



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:46 PM UTC

PDB ID : 5B58 / pdb_00005b58
Title : Inward-facing conformation of ABC heme importer BhuUV in complex with periplasmic heme binding protein BhuT from Burkholderia cenocepacia
Authors : Naoe, Y.; Nakamura, N.; Doi, A.; Shiro, Y.; Sugimoto, H.
Deposited on : 2016-04-25
Resolution : 3.21 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

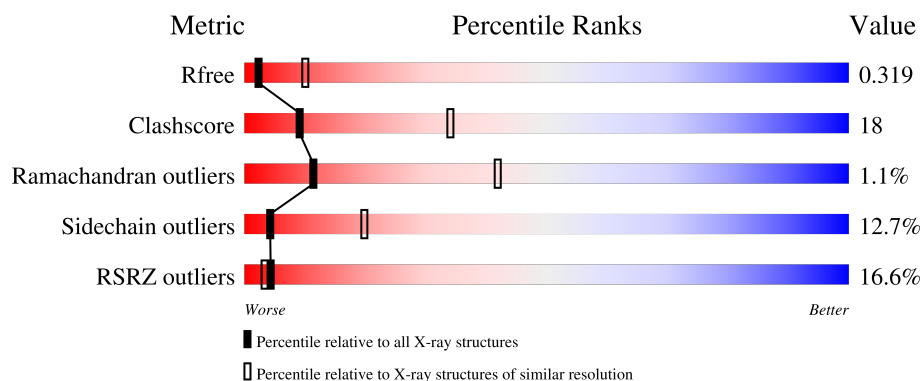
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 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}	180053	1768 (3.24-3.20)
Clashscore	190562	1879 (3.24-3.20)
Ramachandran outliers	187476	1844 (3.24-3.20)
Sidechain outliers	187428	1843 (3.24-3.20)
RSRZ outliers	180081	1768 (3.24-3.20)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$. 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	385	7% 48% 33% 14%
1	B	385	8% 52% 29% 5% 14%
2	C	273	8% 49% 41% 5% 5%
2	D	273	4% 52% 34% 6% 7%
3	T	271	54% 77% 20% ••

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10446 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 Putative hemin ABC transport system, membrane protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2326	1512	413	393	8			
1	B	331	Total	C	N	O	S	0	0	0
			2326	1512	413	393	8			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	expression tag	UNP B4EKB4
A	-21	GLY	-	expression tag	UNP B4EKB4
A	-20	HIS	-	expression tag	UNP B4EKB4
A	-19	HIS	-	expression tag	UNP B4EKB4
A	-18	HIS	-	expression tag	UNP B4EKB4
A	-17	HIS	-	expression tag	UNP B4EKB4
A	-16	HIS	-	expression tag	UNP B4EKB4
A	-15	HIS	-	expression tag	UNP B4EKB4
A	-14	HIS	-	expression tag	UNP B4EKB4
A	-13	HIS	-	expression tag	UNP B4EKB4
A	-12	HIS	-	expression tag	UNP B4EKB4
A	-11	HIS	-	expression tag	UNP B4EKB4
A	-10	SER	-	expression tag	UNP B4EKB4
A	-9	SER	-	expression tag	UNP B4EKB4
A	-8	GLY	-	expression tag	UNP B4EKB4
A	-7	HIS	-	expression tag	UNP B4EKB4
A	-6	ILE	-	expression tag	UNP B4EKB4
A	-5	ASP	-	expression tag	UNP B4EKB4
A	-4	ASP	-	expression tag	UNP B4EKB4
A	-3	ASP	-	expression tag	UNP B4EKB4
A	-2	ASP	-	expression tag	UNP B4EKB4
A	-1	LYS	-	expression tag	UNP B4EKB4
A	0	HIS	-	expression tag	UNP B4EKB4
B	-22	MET	-	expression tag	UNP B4EKB4
B	-21	GLY	-	expression tag	UNP B4EKB4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	HIS	-	expression tag	UNP B4EKB4
B	-19	HIS	-	expression tag	UNP B4EKB4
B	-18	HIS	-	expression tag	UNP B4EKB4
B	-17	HIS	-	expression tag	UNP B4EKB4
B	-16	HIS	-	expression tag	UNP B4EKB4
B	-15	HIS	-	expression tag	UNP B4EKB4
B	-14	HIS	-	expression tag	UNP B4EKB4
B	-13	HIS	-	expression tag	UNP B4EKB4
B	-12	HIS	-	expression tag	UNP B4EKB4
B	-11	HIS	-	expression tag	UNP B4EKB4
B	-10	SER	-	expression tag	UNP B4EKB4
B	-9	SER	-	expression tag	UNP B4EKB4
B	-8	GLY	-	expression tag	UNP B4EKB4
B	-7	HIS	-	expression tag	UNP B4EKB4
B	-6	ILE	-	expression tag	UNP B4EKB4
B	-5	ASP	-	expression tag	UNP B4EKB4
B	-4	ASP	-	expression tag	UNP B4EKB4
B	-3	ASP	-	expression tag	UNP B4EKB4
B	-2	ASP	-	expression tag	UNP B4EKB4
B	-1	LYS	-	expression tag	UNP B4EKB4
B	0	HIS	-	expression tag	UNP B4EKB4

- Molecule 2 is a protein called Hemin import ATP-binding protein HmuV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	258	Total	C	N	O	S	0	0	0
			1951	1228	370	346	7			
2	D	253	Total	C	N	O	S	0	0	0
			1907	1203	357	340	7			

- Molecule 3 is a protein called Putative hemin transport system, substrate-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	265	Total	C	N	O	S	0	0	0
			1936	1216	361	356	3			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	35	GLY	-	expression tag	UNP B4EKB3
T	36	PRO	-	expression tag	UNP B4EKB3
T	37	LEU	-	expression tag	UNP B4EKB3

Continued on next page...

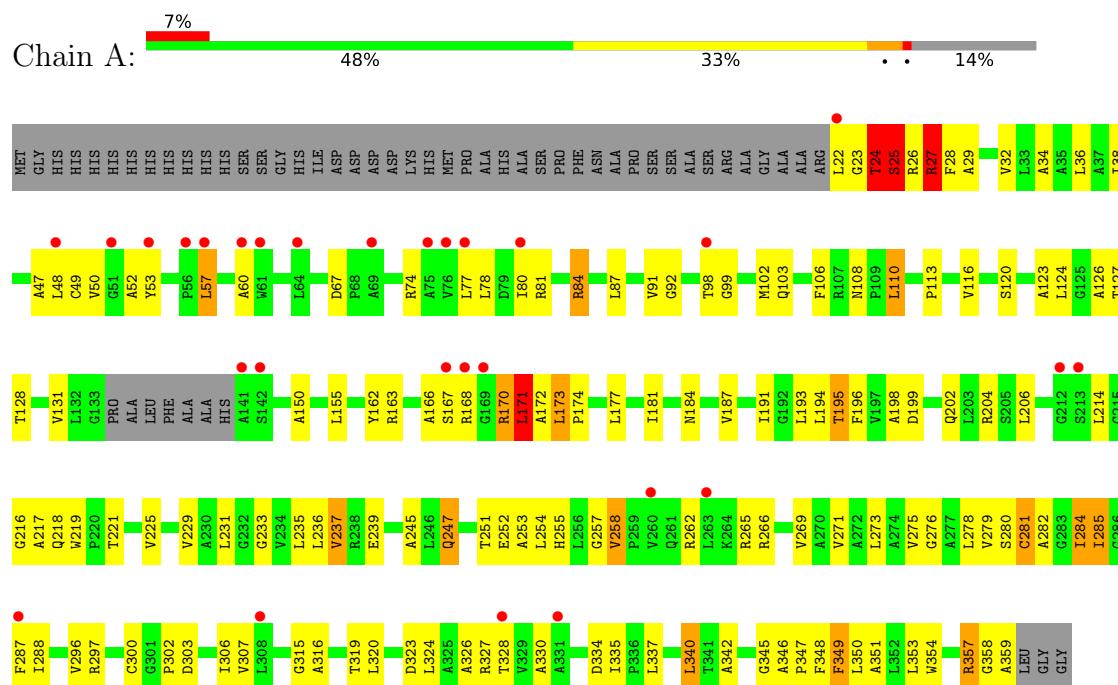
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
T	38	GLY	-	expression tag	UNP B4EKB3
T	39	SER	-	expression tag	UNP B4EKB3

