN
1	D	448	GLN
1	D	449	ASN
1	D	482	ASN
1	D	502	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

25 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	HEM	A	550	1	30,50,50	2.08	6 (20%)	24,82,82	2.64	13 (54%)
3	H4B	A	600	-	13,18,18	0.80	0	11,26,26	2.06	2 (18%)
4	S71	A	800	-	30,30,30	0.72	1 (3%)	37,41,41	1.89	14 (37%)
5	GOL	A	880	-	5,5,5	0.40	0	5,5,5	1.08	0
6	SO4	A	910	-	4,4,4	0.73	0	6,6,6	0.39	0
6	SO4	A	920	-	4,4,4	0.62	0	6,6,6	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	SO4	A	930	-	4,4,4	0.55	0	6,6,6	1.23	1 (16%)
2	HEM	B	550	1	30,50,50	2.11	8 (26%)	24,82,82	2.68	12 (50%)
3	H4B	B	600	-	13,18,18	0.96	1 (7%)	11,26,26	2.58	3 (27%)
4	S71	B	800	-	30,30,30	1.13	2 (6%)	37,41,41	2.12	14 (37%)
5	GOL	B	880	-	5,5,5	0.48	0	5,5,5	0.24	0
6	SO4	B	910	-	4,4,4	0.57	0	6,6,6	0.49	0
6	SO4	B	920	-	4,4,4	0.62	0	6,6,6	0.46	0
2	HEM	C	550	1	30,50,50	2.18	7 (23%)	24,82,82	2.45	13 (54%)
3	H4B	C	600	-	13,18,18	0.95	1 (7%)	11,26,26	2.32	5 (45%)
4	S71	C	800	-	30,30,30	1.00	2 (6%)	37,41,41	2.02	13 (35%)
5	GOL	C	880	-	5,5,5	0.38	0	5,5,5	0.33	0
6	SO4	C	910	-	4,4,4	0.50	0	6,6,6	0.21	0
6	SO4	C	920	-	4,4,4	0.47	0	6,6,6	0.27	0
2	HEM	D	550	1	30,50,50	2.18	6 (20%)	24,82,82	2.42	11 (45%)
3	H4B	D	600	-	13,18,18	0.85	0	11,26,26	2.43	4 (36%)
4	S71	D	800	-	30,30,30	0.92	1 (3%)	37,41,41	2.33	15 (40%)
5	GOL	D	880	-	5,5,5	0.34	0	5,5,5	0.33	0
6	SO4	D	910	-	4,4,4	0.57	0	6,6,6	0.21	0
6	SO4	D	920	-	4,4,4	0.58	0	6,6,6	0.60	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	HEM	A	550	1	-	0/10/54/54	0/0/8/8
3	H4B	A	600	-	-	0/8/17/17	0/2/2/2
4	S71	A	800	-	-	0/15/15/15	0/3/3/3
5	GOL	A	880	-	-	0/4/4/4	0/0/0/0
6	SO4	A	910	-	-	0/0/0/0	0/0/0/0
6	SO4	A	920	-	-	0/0/0/0	0/0/0/0
6	SO4	A	930	-	-	0/0/0/0	0/0/0/0
2	HEM	B	550	1	-	0/10/54/54	0/0/8/8
3	H4B	B	600	-	-	0/8/17/17	0/2/2/2
4	S71	B	800	-	-	0/15/15/15	0/3/3/3
5	GOL	B	880	-	-	0/4/4/4	0/0/0/0
6	SO4	B	910	-	-	0/0/0/0	0/0/0/0
6	SO4	B	920	-	-	0/0/0/0	0/0/0/0
2	HEM	C	550	1	-	0/10/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	H4B	C	600	-	-	0/8/17/17	0/2/2/2
4	S71	C	800	-	-	0/15/15/15	0/3/3/3
5	GOL	C	880	-	-	0/4/4/4	0/0/0/0
6	SO4	C	910	-	-	0/0/0/0	0/0/0/0
6	SO4	C	920	-	-	0/0/0/0	0/0/0/0
2	HEM	D	550	1	-	0/10/54/54	0/0/8/8
3	H4B	D	600	-	-	0/8/17/17	0/2/2/2
4	S71	D	800	-	-	0/15/15/15	0/3/3/3
5	GOL	D	880	-	-	0/4/4/4	0/0/0/0
