Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2021 – 12:39 PM EDT

PDB ID	:	5R1R
Title	:	RIBONUCLEOTIDE REDUCTASE E441A MUTANT R1 PROTEIN FROM ESCHERICHIA COLI
Authors	:	Eriksson, M.; Eklund, H.
Deposited on	:	1997-09-17
Resolution	:	3.10 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 (i) symbol.

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

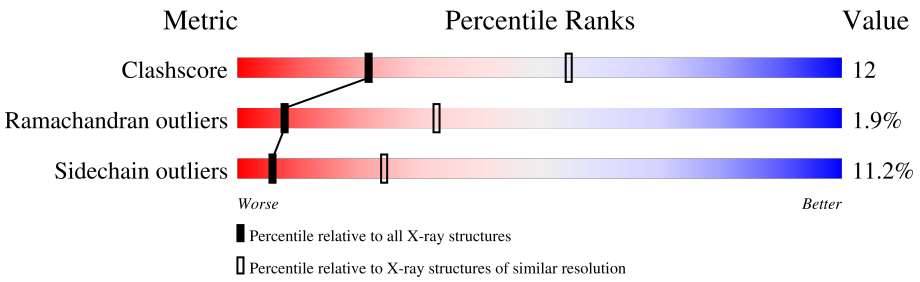
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	761	63% 29% • • •
1	B	761	64% 28% 5% •
1	C	761	62% 30% 5% •
2	D	20	70% 10% 10% 10%
2	E	20	75% 10% 5% 10%
2	F	20	75% 10% 5% 10%
2	P	20	10% 10% 80%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 18154 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 RIBONUCLEOTIDE REDUCTASE R1 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	738	5871	3727	1010	1109	25	0	0	0
1	B	738	5871	3727	1010	1109	25	0	0	0
1	C	738	5871	3727	1010	1109	25	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	441	ALA	GLU	engineered mutation	UNP P00452
B	441	ALA	GLU	engineered mutation	UNP P00452
C	441	ALA	GLU	engineered mutation	UNP P00452

- Molecule 2 is a protein called RIBONUCLEOTIDE REDUCTASE R2 PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	D	18	140	84	21	35	0	0	0
2	E	18	140	84	21	35	0	0	0
2	F	18	140	84	21	35	0	0	0
2	P	4	31	22	4	5	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	28	28	28	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	B	30	30	30	0	0
			Total	O		
3	C	32	32	32	0	0