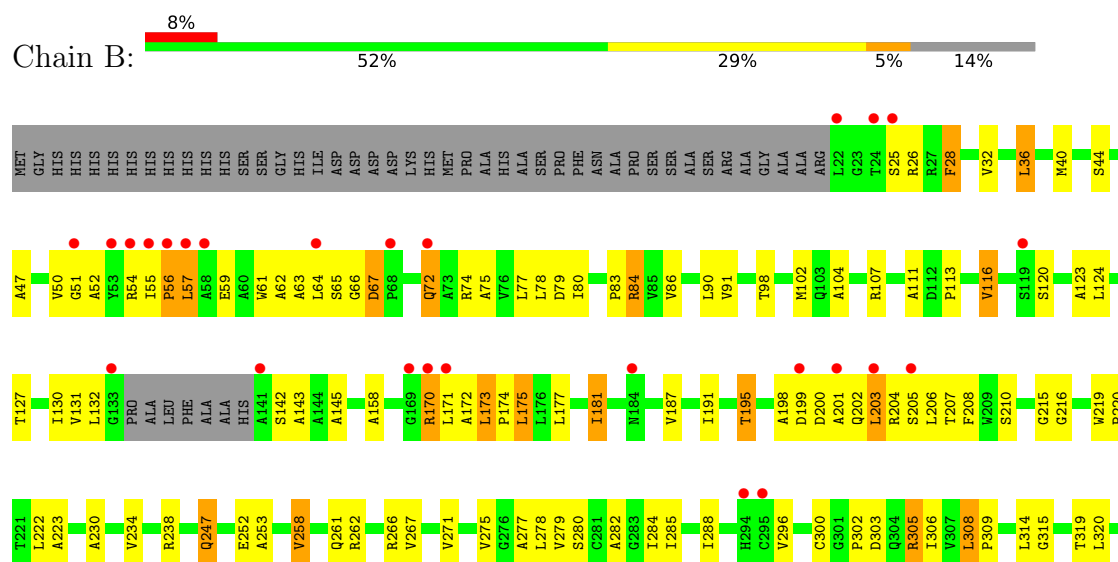
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Putative hemin ABC transport system, membrane protein

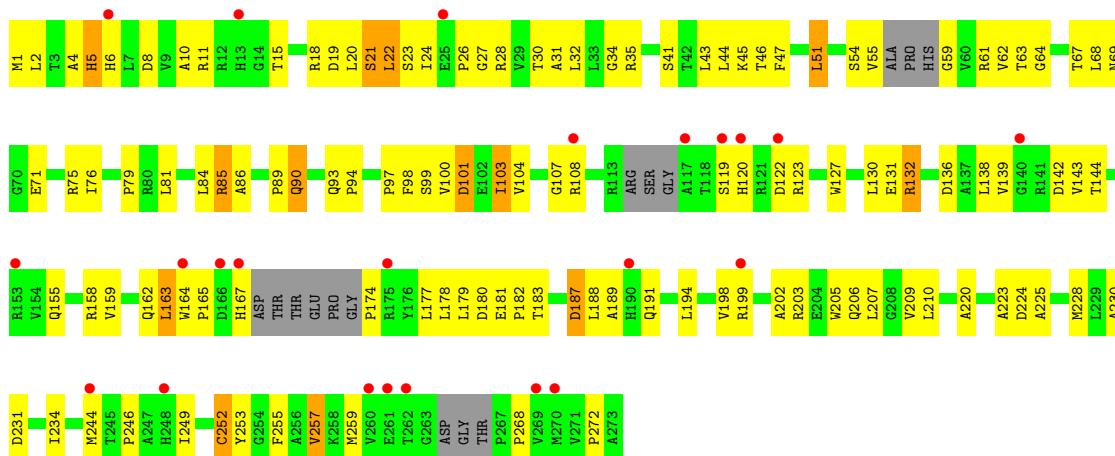


- Molecule 1: Putative hemin ABC transport system, membrane protein

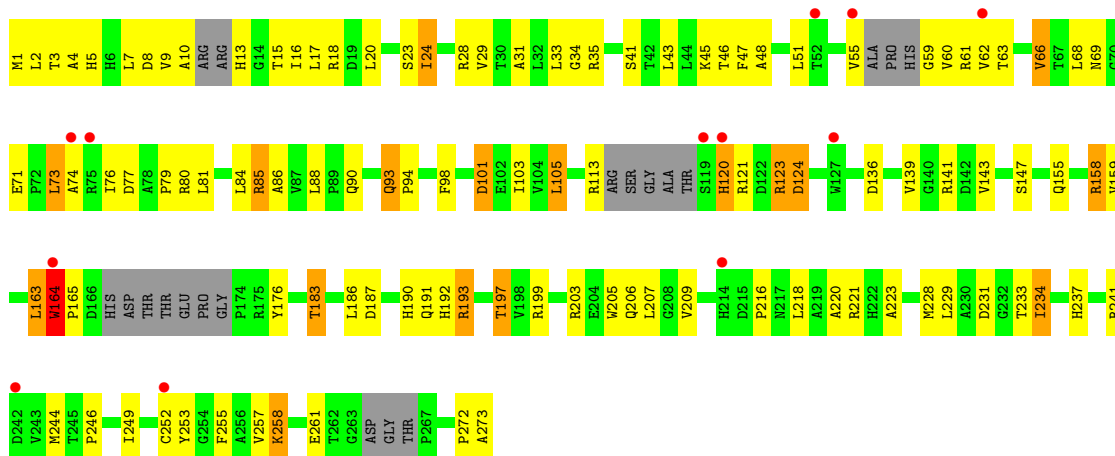




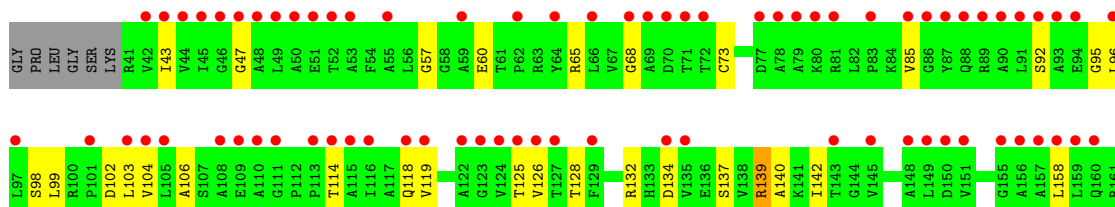
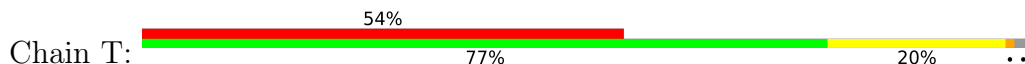
• Molecule 2: Hemin import ATP-binding protein HmuV