6	SO4	D	910	-	-	0/0/0/0	0/0/0/0
6	SO4	D	920	-	-	0/0/0/0	0/0/0/0

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	550	HEM	C2D-C3D	-6.86	1.33	1.54
2	A	550	HEM	C2C-C1C	-6.82	1.39	1.52
2	D	550	HEM	C2D-C3D	-6.80	1.34	1.54
2	A	550	HEM	C2D-C3D	-6.44	1.35	1.54
2	D	550	HEM	C2C-C1C	-6.37	1.40	1.52
2	C	550	HEM	C2D-C3D	-6.32	1.35	1.54
2	B	550	HEM	C2C-C1C	-5.90	1.41	1.52
2	C	550	HEM	C2C-C1C	-5.83	1.41	1.52
2	C	550	HEM	C3B-C4B	-3.97	1.48	1.51
2	D	550	HEM	C3B-C4B	-3.65	1.48	1.51
2	B	550	HEM	C3B-C4B	-3.19	1.49	1.51
2	C	550	HEM	C3D-C4D	-3.17	1.47	1.51
4	B	800	S71	C20-C17	-2.97	1.51	1.54
2	C	550	HEM	C2B-C1B	-2.75	1.42	1.51
2	B	550	HEM	C3C-CAC	-2.60	1.46	1.51
2	A	550	HEM	C2B-C1B	-2.43	1.43	1.51
2	A	550	HEM	C3B-C4B	-2.35	1.49	1.51
2	B	550	HEM	C2B-C1B	-2.19	1.44	1.51
2	D	550	HEM	C2B-C1B	-2.19	1.44	1.51
2	B	550	HEM	C3D-C4D	-2.16	1.48	1.51
4	A	800	S71	C20-C17	-2.08	1.52	1.54
4	D	800	S71	C16-C15	2.05	1.41	1.38
3	B	600	H4B	C4-N3	2.05	1.36	1.33
2	B	550	HEM	FE-NB	2.05	2.08	1.97
2	A	550	HEM	FE-NB	2.22	2.09	1.97
2	C	550	HEM	FE-NB	2.32	2.09	1.97
4	C	800	S71	C16-C15	2.33	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	600	H4B	C4-N3	2.38	1.37	1.33
4	C	800	S71	C12-C13	2.39	1.42	1.38
2	A	550	HEM	FE-NC	2.40	2.05	1.95
2	B	550	HEM	FE-NC	2.81	2.06	1.95
2	D	550	HEM	FE-NB	2.83	2.12	1.97
2	D	550	HEM	FE-NC	2.93	2.07	1.95
2	C	550	HEM	FE-NC	3.24	2.08	1.95
4	B	800	S71	C22-N21	3.31	1.41	1.35

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	550	HEM	CBA-CAA-C2A	-5.58	102.53	112.53
2	B	550	HEM	C3C-CAC-CBC	-4.61	117.39	124.46
4	D	800	S71	C04-C05-C06	-4.45	117.49	120.28
2	A	550	HEM	CBD-CAD-C3D	-4.21	101.30	113.55
4	B	800	S71	C04-C05-C06	-4.17	117.67	120.28
2	D	550	HEM	C1D-CHD-C4C	-4.17	118.86	125.82
4	D	800	S71	C14-C15-C17	-3.94	115.11	120.89
4	B	800	S71	C25-C26-N21	-3.77	118.71	122.96
4	C	800	S71	C14-C15-C17	-3.74	115.40	120.89
2	D	550	HEM	C3C-CAC-CBC	-3.73	118.73	124.46
2	A	550	HEM	C3C-CAC-CBC	-3.73	118.74	124.46
4	D	800	S71	C25-C26-N21	-3.46	119.06	122.96
4	A	800	S71	C14-C15-C17	-3.42	115.86	120.89
2	C	550	HEM	C3B-CAB-CBB	-3.23	119.50	124.46
2	A	550	HEM	CMA-C3A-C4A	-3.16	123.13	128.36
2	C	550	HEM	CBD-CAD-C3D	-3.08	104.59	113.55
2	A	550	HEM	C1D-CHD-C4C	-3.08	120.68	125.82
3	C	600	H4B	N3-C2-N1	-3.02	120.58	125.53
2	B	550	HEM	C1D-CHD-C4C	-2.94	120.91	125.82