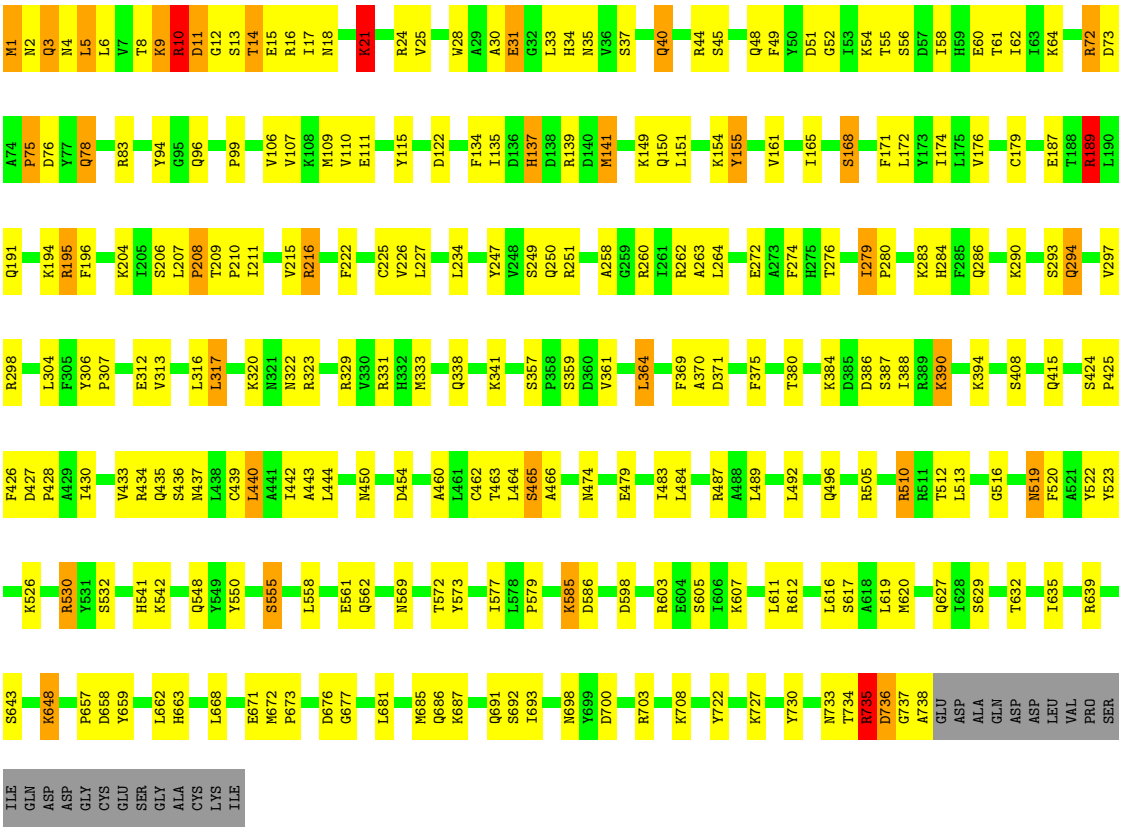
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

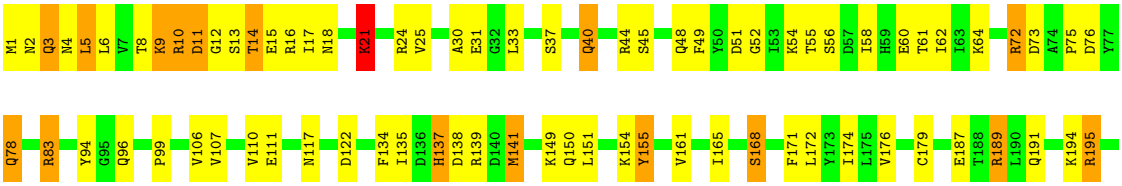
• Molecule 1: RIBONUCLEOTIDE REDUCTASE R1 PROTEIN

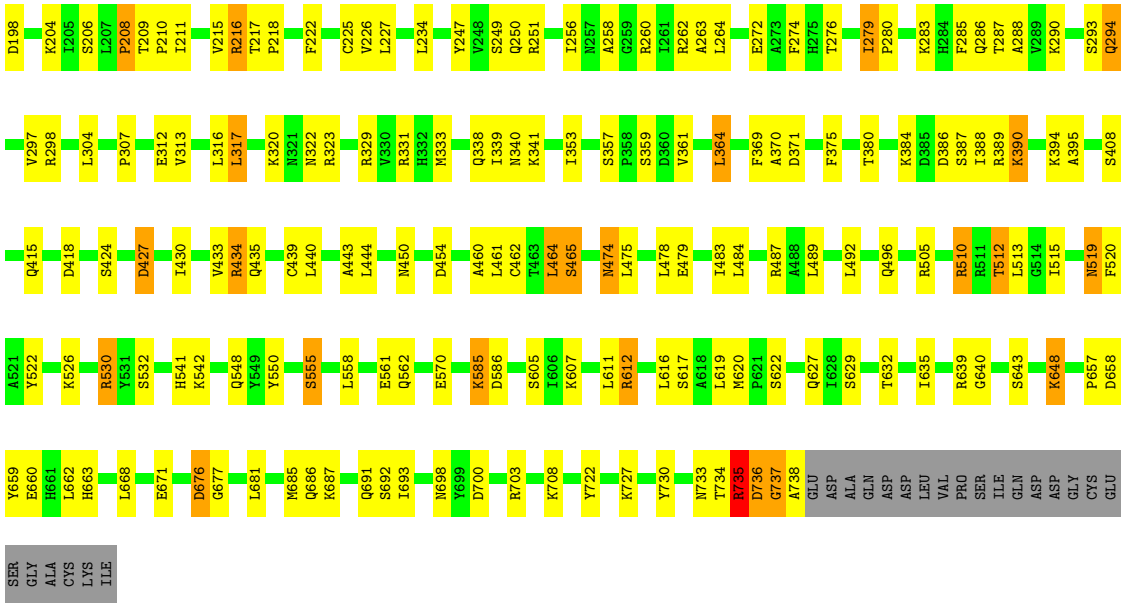
Chain A:



• Molecule 1: RIBONUCLEOTIDE REDUCTASE R1 PROTEIN

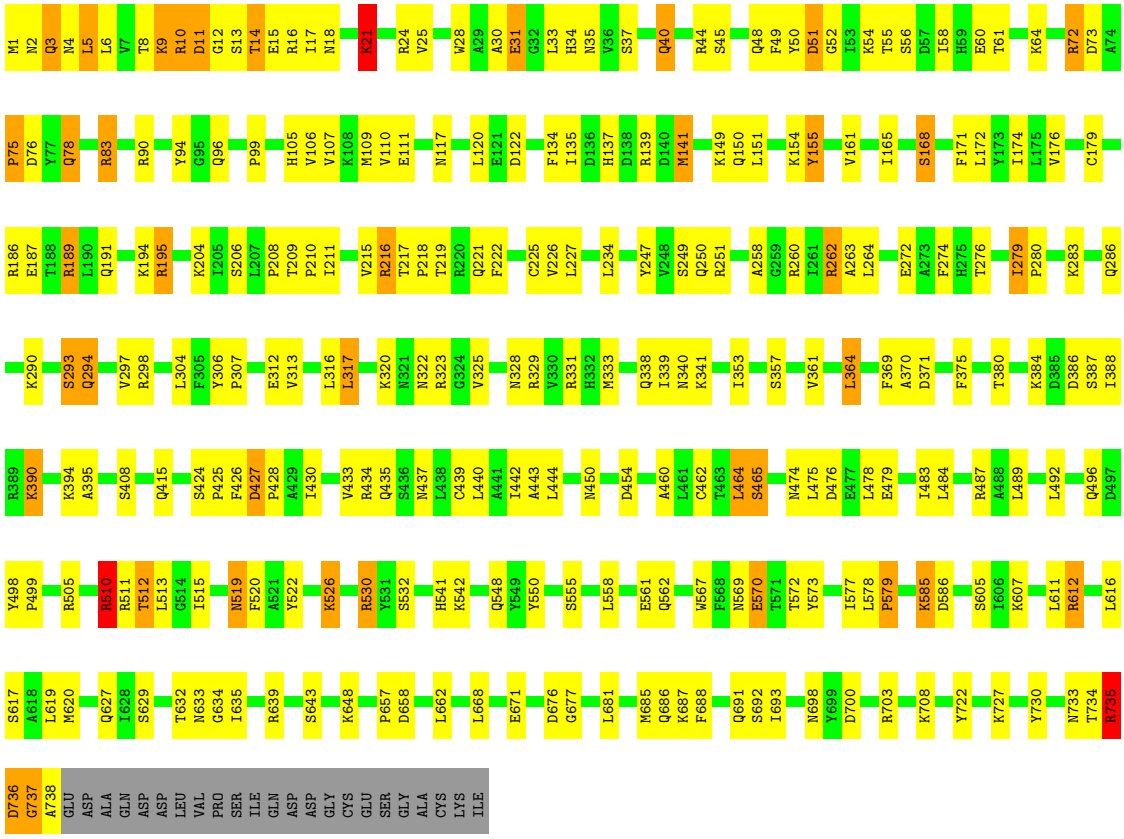
Chain B:





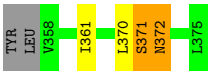
- Molecule 1: RIBONUCLEOTIDE REDUCTASE R1 PROTEIN

Chain C: 62% 30% 5% •



- Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN

Chain D: 70% 10% 10% 10%



• Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN

Chain E:

• Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN

Chain F:

• Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN

Chain P:

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	223.81Å 223.81Å 334.26Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.10	Depositor
% Data completeness (in resolution range)	90.9 (20.00-3.10)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
Refinement program	TNT, REFMAC	Depositor
R, R_{free}	0.196 , 0.227	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18154	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

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	0.44	0/5999	1.18	24/8125 (0.3%)
1	B	0.42	0/5999	1.20	29/8125 (0.4%)
1	C	0.44	0/5999	1.22	27/8125 (0.3%)
2	D	0.42	0/140	1.01	0/188
2	E	0.42	0/140	1.02	0/188
2	F	0.43	0/140	1.08	0/188
2	P	0.83	0/31	2.38	2/41 (4.9%)
All	All	0.43	0/18448	1.20	82/24980 (0.3%)

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	3
1	B	0	1
1	C	0	2
All	All	0	6

There are no bond length outliers.

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	530	ARG	NE-CZ-NH1	16.54	128.57	120.30
1	A	530	ARG	NE-CZ-NH1	15.10	127.85	120.30
1	B	530	ARG	NE-CZ-NH1	14.97	127.79	120.30
1	B	703	ARG	NE-CZ-NH2	-13.91	113.34	120.30
1	A	703	ARG	NE-CZ-NH2	-12.18	114.21	120.30
1	C	530	ARG	NE-CZ-NH2	-12.06	114.27	120.30
1	B	530	ARG	NE-CZ-NH2	-10.17	115.21	120.30
1	C	703	ARG	NE-CZ-NH2	-10.04	115.28	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	195	ARG	CD-NE-CZ	10.01	137.62	123.60
1	C	703	ARG	NE-CZ-NH1	9.61	125.10	120.30
1	B	195	ARG	CD-NE-CZ	9.51	136.91	123.60
1	A	530	ARG	NE-CZ-NH2	-9.24	115.68	120.30
1	A	703	ARG	NE-CZ-NH1	8.77	124.69	120.30
1	B	703	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	B	612	ARG	NE-CZ-NH2	-8.27	116.17	120.30
1	B	195	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	C	530	ARG	CD-NE-CZ	8.20	135.07	123.60
1	B	83	ARG	NE-CZ-NH2	-8.16	116.22	120.30
1	B	24	ARG	NE-CZ-NH1	8.01	124.30	120.30
1	C	83	ARG	NE-CZ-NH2	-7.73	116.43	120.30
1	B	72	ARG	NE-CZ-NH1	-7.73	116.44	120.30
1	A	24	ARG	CD-NE-CZ	7.36	133.91	123.60
1	A	195	ARG	CD-NE-CZ	7.34	133.88	123.60
1	C	427	ASP	CB-CG-OD2	-7.32	111.71	118.30
1	B	72	ARG	NE-CZ-NH2	7.26	123.93	120.30
1	C	24	ARG	NE-CZ-NH1	7.23	123.92	120.30
1	A	371	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	B	530	ARG	CD-NE-CZ	6.90	133.26	123.60
1	C	262	ARG	NE-CZ-NH2	-6.85	116.87	120.30
2	P	1	TYR	CA-CB-CG	6.72	126.17	113.40
1	B	24	ARG	CD-NE-CZ	6.60	132.83	123.60
1	C	371	ASP	CB-CG-OD2	-6.55	112.41	118.30
1	B	371	ASP	CB-CG-OD2	-6.36	112.57	118.30
1	C	510	ARG	NE-CZ-NH1	-6.31	117.15	120.30
1	C	195	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	C	510	ARG	NE-CZ-NH2	6.22	123.41	120.30
1	C	620	MET	CB-CA-C	-6.21	97.99	110.40
1	A	530	ARG	CD-NE-CZ	6.17	132.24	123.60
1	C	612	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	B	198	ASP	CB-CG-OD1	6.04	123.73	118.30
1	C	24	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	C	676	ASP	CB-CG-OD2	-5.86	113.02	118.30
1	A	510	ARG	NE-CZ-NH2	5.85	123.22	120.30
1	A	21	LYS	CA-CB-CG	5.82	126.21	113.40
1	A	72	ARG	NE-CZ-NH2	5.82	123.21	120.30
1	B	293	SER	C-N-CA	5.78	136.15	121.70
1	B	21	LYS	CA-CB-CG	5.78	126.10	113.40
1	A	293	SER	C-N-CA	5.72	135.99	121.70
1	A	155	TYR	CB-CG-CD1	5.70	124.42	121.00
1	A	72	ARG	NE-CZ-NH1	-5.69	117.45	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	24	ARG	CD-NE-CZ	5.65	131.51	123.60
1	B	24	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	C	293	SER	C-N-CA	5.62	135.75	121.70
1	B	434	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	C	90	ARG	NE-CZ-NH2	5.61	123.11	120.30
1	C	21	LYS	CA-CB-CG	5.56	125.62	113.40
1	A	10	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	A	676	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	C	72	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	B	276	THR	CA-CB-CG2	-5.42	104.82	112.40
1	B	208	PRO	N-CA-CB	5.39	109.77	103.30
1	A	208	PRO	N-CA-CB	5.37	109.75	103.30
1	C	155	TYR	CB-CG-CD1	5.33	124.20	121.00
1	B	676	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	A	598	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	A	523	TYR	CB-CG-CD2	-5.28	117.83	121.00
1	B	155	TYR	CB-CG-CD1	5.28	124.17	121.00
2	P	2	LEU	CA-CB-CG	5.26	127.39	115.30
1	A	189	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	B	620	MET	CA-CB-CG	5.25	122.22	113.30
1	A	620	MET	CB-CA-C	-5.23	99.94	110.40
1	B	138	ASP	CB-CG-OD2	-5.23	113.60	118.30
1	C	511	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	603	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	C	476	ASP	CB-CG-OD1	5.16	122.94	118.30
1	A	195	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	389	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	C	276	THR	CA-CB-CG2	-5.09	105.28	112.40
1	B	418	ASP	CB-CG-OD2	-5.08	113.72	118.30
1	B	427	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	A	276	THR	CA-CB-CG2	-5.04	105.34	112.40
1	B	293	SER	CA-C-O	5.02	130.65	120.10