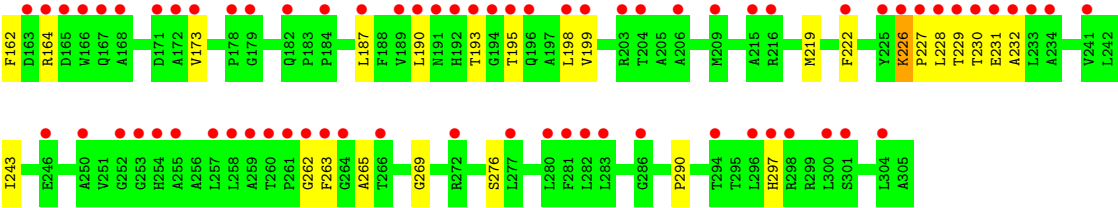


• Molecule 2: Hemin import ATP-binding protein HmuV



• Molecule 3: Putative hemin transport system, substrate-binding protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.02Å 99.75Å 253.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.61 – 3.21 32.61 – 3.21	Depositor EDS
% Data completeness (in resolution range)	76.1 (32.61-3.21) 76.0 (32.61-3.21)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.18Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.269 , 0.309 0.272 , 0.319	Depositor DCC
R_{free} test set	1066 reflections (1.73%)	wwPDB-VP
Wilson B-factor (Å ²)	61.8	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	10446	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.38	0/2363	0.63	0/3232
1	B	0.41	0/2363	0.66	0/3232
2	C	0.41	0/1988	0.61	0/2704
2	D	0.40	0/1942	0.67	2/2641 (0.1%)
3	T	0.16	0/1970	0.39	0/2684
All	All	0.37	0/10626	0.60	2/14493 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	164	TRP	CA-C-N	5.09	139.21	127.00
2	D	164	TRP	C-N-CA	5.09	139.21	127.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	348	PHE	Peptide
1	A	52	ALA	Peptide

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	2326	0	2502	108	0
1	B	2326	0	2502	112	0
2	C	1951	0	1987	92	0
2	D	1907	0	1941	75	0
3	T	1936	0	1974	50	0
All	All	10446	0	10906	391	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 18.