4	A	800	S71	C27-C24-C25	-2.91	116.53	120.95
4	D	800	S71	C09-C13-C14	-2.90	115.69	120.56
2	D	550	HEM	CBA-CAA-C2A	-2.87	107.38	112.53
4	A	800	S71	C15-C16-N11	-2.87	119.65	124.27
2	C	550	HEM	C1D-CHD-C4C	-2.84	121.07	125.82
4	D	800	S71	C15-C16-N11	-2.83	119.70	124.27
4	C	800	S71	C05-C06-N01	-2.80	119.80	122.96
2	A	550	HEM	CAA-C2A-C1A	-2.76	124.01	127.01
4	B	800	S71	C23-C22-N22	-2.71	113.42	121.56
2	B	550	HEM	CBD-CAD-C3D	-2.69	105.73	113.55
4	B	800	S71	C08-C09-C13	-2.69	104.42	113.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	800	S71	C09-C13-C14	-2.67	116.08	120.56
4	A	800	S71	C13-C12-N11	-2.60	118.81	123.66
2	A	550	HEM	CBA-CAA-C2A	-2.56	107.93	112.53
4	B	800	S71	C13-C12-N11	-2.52	118.95	123.66
4	A	800	S71	C04-C05-C06	-2.46	118.74	120.28
2	C	550	HEM	CMA-C3A-C4A	-2.36	124.46	128.36
4	C	800	S71	C15-C16-N11	-2.33	120.52	124.27
4	A	800	S71	C20-C26-C25	-2.25	115.12	120.88
2	C	550	HEM	CAA-C2A-C1A	-2.21	124.61	127.01
4	D	800	S71	C08-C09-C13	-2.21	106.00	113.27
4	A	800	S71	C09-C13-C14	-2.20	116.88	120.56
2	C	550	HEM	C3B-C4B-NB	-2.17	107.49	111.63
2	C	550	HEM	CBA-CAA-C2A	-2.16	108.65	112.53
2	D	550	HEM	CBD-CAD-C3D	-2.15	107.30	113.55
4	A	800	S71	C08-C09-C13	-2.02	106.61	113.27
2	B	550	HEM	CAD-CBD-CGD	2.05	121.37	113.02
2	B	550	HEM	CHC-C4B-NB	2.07	129.51	124.52
4	C	800	S71	C22-N21-C26	2.11	119.73	118.23
2	A	550	HEM	C2D-C3D-C4D	2.11	105.08	101.50
4	D	800	S71	C12-N11-C16	2.12	120.69	117.50
4	B	800	S71	C25-C24-C23	2.16	120.84	118.08
4	D	800	S71	N22-C22-N21	2.17	120.45	116.50
2	A	550	HEM	CAD-CBD-CGD	2.18	121.89	113.02
3	D	600	H4B	C2-N1-C8A	2.18	119.45	114.54
2	D	550	HEM	C2D-C3D-C4D	2.19	105.21	101.50
4	A	800	S71	C27-C24-C23	2.21	124.30	120.95
2	C	550	HEM	C2D-C3D-C4D	2.22	105.27	101.50
4	B	800	S71	C24-C25-C26	2.26	121.69	120.28
4	C	800	S71	C12-N11-C16	2.26	120.90	117.50
3	C	600	H4B	C2-N1-C8A	2.28	119.66	114.54
4	C	800	S71	C09-C08-C06	2.31	116.97	112.53
2	D	550	HEM	CHD-C1D-ND	2.32	130.10	124.52
3	C	600	H4B	N2-C2-N3	2.33	121.06	117.20
4	C	800	S71	C14-C15-C16	2.34	119.35	116.78
4	B	800	S71	C08-C06-N01	2.35	119.16	115.69
4	B	800	S71	C03-C04-C05	2.36	121.09	118.08
4	A	800	S71	N02-C02-N01	2.40	120.88	116.50
2	D	550	HEM	C3B-CAB-CBB	2.42	128.16	124.46
4	A	800	S71	C18-C17-C20	2.42	115.12	110.11
4	D	800	S71	C14-C13-C12	2.43	119.22	116.57