All (391) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ARG:O	1:A:29:ALA:N	1.90	1.03
1:A:334:ASP:HB2	3:T:92:SER:HB2	1.42	1.00
1:B:63:ALA:HB1	1:B:74:ARG:HB2	1.51	0.91
1:B:59:GLU:HG2	1:B:72:GLN:HB3	1.52	0.89
1:B:84:ARG:HH22	1:B:215:GLY:HA2	1.38	0.89
1:A:23:GLY:HA2	1:A:24:THR:HB	1.59	0.84
1:B:61:TRP:HB3	1:B:67:ASP:HB3	1.61	0.81
2:C:183:THR:HG22	2:C:194:LEU:HD23	1.64	0.80
2:C:1:MET:N	2:C:69:ASN:OD1	2.17	0.78
1:B:247:GLN:HB2	2:D:98:PHE:HE2	1.47	0.78
2:D:48:ALA:O	2:D:85:ARG:NH1	2.17	0.78
2:D:155:GLN:OE1	2:D:158:ARG:NH1	2.18	0.77
1:B:78:LEU:O	1:B:219:TRP:NE1	2.17	0.77
1:B:201:ALA:O	1:B:205:SER:OG	2.03	0.76
2:D:187:ASP:OD1	2:D:190:HIS:ND1	2.18	0.76
2:C:2:LEU:HD23	2:C:24:ILE:HD12	1.68	0.75
2:C:8:ASP:OD1	2:C:19:ASP:N	2.19	0.75
2:C:199:ARG:HH21	2:C:203:ARG:HH22	1.32	0.75
1:A:204:ARG:HD2	1:B:203:LEU:HD22	1.69	0.74
2:C:119:SER:HB2	2:C:120:HIS:HA	1.67	0.74
1:B:333:ALA:HB2	3:T:226:LYS:HD3	1.69	0.74
3:T:68:GLY:HA3	3:T:99:LEU:HD13	1.68	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:PHE:HD1	1:B:28:PHE:H	1.35	0.72
2:C:32:LEU:HD21	2:C:43:LEU:HD13	1.73	0.71
1:B:63:ALA:HB1	1:B:74:ARG:CB	2.21	0.71
1:B:120:SER:HB3	1:B:187:VAL:HG11	1.72	0.71
1:A:29:ALA:HA	1:A:32:VAL:HG12	1.73	0.70
2:C:220:ALA:HB2	2:C:244:MET:HE3	1.73	0.69
3:T:43:ILE:HD11	3:T:99:LEU:HB2	1.73	0.68
1:A:288:ILE:HG12	1:A:319:THR:HG22	1.76	0.68
1:B:26:ARG:HH11	1:B:300:CYS:HA	1.57	0.68
1:A:323:ASP:O	1:A:326:ALA:N	2.25	0.68
1:A:204:ARG:NH2	1:B:198:ALA:O	2.26	0.68
1:A:170:ARG:HH22	2:C:59:GLY:N	1.92	0.67
2:D:120:HIS:HA	2:D:123:ARG:HB2	1.75	0.67
2:D:101:ASP:O	2:D:105:LEU:HB2	1.94	0.66
1:A:98:THR:HB	1:A:271:VAL:HG23	1.77	0.66
1:B:52:ALA:HB3	3:T:231:GLU:HB3	1.77	0.66
1:A:253:ALA:O	1:A:258:VAL:HG13	1.96	0.66
1:A:199:ASP:C	1:B:204:ARG:HH22	2.04	0.66
2:D:15:THR:HG21	2:D:18:ARG:HH12	1.59	0.66
2:D:193:ARG:O	2:D:197:THR:OG1	2.13	0.65
1:A:27:ARG:HH11	1:A:27:ARG:HB2	1.61	0.65
1:A:78:LEU:O	1:A:219:TRP:NE1	2.28	0.65
1:B:170:ARG:HH22	2:D:59:GLY:N	1.94	0.65
2:D:203:ARG:HA	2:D:203:ARG:HH21	1.62	0.65
3:T:96:LEU:HD13	3:T:119:VAL:HG21	1.78	0.64
1:B:62:ALA:N	1:B:67:ASP:OD1	2.31	0.64
1:B:332:PRO:HB2	3:T:232:ALA:HB2	1.80	0.64
2:D:2:LEU:HD23	2:D:24:ILE:HD13	1.80	0.64
1:A:124:LEU:HB2	1:A:187:VAL:HG13	1.80	0.64
2:C:187:ASP:OD1	2:C:187:ASP:N	2.29	0.64
1:A:357:ARG:HA	1:B:175:LEU:HD11	1.80	0.63
3:T:164:ARG:O	3:T:164:ARG:NH1	2.32	0.63
1:A:25:SER:HA	1:A:27:ARG:NH1	2.14	0.63
2:D:77:ASP:HB3	2:D:79:PRO:HD2	1.80	0.63
2:D:164:TRP:HB3	2:D:165:PRO:HA	1.80	0.63
2:D:93:GLN:CD	2:D:94:PRO:HD2	2.24	0.62
1:B:40:MET:O	1:B:44:SER:OG	2.16	0.62
2:C:24:ILE:HD13	2:C:210:LEU:HB2	1.82	0.62
1:A:204:ARG:HH12	1:B:199:ASP:C	2.07	0.62
2:C:46:THR:HG22	2:C:51:LEU:HD12	1.82	0.62
3:T:132:ARG:HB2	3:T:137:SER:HB2	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:HIS:O	2:C:85:ARG:NH2	2.33	0.61
1:B:253:ALA:O	1:B:258:VAL:HG13	2.00	0.61
2:C:98:PHE:O	2:C:143:VAL:HG22	2.00	0.61
1:B:335:ILE:H	1:B:335:ILE:HD12	1.64	0.61
1:A:196:PHE:CE1	3:T:227:PRO:HD2	2.36	0.60
1:B:63:ALA:O	1:B:74:ARG:NE	2.34	0.60
1:B:84:ARG:HE	1:B:327:ARG:HD2	1.66	0.60
1:B:98:THR:HB	1:B:271:VAL:HG23	1.83	0.60
2:C:199:ARG:HH21	2:C:203:ARG:NH2	1.98	0.60
1:A:181:ILE:HA	1:A:184:ASN:HB2	1.83	0.60
1:A:202:GLN:O	1:A:206:LEU:HG	2.02	0.60
1:B:36:LEU:HD21	1:B:314:LEU:HB2	1.84	0.60
1:B:142:SER:OG	1:B:143:ALA:N	2.34	0.59
1:B:61:TRP:HB3	1:B:67:ASP:CB	2.29	0.59
1:B:91:VAL:HG11	1:B:285:ILE:HD12	1.84	0.59
1:B:282:ALA:HB1	1:B:285:ILE:HD11	1.85	0.59
2:D:120:HIS:O	2:D:120:HIS:ND1	2.35	0.59
1:B:102:MET:HG3	1:B:113:PRO:HA	1.85	0.59
1:B:204:ARG:HD2	3:T:198:LEU:HD22	1.85	0.58
1:B:75:ALA:HB1	3:T:265:ALA:HB1	1.85	0.58
1:A:199:ASP:C	1:B:204:ARG:NH2	2.61	0.58
1:B:80:ILE:HD11	3:T:262:GLY:HA2	1.85	0.58
1:B:124:LEU:HD22	1:B:187:VAL:HG23	1.86	0.58
2:D:86:ALA:HB3	2:D:163:LEU:HD21	1.85	0.58
2:C:189:ALA:HB2	2:D:255:PHE:HB2	1.84	0.58
3:T:219:MET:HE1	3:T:232:ALA:HB1	1.86	0.58
2:C:108:ARG:NE	2:C:122:ASP:OD1	2.33	0.58
2:C:132:ARG:HG2	2:C:164:TRP:HH2	1.69	0.58
2:D:7:LEU:HD21	2:D:46:THR:HG21	1.86	0.58
1:A:275:VAL:O	1:A:279:VAL:HG12	2.04	0.58
1:B:59:GLU:CG	1:B:72:GLN:HB3	2.31	0.58
1:A:265:ARG:O	1:A:269:VAL:HG23	2.03	0.57
1:A:23:GLY:HA2	1:A:24:THR:CB	2.33	0.57
2:C:249:ILE:HG21	2:C:257:VAL:HG21	1.85	0.57
1:A:326:ALA:HB2	1:A:340:LEU:HD13	1.85	0.57
1:A:91:VAL:HA	1:A:278:LEU:HD22	1.86	0.57
1:A:131:VAL:HG21	1:A:194:LEU:HD22	1.85	0.56
1:B:216:GLY:HA3	3:T:195:THR:OG1	2.04	0.56
1:B:347:PRO:O	1:B:351:ALA:N	2.37	0.56
1:B:57:LEU:HG	1:B:77:LEU:HD21	1.87	0.56
2:C:178:LEU:HD23	2:C:210:LEU:HB3	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:81:LEU:O	2:D:84:LEU:N	2.37	0.56
2:C:103:ILE:HD12	2:C:143:VAL:HG11	1.87	0.56
1:B:247:GLN:HB2	2:D:98:PHE:CE2	2.35	0.56
1:B:285:ILE:HD13	1:B:337:LEU:HD11	1.87	0.56
1:B:47:ALA:HA	1:B:324:LEU:CD1	2.36	0.56
2:C:28:ARG:HG2	2:C:224:ASP:HB2	1.88	0.56
2:D:220:ALA:HB2	2:D:244:MET:HE3	1.86	0.56
1:B:198:ALA:HB1	1:B:202:GLN:CB	2.35	0.56
1:A:49:CYS:SG	1:A:57:LEU:HD12	2.46	0.56
1:A:303:ASP:O	1:A:307:VAL:HG23	2.06	0.55
2:D:9:VAL:HG22	2:D:17:LEU:HB3	1.89	0.55
3:T:222:PHE:CE2	3:T:226:LYS:HD2	2.41	0.55
2:D:255:PHE:CZ	2:D:272:PRO:HB3	2.42	0.55
2:D:2:LEU:HD21	2:D:47:PHE:HB3	1.88	0.55
1:A:102:MET:HG3	1:A:113:PRO:HA	1.89	0.54
1:A:162:TYR:CE1	1:A:166:ALA:HB2	2.43	0.54
1:B:191:ILE:O	1:B:195:THR:HG23	2.07	0.54
1:B:219:TRP:CE3	1:B:222:LEU:HD11	2.42	0.54
2:C:1:MET:HE3	2:C:23:SER:HB2	1.88	0.54
2:D:15:THR:HG21	2:D:18:ARG:NH1	2.22	0.54
3:T:187:LEU:HD11	3:T:199:VAL:HG11	1.90	0.54
1:A:191:ILE:O	1:A:195:THR:HG23	2.08	0.54
1:B:84:ARG:NH2	1:B:215:GLY:HA2	2.17	0.54
2:C:68:LEU:HD11	2:C:84:LEU:HD13	1.89	0.54
1:B:28:PHE:CD1	1:B:28:PHE:N	2.76	0.53
1:B:303:ASP:OD1	1:B:305:ARG:HB2	2.07	0.53
2:C:93:GLN:HE21	2:C:144:THR:HB	1.73	0.53
2:C:99:SER:OG	2:C:101:ASP:OD1	2.23	0.53
2:D:51:LEU:HA	2:D:55:VAL:HG22	1.90	0.53
1:A:126:ALA:HB2	1:A:150:ALA:HB2	1.90	0.53
2:C:8:ASP:HB2	2:C:63:THR:OG1	2.09	0.53
2:C:183:THR:HB	2:C:191:GLN:HG2	1.89	0.53
2:D:1:MET:HA	2:D:176:TYR:OH	2.08	0.53
2:D:234:ILE:HD11	2:D:237:HIS:HB2	1.90	0.53
1:A:214:LEU:HG	1:A:337:LEU:HD21	1.91	0.53
2:C:228:MET:HE1	2:C:249:ILE:HD13	1.89	0.53
1:A:84:ARG:NH2	1:A:327:ARG:HG2	2.24	0.53
1:B:308:LEU:HB3	1:B:309:PRO:HD3	1.89	0.53
2:C:188:LEU:HD11	2:D:216:PRO:HG2	1.91	0.53
3:T:263:PHE:O	3:T:269:GLY:HA3	2.09	0.53
2:C:107:GLY:O	2:C:162:GLN:HG3	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:SER:HB2	1:A:170:ARG:HG2	1.90	0.52
1:A:233:GLY:O	1:A:237:VAL:HG12	2.10	0.52
3:T:162:PHE:CE2	3:T:290:PRO:HD3	2.44	0.52
1:A:262:ARG:O	1:A:266:ARG:HG3	2.10	0.52
2:D:4:ALA:HA	2:D:66:VAL:HA	1.92	0.52
1:A:103:GLN:OE1	1:A:297:ARG:NH2	2.43	0.52
1:A:173:LEU:HG	1:A:174:PRO:HD3	1.92	0.52
2:D:249:ILE:HG21	2:D:257:VAL:HG21	1.92	0.52
1:A:27:ARG:HH11	1:A:27:ARG:CB	2.23	0.51
1:B:267:VAL:O	1:B:271:VAL:HG12	2.10	0.51
2:C:4:ALA:HB2	2:C:47:PHE:HE1	1.76	0.51
1:A:87:LEU:HD23	1:A:214:LEU:HB3	1.92	0.51
1:A:170:ARG:O	1:A:171:LEU:HB2	2.10	0.51
2:C:120:HIS:O	2:C:123:ARG:N	2.43	0.51
2:D:9:VAL:HG12	2:D:62:VAL:HG22	1.91	0.51
1:A:24:THR:HG23	1:A:25:SER:N	2.26	0.51
2:D:98:PHE:O	2:D:143:VAL:HG23	2.10	0.51
1:B:32:VAL:HG11	1:B:300:CYS:SG	2.50	0.51
1:B:344:LEU:O	1:B:347:PRO:HD2	2.10	0.51
1:A:24:THR:HG22	2:C:101:ASP:OD2	2.11	0.51
1:A:302:PRO:HG2	2:C:98:PHE:CD1	2.46	0.50
2:C:94:PRO:HG3	2:C:143:VAL:HG21	1.92	0.50
2:C:22:LEU:HG	2:C:234:ILE:CD1	2.41	0.50
1:B:107:ARG:NH1	1:B:107:ARG:HB2	2.27	0.50
2:C:31:ALA:HB2	2:C:223:ALA:HB2	1.93	0.50
1:A:50:VAL:HG11	1:A:328:THR:HG21	1.93	0.50
2:C:230:ALA:HB2	2:C:252:CYS:HA	1.93	0.50
1:A:315:GLY:O	1:A:319:THR:HG23	2.12	0.50
2:C:155:GLN:OE1	2:C:158:ARG:NH1	2.45	0.50
1:B:170:ARG:HA	1:B:261:GLN:OE1	2.12	0.50
3:T:229:THR:HB	3:T:231:GLU:OE1	2.11	0.49
2:C:2:LEU:HA	2:C:68:LEU:HA	1.93	0.49
2:D:2:LEU:HD13	2:D:68:LEU:HD13	1.94	0.49
2:D:136:ASP:O	2:D:139:VAL:HG13	2.12	0.49
2:D:203:ARG:HA	2:D:203:ARG:NH2	2.25	0.49
3:T:95:GLY:O	3:T:98:SER:OG	2.26	0.49
1:A:236:LEU:O	1:A:239:GLU:N	2.40	0.49
1:B:332:PRO:HB2	3:T:232:ALA:CB	2.43	0.49
2:D:34:GLY:HA2	2:D:252:CYS:SG	2.52	0.49
1:A:163:ARG:NH1	1:A:168:ARG:HH12	2.11	0.49
1:B:84:ARG:HH11	1:B:84:ARG:HB2	1.76	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:VAL:O	1:B:279:VAL:HG12	2.12	0.49
1:A:282:ALA:HB3	1:A:285:ILE:HD11	1.94	0.49
1:A:27:ARG:C	1:A:29:ALA:N	2.70	0.49
1:B:173:LEU:HB3	1:B:174:PRO:HD3	1.95	0.49
2:C:94:PRO:HG3	2:C:143:VAL:CG2	2.43	0.49
1:A:351:ALA:O	1:A:354:TRP:HB3	2.12	0.49
2:C:97:PRO:HB3	2:C:142:ASP:OD2	2.13	0.49
1:A:99:GLY:O	1:A:103:GLN:HG3	2.13	0.48
2:D:101:ASP:OD1	2:D:101:ASP:N	2.45	0.48
2:D:164:TRP:HB3	2:D:165:PRO:CA	2.42	0.48
1:B:44:SER:HA	1:B:320:LEU:HD21	1.94	0.48
1:B:177:LEU:O	1:B:181:ILE:HG12	2.13	0.48
1:B:208:PHE:CD2	3:T:227:PRO:HG3	2.48	0.48
2:C:130:LEU:HD13	2:C:139:VAL:HG12	1.95	0.48
2:D:205:TRP:HE3	2:D:207:LEU:HD13	1.78	0.48
2:C:5:HIS:HA	2:C:21:SER:HB3	1.95	0.48
2:D:35:ARG:NH1	2:D:253:TYR:O	2.46	0.48
1:A:330:ALA:HB3	1:A:335:ILE:HD11	1.95	0.48
1:A:113:PRO:HB3	1:A:275:VAL:HG21	1.96	0.48
1:B:26:ARG:NH1	1:B:300:CYS:O	2.47	0.48
1:B:104:ALA:CB	1:B:247:GLN:HE22	2.27	0.48
1:A:346:ALA:HB3	1:A:347:PRO:HD3	1.96	0.48
1:B:355:LYS:HG2	1:B:355:LYS:O	2.14	0.48
2:C:206:GLN:HA	2:C:206:GLN:OE1	2.14	0.47
1:B:80:ILE:HD13	3:T:230:THR:HB	1.96	0.47
2:C:67:THR:HG23	2:C:71:GLU:C	2.39	0.47
3:T:60:GLU:HB3	3:T:65:ARG:HG2	1.96	0.47
1:A:196:PHE:HZ	1:B:333:ALA:HB1	1.79	0.47
1:B:130:ILE:HG22	1:B:202:GLN:OE1	2.14	0.47
2:D:191:GLN:OE1	2:D:218:LEU:HD11	2.14	0.47
3:T:243:ILE:O	3:T:276:SER:HA	2.15	0.47
1:B:91:VAL:HA	1:B:278:LEU:HD22	1.95	0.47
2:D:8:ASP:HB2	2:D:63:THR:OG1	2.14	0.47
1:A:231:LEU:HD23	1:A:273:LEU:HD21	1.96	0.47
1:B:123:ALA:O	1:B:127:THR:HG22	2.13	0.47
2:D:29:VAL:HG22	2:D:209:VAL:HB	1.95	0.47
2:D:85:ARG:HG2	2:D:86:ALA:N	2.29	0.47
3:T:104:VAL:HB	3:T:126:VAL:HG22	1.96	0.47
1:B:204:ARG:HD2	3:T:198:LEU:CD2	2.45	0.47
1:B:84:ARG:NE	1:B:327:ARG:HD2	2.28	0.46
2:C:120:HIS:ND1	2:C:120:HIS:C	2.73	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:228:MET:HE2	2:D:252:CYS:SG	2.55	0.46
1:B:210:SER:O	1:B:284:ILE:HB	2.15	0.46
2:C:41:SER:O	2:C:45:LYS:HG3	2.16	0.46
3:T:142:ILE:HG23	3:T:158:LEU:HD23	1.97	0.46
1:A:216:GLY:CA	3:T:114:THR:HB	2.46	0.46
1:B:315:GLY:O	1:B:319:THR:HG23	2.15	0.46
1:A:47:ALA:HA	1:A:324:LEU:CD1	2.46	0.46
1:B:104:ALA:HB1	1:B:247:GLN:HE22	1.79	0.46
2:C:10:ALA:HB2	2:C:15:THR:HG22	1.96	0.46
2:C:244:MET:HE2	2:C:244:MET:HB2	1.69	0.46
1:B:86:VAL:HG13	1:B:222:LEU:HD22	1.98	0.46
2:C:86:ALA:HB1	2:C:159:VAL:HG23	1.97	0.46
2:D:76:ILE:HG21	2:D:81:LEU:HD13	1.97	0.46
1:A:60:ALA:HB1	1:A:77:LEU:HD11	1.98	0.46
1:B:220:PRO:HA	1:B:223:ALA:HB3	1.96	0.46
2:C:71:GLU:HG3	2:C:76:ILE:HD11	1.98	0.46
3:T:173:VAL:HG13	3:T:297:HIS:CD2	2.50	0.46
1:B:277:ALA:O	1:B:280:SER:OG	2.21	0.46
2:C:131:GLU:HB3	2:C:132:ARG:HH11	1.81	0.46
3:T:190:LEU:HD23	3:T:198:LEU:HD23	1.97	0.46
1:A:92:GLY:HA3	1:A:316:ALA:HA	1.96	0.46
1:A:245:ALA:O	1:A:253:ALA:HB2	2.15	0.46
1:B:57:LEU:HG	1:B:77:LEU:CD2	2.46	0.46
2:D:31:ALA:HB2	2:D:223:ALA:HB2	1.98	0.45
1:A:22:LEU:HD12	2:C:127:TRP:CG	2.51	0.45
1:B:205:SER:HA	3:T:193:THR:OG1	2.16	0.45
2:C:26:PRO:HB3	2:C:206:GLN:O	2.16	0.45
1:B:195:THR:O	1:B:203:LEU:HD11	2.16	0.45
2:C:136:ASP:C	2:C:138:LEU:H	2.25	0.45
2:D:3:THR:O	2:D:66:VAL:HA	2.16	0.45
1:A:262:ARG:O	1:A:265:ARG:HB2	2.16	0.45
1:B:124:LEU:HA	1:B:127:THR:HG22	1.99	0.45
1:B:332:PRO:O	3:T:232:ALA:HB2	2.16	0.45
1:A:34:ALA:O	1:A:38:ILE:HG12	2.16	0.45
1:A:358:GLY:HA2	1:A:359:ALA:HA	1.63	0.45
2:C:249:ILE:HG23	2:C:253:TYR:HD2	1.81	0.45
1:A:29:ALA:HB1	1:A:306:ILE:HG21	1.99	0.45
2:D:192:HIS:HE1	2:D:221:ARG:NE	2.15	0.45