4	D	800	S71	C09-C08-C06	2.49	117.32	112.53
4	C	800	S71	C08-C06-N01	2.51	119.40	115.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	930	SO4	O2-S-O1	2.57	117.64	109.50
2	A	550	HEM	CMD-C2D-C3D	2.68	126.19	114.35
2	D	550	HEM	CMD-C2D-C3D	2.72	126.37	114.35
2	C	550	HEM	CMD-C2D-C3D	2.78	126.65	114.35
2	B	550	HEM	CMB-C2B-C3B	2.81	123.55	116.53
2	B	550	HEM	C2D-C3D-C4D	2.85	106.33	101.50
4	C	800	S71	N22-C22-N21	2.86	121.71	116.50
4	A	800	S71	C14-C13-C12	2.87	119.70	116.57
3	D	600	H4B	C4A-C8A-N8	2.94	121.89	118.43
4	C	800	S71	C14-C13-C12	2.94	119.78	116.57
4	B	800	S71	C14-C13-C12	3.03	119.88	116.57
4	C	800	S71	N02-C02-N01	3.05	122.06	116.50
2	B	550	HEM	CMD-C2D-C3D	3.10	128.05	114.35
3	B	600	H4B	N2-C2-N3	3.10	122.33	117.20
3	D	600	H4B	C4-N3-C2	3.13	120.28	115.94
2	C	550	HEM	CMB-C2B-C3B	3.13	124.34	116.53
4	D	800	S71	C14-C15-C16	3.16	120.25	116.78
4	B	800	S71	C12-N11-C16	3.30	122.47	117.50
2	A	550	HEM	CMB-C2B-C3B	3.32	124.82	116.53
3	A	600	H4B	C4-N3-C2	3.35	120.58	115.94
4	B	800	S71	N02-C02-N01	3.40	122.69	116.50
3	B	600	H4B	C4-N3-C2	3.45	120.73	115.94
4	D	800	S71	N02-C02-N01	3.46	122.81	116.50
4	A	800	S71	C12-N11-C16	3.52	122.81	117.50
4	A	800	S71	C02-N01-C06	3.66	120.83	118.23
2	B	550	HEM	CMC-C2C-C3C	3.71	125.78	116.53
2	B	550	HEM	CAD-C3D-C2D	3.72	123.93	113.22
4	B	800	S71	N22-C22-N21	3.74	123.31	116.50
2	C	550	HEM	CMC-C2C-C3C	3.81	126.03	116.53
2	D	550	HEM	CAD-C3D-C2D	3.93	124.50	113.22
4	D	800	S71	C18-C17-C20	3.95	118.30	110.11
3	C	600	H4B	C4-N3-C2	4.01	121.50	115.94
2	C	550	HEM	CAD-C3D-C4D	4.08	126.88	112.47
2	D	550	HEM	CMC-C2C-C3C	4.16	126.91	116.53
4	B	800	S71	C02-N01-C06	4.18	121.20	118.23
2	A	550	HEM	CMC-C2C-C3C	4.38	127.48	116.53
3	C	600	H4B	C4-C4A-C8A	4.40	118.54	114.56
4	D	800	S71	C22-N21-C26	4.43	121.38	118.23
2	A	550	HEM	CAD-C3D-C4D	4.51	128.37	112.47
2	A	550	HEM	CAD-C3D-C2D	4.61	126.47	113.22
3	A	600	H4B	C4-C4A-C8A	4.74	118.86	114.56
2	B	550	HEM	CAD-C3D-C4D	4.89	129.73	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	800	S71	C02-N01-C06	4.93	121.73	118.23
2	D	550	HEM	CAD-C3D-C4D	5.04	130.26	112.47
2	C	550	HEM	CAD-C3D-C2D	5.08	127.83	113.22
4	C	800	S71	C02-N01-C06	5.56	122.18	118.23
3	D	600	H4B	C4-C4A-C8A	5.62	119.65	114.56
3	B	600	H4B	C4-C4A-C8A	6.19	120.16	114.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	550	HEM	2	0