1:A:25:SER:HA	1:A:27:ARG:CZ	2.47	0.45
1:B:230:ALA:O	1:B:234:VAL:HG23	2.17	0.45
2:C:90:GLN:OE1	2:C:90:GLN:N	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:244:MET:HG3	2:C:259:MET:HE1	1.97	0.45
2:D:69:ASN:OD1	2:D:176:TYR:OH	2.11	0.45
1:A:225:VAL:HG21	1:A:281:CYS:SG	2.57	0.45
2:C:34:GLY:HA2	2:C:252:CYS:SG	2.56	0.45
2:D:33:LEU:HB3	2:D:228:MET:HE3	1.98	0.45
1:B:302:PRO:HG2	2:D:98:PHE:CD1	2.52	0.44
2:C:30:THR:HA	2:C:225:ALA:O	2.17	0.44
2:D:20:LEU:HD13	2:D:43:LEU:HD13	1.98	0.44
1:A:123:ALA:O	1:A:127:THR:HG22	2.17	0.44
1:B:247:GLN:H	1:B:247:GLN:HG2	1.42	0.44
2:C:90:GLN:HG3	2:C:180:ASP:O	2.17	0.44
2:D:183:THR:O	2:D:186:LEU:HB2	2.17	0.44
2:D:246:PRO:HB3	2:D:257:VAL:O	2.17	0.44
2:C:2:LEU:CD1	2:C:68:LEU:HB3	2.48	0.44
2:C:47:PHE:HD2	2:C:210:LEU:HD22	1.82	0.44
2:C:100:VAL:O	2:C:104:VAL:HG23	2.17	0.44
1:A:23:GLY:C	2:C:123:ARG:HH21	2.26	0.44
2:C:2:LEU:HD12	2:C:68:LEU:HB3	1.99	0.44
2:C:35:ARG:HG3	2:C:252:CYS:O	2.18	0.44
2:C:89:PRO:O	2:C:90:GLN:C	2.61	0.44
2:C:93:GLN:HE21	2:C:144:THR:CB	2.30	0.44
3:T:60:GLU:CB	3:T:65:ARG:HG2	2.48	0.44
2:C:179:LEU:HD13	2:C:182:PRO:HG3	1.99	0.44
3:T:132:ARG:H	3:T:137:SER:CB	2.31	0.44
1:B:219:TRP:HE3	1:B:222:LEU:HD11	1.82	0.44
1:B:262:ARG:HD2	1:B:266:ARG:HG3	2.00	0.44
2:C:255:PHE:CZ	2:C:272:PRO:HB3	2.52	0.44
1:A:124:LEU:HA	1:A:127:THR:HG22	1.99	0.44
1:A:287:PHE:CD2	1:A:342:ALA:HA	2.53	0.44
1:A:345:GLY:O	1:A:349:PHE:N	2.51	0.44
1:B:302:PRO:HG2	2:D:98:PHE:CE1	2.53	0.44
3:T:173:VAL:HG22	3:T:297:HIS:CG	2.52	0.44
1:B:63:ALA:CB	1:B:74:ARG:HB2	2.35	0.43
1:B:171:LEU:HD23	1:B:261:GLN:HE22	1.83	0.43
3:T:103:LEU:HD12	3:T:125:THR:O	2.17	0.43
1:A:163:ARG:HH12	1:A:168:ARG:HH12	1.66	0.43
1:A:287:PHE:N	1:A:287:PHE:CD1	2.86	0.43
1:A:24:THR:O	1:A:26:ARG:N	2.51	0.43
1:A:198:ALA:HB1	1:A:202:GLN:HB2	2.00	0.43
1:B:203:LEU:O	1:B:207:THR:HG23	2.19	0.43
2:C:69:ASN:ND2	2:C:174:PRO:HD2	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:241:ARG:HH12	2:D:261:GLU:CD	2.25	0.43
1:B:351:ALA:O	1:B:354:TRP:N	2.52	0.43
2:C:20:LEU:HD11	2:C:234:ILE:HG13	1.99	0.43
2:D:3:THR:HG23	2:D:23:SER:HB3	2.00	0.43
1:A:288:ILE:HG12	1:A:319:THR:CG2	2.45	0.43
2:D:121:ARG:HH11	2:D:121:ARG:HG3	1.84	0.43
1:A:80:ILE:HG23	3:T:118:GLN:HE21	1.84	0.43
2:C:20:LEU:HD12	2:C:20:LEU:HA	1.79	0.43
2:D:3:THR:OG1	2:D:23:SER:HB2	2.19	0.43
1:B:355:LYS:HE2	1:B:356:ASN:HD21	1.84	0.43
2:C:108:ARG:HG3	2:C:122:ASP:HB3	2.01	0.43
2:D:73:LEU:O	2:D:76:ILE:N	2.51	0.43
1:A:251:THR:HG22	1:A:255:HIS:CE1	2.54	0.42
2:D:41:SER:O	2:D:45:LYS:HG3	2.19	0.42
2:D:120:HIS:O	2:D:120:HIS:CG	2.71	0.42
1:A:247:GLN:H	1:A:247:GLN:HG2	1.60	0.42
1:B:170:ARG:H	1:B:170:ARG:HG3	1.42	0.42
3:T:106:ALA:O	3:T:128:THR:HA	2.19	0.42
1:A:108:ASN:OD1	1:A:110:LEU:HB2	2.19	0.42
1:A:198:ALA:O	1:B:204:ARG:NH1	2.47	0.42
3:T:199:VAL:HG13	3:T:228:LEU:HB2	2.00	0.42
3:T:222:PHE:CD2	3:T:226:LYS:HD2	2.55	0.42
1:A:47:ALA:CB	1:A:320:LEU:HD11	2.48	0.42
1:B:116:VAL:O	1:B:158:ALA:HA	2.18	0.42
2:C:68:LEU:HD21	2:C:81:LEU:HD11	1.99	0.42
2:C:246:PRO:HB3	2:C:257:VAL:O	2.19	0.42
2:D:228:MET:HE1	2:D:249:ILE:HD13	2.00	0.42
1:A:214:LEU:HG	1:A:337:LEU:CD2	2.49	0.42
3:T:47:GLY:HA2	3:T:73:CYS:SG	2.59	0.42
2:C:132:ARG:HD3	2:C:132:ARG:N	2.34	0.42
1:B:62:ALA:HB2	1:B:67:ASP:O	2.19	0.42
2:D:206:GLN:OE1	2:D:206:GLN:HA	2.19	0.42
3:T:164:ARG:HA	3:T:164:ARG:HD2	1.94	0.42
1:A:25:SER:HA	1:A:27:ARG:HH12	1.83	0.42
2:D:258:LYS:HB3	2:D:273:ALA:HB2	2.00	0.42
1:A:80:ILE:HG23	3:T:118:GLN:NE2	2.34	0.42
1:B:79:ASP:O	1:B:83:PRO:HG2	2.19	0.42
1:B:131:VAL:HG22	1:B:202:GLN:OE1	2.20	0.42
1:B:206:LEU:HD23	1:B:206:LEU:HA	1.87	0.42
2:C:6:HIS:O	2:C:64:GLY:HA3	2.20	0.42
2:C:2:LEU:O	2:C:23:SER:HA	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:163:LEU:HD12	2:C:163:LEU:HA	1.89	0.41
2:D:88:LEU:HD23	2:D:159:VAL:HG11	2.01	0.41
1:A:106:PHE:CE2	1:A:177:LEU:HD21	2.55	0.41
1:B:107:ARG:HB2	1:B:107:ARG:HH11	1.85	0.41
2:C:27:GLY:HA2	2:C:202:ALA:O	2.20	0.41
2:D:81:LEU:HD12	2:D:81:LEU:HA	1.86	0.41
3:T:198:LEU:HD12	3:T:226:LYS:C	2.46	0.41
1:A:127:THR:HG21	1:A:191:ILE:HG12	2.01	0.41
1:B:288:ILE:HG12	1:B:319:THR:HG22	2.02	0.41
1:A:247:GLN:HB2	2:C:98:PHE:HE2	1.86	0.41
1:A:276:GLY:O	1:A:280:SER:OG	2.34	0.41
1:B:61:TRP:O	1:B:66:GLY:N	2.53	0.41
1:A:87:LEU:HD22	1:A:217:ALA:HB2	2.02	0.41
1:B:55:ILE:HA	1:B:56:PRO:HD3	1.93	0.41
3:T:139:ARG:HG3	3:T:140:ALA:N	2.36	0.41
1:A:235:LEU:O	1:A:239:GLU:HG2	2.21	0.41
1:A:247:GLN:HB2	2:C:98:PHE:CE2	2.56	0.41
1:A:284:ILE:H	1:A:284:ILE:HG12	1.70	0.41
2:D:55:VAL:HG11	2:D:60:VAL:HG22	2.03	0.41
1:B:143:ALA:C	1:B:145:ALA:H	2.29	0.41
1:B:333:ALA:HB2	3:T:226:LYS:CD	2.45	0.41
1:A:23:GLY:N	2:C:123:ARG:NH2	2.69	0.41
1:A:84:ARG:HH21	1:A:327:ARG:HG2	1.83	0.41
1:A:196:PHE:HA	1:B:208:PHE:CE1	2.56	0.41
1:A:257:GLY:HA3	2:C:79:PRO:HA	2.03	0.41
1:A:335:ILE:H	1:A:335:ILE:HG12	1.61	0.41
2:C:205:TRP:CD1	2:C:205:TRP:N	2.87	0.41
2:D:10:ALA:HB2	2:D:15:THR:HG22	2.03	0.41
2:D:120:HIS:HE1	2:D:124:ASP:OD2	2.04	0.41
1:A:163:ARG:HH11	1:A:168:ARG:HH22	1.69	0.41
2:D:71:GLU:HG3	2:D:76:ILE:HD11	2.03	0.41
1:A:48:LEU:O	1:A:81:ARG:HD2	2.21	0.40
1:A:23:GLY:O	2:C:123:ARG:NH2	2.54	0.40
1:B:198:ALA:HB1	1:B:202:GLN:HB2	2.03	0.40
3:T:85:VAL:HG13	3:T:99:LEU:HD11	2.03	0.40
3:T:134:ASP:N	3:T:134:ASP:OD1	2.53	0.40
2:D:1:MET:N	2:D:69:ASN:HA	2.35	0.40
2:C:8:ASP:O	2:C:62:VAL:HA	2.21	0.40
2:D:71:GLU:OE1	2:D:80:ARG:NH2	2.55	0.40
1:B:204:ARG:HG2	1:B:208:PHE:CE2	2.56	0.40
2:C:177:LEU:O	2:C:209:VAL:HA	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	327/385 (85%)	284 (87%)	37 (11%)	6 (2%)	6	33
1	B	327/385 (85%)	294 (90%)	28 (9%)	5 (2%)	8	36
2	C	248/273 (91%)	232 (94%)	14 (6%)	2 (1%)	16	48
2	D	241/273 (88%)	227 (94%)	12 (5%)	2 (1%)	16	48
3	T	263/271 (97%)	255 (97%)	7 (3%)	1 (0%)	30	61
All	All	1406/1587 (89%)	1292 (92%)	98 (7%)	16 (1%)	11	42

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	SER
1	A	28	PHE
1	A	171	LEU
1	B	357	ARG
2	D	164	TRP
1	A	27	ARG
2	D	74	ALA
1	A	24	THR
1	A	172	ALA
1	B	111	ALA
1	B	172	ALA
3	T	57	GLY
2	C	165	PRO
1	B	56	PRO
2	C	268	PRO
1	B	51	GLY

5.3.2 Protein sidechains ⓘ

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	220/259 (85%)	183 (83%)	37 (17%)	2	10
1	B	220/259 (85%)	187 (85%)	33 (15%)	3	14
2	C	198/209 (95%)	173 (87%)	25 (13%)	4	20
2	D	194/209 (93%)	163 (84%)	31 (16%)	2	12
3	T	186/190 (98%)	183 (98%)	3 (2%)	55	73
All	All	1018/1126 (90%)	889 (87%)	129 (13%)	4	20

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	THR
1	A	25	SER
1	A	27	ARG
1	A	36	LEU
1	A	53	TYR
1	A	57	LEU
1	A	67	ASP
1	A	74	ARG
1	A	84	ARG
1	A	110	LEU
1	A	116	VAL
1	A	120	SER
1	A	128	THR
1	A	155	LEU
1	A	170	ARG
1	A	171	LEU
1	A	173	LEU
1	A	193	LEU
1	A	195	THR
1	A	218	GLN
1	A	221	THR
1	A	229	VAL
1	A	237	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	247	GLN
1	A	252	GLU
1	A	254	LEU
1	A	258	VAL
1	A	281	CYS
1	A	284	ILE
1	A	285	ILE
1	A	296	VAL
1	A	300	CYS
1	A	340	LEU
1	A	349	PHE
1	A	350	LEU
1	A	353	LEU
1	A	357	ARG
1	B	25	SER
1	B	28	PHE
1	B	36	LEU
1	B	50	VAL
1	B	54	ARG
1	B	57	LEU
1	B	64	LEU
1	B	65	SER
1	B	67	ASP
1	B	72	GLN
1	B	84	ARG
1	B	90	LEU
1	B	116	VAL
1	B	132	LEU
1	B	170	ARG
1	B	173	LEU
1	B	175	LEU
1	B	181	ILE
1	B	195	THR
1	B	200	ASP
1	B	203	LEU
1	B	238	ARG
1	B	247	GLN
1	B	252	GLU
1	B	258	VAL
1	B	296	VAL
1	B	305	ARG
1	B	306	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	308	LEU
1	B	334	ASP
1	B	350	LEU
1	B	353	LEU
1	B	355	LYS
2	C	5	HIS
2	C	11	ARG
2	C	18	ARG
2	C	21	SER
2	C	22	LEU
2	C	44	LEU
2	C	51	LEU
2	C	54	SER
2	C	55	VAL
2	C	61	ARG
2	C	75	ARG
2	C	85	ARG
2	C	90	GLN
2	C	101	ASP
2	C	103	ILE
2	C	132	ARG
2	C	163	LEU
2	C	167	HIS
2	C	181	GLU
2	C	187	ASP
2	C	198	VAL
2	C	207	LEU
2	C	231	ASP
2	C	252	CYS
2	C	257	VAL
2	D	5	HIS
2	D	13	HIS
2	D	16	ILE
2	D	24	ILE
2	D	28	ARG
2	D	61	ARG
2	D	66	VAL
2	D	73	LEU
2	D	85	ARG
2	D	90	GLN
2	D	93	GLN
2	D	101	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	103	ILE
2	D	105	LEU
2	D	113	ARG
2	D	120	HIS
2	D	123	ARG
2	D	124	ASP
2	D	141	ARG
2	D	147	SER
2	D	158	ARG
2	D	163	LEU
2	D	183	THR
2	D	193	ARG
2	D	197	THR
2	D	199	ARG
2	D	229	LEU
2	D	231	ASP
2	D	233	THR
2	D	234	ILE
2	D	258	LYS
3	T	102	ASP
3	T	139	ARG
3	T	226	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	72	GLN
1	B	247	GLN
1	B	261	GLN
2	C	93	GLN
2	C	162	GLN
3	T	118	GLN
3	T	192	HIS
3	T	196	GLN
3	T	254	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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, 95th 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	331/385 (85%)	0.53	28 (8%)	16 11	34, 64, 170, 254	0
1	B	331/385 (85%)	0.39	29 (8%)	15 10	13, 52, 166, 199	0
2	C	258/273 (94%)	0.50	23 (8%)	15 10	27, 59, 124, 170	0
2	D	253/273 (92%)	0.35	12 (4%)	36 23	13, 52, 107, 143	0
3	T	265/271 (97%)	2.73	146 (55%)	0 1	46, 65, 77, 84	265 (100%)
All	All	1438/1587 (90%)	0.86	238 (16%)	4 3	13, 60, 137, 254	265 (18%)