3	A	600	H4B	1	0
4	A	800	S71	3	0
5	A	880	GOL	3	0
2	B	550	HEM	5	0
4	B	800	S71	1	0
5	B	880	GOL	1	0
2	C	550	HEM	3	0
4	C	800	S71	1	0
5	C	880	GOL	1	0
2	D	550	HEM	2	0
4	D	800	S71	1	0
5	D	880	GOL	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	414/431 (96%)	-0.37	3 (0%) 89 82	43, 65, 113, 147	0
1	B	414/431 (96%)	-0.42	1 (0%) 95 94	45, 67, 98, 131	0
1	C	414/431 (96%)	-0.02	10 (2%) 62 45	51, 97, 145, 175	0
1	D	414/431 (96%)	-0.41	1 (0%) 95 94	45, 69, 103, 132	0
All	All	1656/1724 (96%)	-0.30	15 (0%) 85 77	43, 72, 126, 175	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	177	GLY	2.7
1	A	107	ILE	2.7
1	C	85	VAL	2.7
1	C	151	TYR	2.6
1	C	97	GLN	2.4
1	C	176	THR	2.4
1	C	84	HIS	2.4
1	D	97	GLN	2.4
1	C	502	GLN	2.3
1	A	159	ILE	2.3
1	B	102	HIS	2.2
1	A	140	LEU	2.2
1	C	96	PHE	2.2
1	C	136	PRO	2.1
1	C	175	THR	2.1

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

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

6.3 Carbohydrates (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
5	GOL	B	880	6/6	0.93	0.44	4.00	56,76,89,97	0
6	SO4	D	920	5/5	0.95	0.28	2.21	120,123,135,138	0
3	H4B	B	600	17/17	0.96	0.23	1.65	43,49,53,55	0
5	GOL	C	880	6/6	0.93	0.33	1.60	70,79,84,86	0
3	H4B	D	600	17/17	0.94	0.24	1.36	62,67,72,72	0
4	S71	D	800	28/28	0.97	0.26	1.27	47,68,78,80	0
3	H4B	C	600	17/17	0.94	0.24	1.19	58,64,73,77	0
2	HEM	B	550	43/43	0.98	0.26	1.04	46,58,67,87	0
2	HEM	D	550	43/43	0.98	0.23	0.94	51,57,78,85	0
4	S71	B	800	28/28	0.97	0.25	0.93	47,56,69,71	0
3	H4B	A	600	17/17	0.96	0.21	0.92	44,48,51,52	0
4	S71	C	800	28/28	0.96	0.28	0.79	66,74,82,91	0
2	HEM	A	550	43/43	0.98	0.21	0.36	47,53,67,79	0
2	HEM	C	550	43/43	0.98	0.24	0.33	68,84,102,110	0
6	SO4	A	930	5/5	0.92	0.22	-0.08	75,82,87,97	0
4	S71	A	800	28/28	0.97	0.20	-0.14	48,58,67,69	0
6	SO4	A	910	5/5	0.96	0.12	-1.11	82,88,99,100	0
6	SO4	B	920	5/5	0.90	0.21	-1.15	105,129,142,162	0
6	SO4	B	910	5/5	0.89	0.17	-	117,120,140,148	0
5	GOL	A	880	6/6	0.94	0.26	-	60,67,84,85	0
6	SO4	D	910	5/5	0.92	0.17	-	114,119,142,142	0
6	SO4	C	920	5/5	0.78	0.31	-	155,161,183,196	0
6	SO4	C	910	5/5	0.84	0.23	-	121,143,163,168	0
5	GOL	D	880	6/6	0.91	0.34	-	64,79,84,85	0
6	SO4	A	920	5/5	0.84	0.18	-	98,127,139,151	0

6.5 Other polymers (i)

There are no such residues in this entry.