All (238) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	T	193	THR	15.0
3	T	191	ASN	13.1
3	T	49	LEU	12.7
3	T	149	LEU	11.5
3	T	122	ALA	11.5
3	T	196	GLN	9.8
3	T	89	ARG	9.1
3	T	192	HIS	9.0
1	A	77	LEU	8.2
3	T	48	ALA	7.5
3	T	215	ALA	7.2
3	T	109	GLU	6.7
3	T	187	LEU	6.7
2	D	75	ARG	6.6
1	A	57	LEU	6.5
3	T	151	VAL	6.4
3	T	118	GLN	6.2
3	T	77	ASP	6.0
3	T	190	LEU	6.0
3	T	296	LEU	6.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	T	64	TYR	5.9
3	T	156	ALA	5.8
3	T	72	THR	5.8
3	T	194	GLY	5.8
2	C	166	ASP	5.7
3	T	119	VAL	5.5
3	T	254	HIS	5.4
2	D	242	ASP	5.3
3	T	46	GLY	5.3
3	T	228	LEU	5.3
3	T	81	ARG	5.2
3	T	264	GLY	5.1
3	T	87	TYR	5.0
3	T	80	LYS	4.8
3	T	298	ARG	4.8
3	T	88	GLN	4.8
3	T	85	VAL	4.8
1	A	75	ALA	4.7
3	T	91	LEU	4.7
3	T	160	GLN	4.7
3	T	165	ASP	4.6
3	T	51	GLU	4.6
3	T	300	LEU	4.5
3	T	145	VAL	4.4
3	T	116	ILE	4.4
3	T	59	ALA	4.3
1	A	60	ALA	4.3
3	T	259	ALA	4.3
3	T	255	ALA	4.2
3	T	282	LEU	4.1
3	T	97	LEU	4.1
3	T	286	GLY	4.1
3	T	260	THR	4.1
3	T	71	THR	4.1
3	T	104	VAL	4.0
2	C	167	HIS	4.0
2	C	190	HIS	4.0
1	B	25	SER	4.0
3	T	96	LEU	4.0
1	A	76	VAL	4.0
3	T	226	LYS	4.0
3	T	150	ASP	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	T	111	GLY	4.0
2	C	164	TRP	4.0
1	A	22	LEU	4.0
3	T	261	PRO	3.9
1	A	80	ILE	3.9
3	T	263	PHE	3.9
3	T	168	ALA	3.9
1	B	332	PRO	3.8
3	T	230	THR	3.8
3	T	148	ALA	3.8
3	T	92	SER	3.8
3	T	231	GLU	3.8
3	T	258	LEU	3.8
1	A	169	GLY	3.7
3	T	115	ALA	3.7
2	D	127	TRP	3.7
1	A	141	ALA	3.7
3	T	47	GLY	3.7
3	T	277	LEU	3.7
1	B	58	ALA	3.6
3	T	158	LEU	3.6
3	T	114	THR	3.6
1	B	51	GLY	3.6
2	C	244	MET	3.5
3	T	143	THR	3.5
3	T	123	GLY	3.5
2	D	119	SER	3.5
3	T	257	LEU	3.5
3	T	179	GLY	3.5
1	A	61	TRP	3.4
3	T	195	THR	3.4
1	B	56	PRO	3.4
3	T	172	ALA	3.4
3	T	79	ALA	3.3
3	T	164	ARG	3.3
1	B	57	LEU	3.3
3	T	66	LEU	3.3
2	C	119	SER	3.2
1	B	170	ARG	3.2
2	C	175	ARG	3.2
1	A	213	SER	3.2
3	T	134	ASP	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	T	163	ASP	3.2
3	T	110	ALA	3.2
1	A	64	LEU	3.2
3	T	157	ALA	3.1
3	T	234	ALA	3.1
2	C	262	THR	3.1
3	T	225	TYR	3.1
3	T	68	GLY	3.0
3	T	45	ILE	3.0
2	C	117	ALA	3.0
3	T	155	GLY	3.0
3	T	246	GLU	3.0
3	T	113	PRO	3.0
3	T	78	ALA	3.0
3	T	90	ALA	3.0
3	T	125	THR	3.0
3	T	135	VAL	3.0
3	T	159	LEU	2.9
3	T	55	ALA	2.9
1	B	133	GLY	2.9
2	C	108	ARG	2.9
3	T	53	ALA	2.9
1	A	167	SER	2.9
3	T	103	LEU	2.9
3	T	272	ARG	2.9
1	B	205	SER	2.9
3	T	86	GLY	2.9
3	T	69	ALA	2.9
3	T	301	SER	2.8
1	A	308	LEU	2.8
3	T	222	PHE	2.8
3	T	166	TRP	2.8
3	T	281	PHE	2.8
3	T	70	ASP	2.8
2	D	252	CYS	2.8
1	B	55	ILE	2.8
3	T	43	ILE	2.8
1	B	169	GLY	2.8
1	B	199	ASP	2.7
3	T	50	ALA	2.7
3	T	42	VAL	2.7
3	T	199	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	T	241	VAL	2.7
3	T	227	PRO	2.7
1	B	54	ARG	2.7
1	A	48	LEU	2.7
3	T	304	LEU	2.7
3	T	105	LEU	2.7
3	T	101	PRO	2.7
1	B	334	ASP	2.7
1	B	68	PRO	2.7
2	C	140	GLY	2.7
3	T	52	THR	2.7
3	T	62	PRO	2.6
3	T	204	THR	2.6
2	C	260	VAL	2.6
3	T	173	VAL	2.6
2	D	120	HIS	2.6
3	T	83	PRO	2.6
1	A	260	VAL	2.6
1	A	328	THR	2.6
3	T	93	ALA	2.6
1	B	184	ASN	2.6
3	T	262	GLY	2.6
1	B	141	ALA	2.6
2	D	55	VAL	2.6
1	A	69	ALA	2.6
3	T	198	LEU	2.5
1	B	24	THR	2.5
2	C	25	GLU	2.5
2	C	120	HIS	2.5
3	T	108	ALA	2.5
2	C	122	ASP	2.5
3	T	294	THR	2.5
3	T	189	VAL	2.5
1	B	201	ALA	2.4
2	D	62	VAL	2.4
3	T	124	VAL	2.4
3	T	253	GLY	2.4
3	T	182	GLN	2.4
1	A	98	THR	2.4
3	T	178	PRO	2.4
1	B	72	GLN	2.4
3	T	209	MET	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	287	PHE	2.4
1	A	53	TYR	2.4
1	A	168	ARG	2.4
1	B	22	LEU	2.3
3	T	94	GLU	2.3
2	C	6	HIS	2.3
3	T	129	PHE	2.3
2	C	261	GLU	2.3
3	T	127	THR	2.3
3	T	232	ALA	2.3
1	A	263	LEU	2.3
3	T	250	ALA	2.3
2	D	74	ALA	2.3
1	B	64	LEU	2.3
3	T	229	THR	2.3
1	B	295	CYS	2.3
2	D	164	TRP	2.2
1	B	294	HIS	2.2
1	A	331	ALA	2.2
3	T	266	THR	2.2
2	C	199	ARG	2.2
3	T	203	ARG	2.2
1	B	119	SER	2.2
2	C	153	ARG	2.2
2	D	52	THR	2.2
1	B	53	TYR	2.2
3	T	280	LEU	2.2
3	T	283	LEU	2.2
2	C	270	MET	2.2
3	T	297	HIS	2.2
3	T	126	VAL	2.1
1	A	142	SER	2.1
3	T	206	ALA	2.1
1	A	51	GLY	2.1
1	A	56	PRO	2.1
3	T	184	PRO	2.1
1	B	328	THR	2.1
3	T	171	ASP	2.1
2	C	248	HIS	2.1
3	T	167	GLN	2.1
1	B	203	LEU	2.1
3	T	233	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	T	44	VAL	2.1
1	B	171	LEU	2.1
2	D	214	HIS	2.1
1	A	212	GLY	2.1
3	T	216	ARG	2.0
2	C	13	HIS	2.0
3	T	252	GLY	2.0
2	C	269	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.