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	HIS	Mainchain
1	A	579	PRO	Mainchain
1	A	75	PRO	Mainchain
1	B	137	HIS	Mainchain
1	C	579	PRO	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	C	75	PRO	Mainchain

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	5871	0	5798	140	0
1	B	5871	0	5798	138	0
1	C	5871	0	5798	148	0
2	D	140	0	123	2	0
2	E	140	0	123	1	0
2	F	140	0	123	1	0
2	P	31	0	34	5	0
3	A	28	0	0	3	0
3	B	30	0	0	4	0
3	C	32	0	0	6	0
All	All	18154	0	17797	428	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 12.

All (428) 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:37:SER:HB3	1:B:40:GLN:HB2	1.47	0.96
1:A:37:SER:HB3	1:A:40:GLN:HB2	1.51	0.93
1:C:37:SER:HB3	1:C:40:GLN:HB2	1.51	0.93
1:A:83:ARG:HG2	1:A:141:MET:HG3	1.56	0.87
1:A:698:ASN:ND2	1:A:733:ASN:HD22	1.72	0.86
1:C:191:GLN:HE21	1:C:195:ARG:HH21	1.21	0.86
1:B:83:ARG:HG2	1:B:141:MET:HG3	1.58	0.85
1:B:698:ASN:ND2	1:B:733:ASN:HD22	1.74	0.85
1:A:191:GLN:HE21	1:A:195:ARG:HH21	1.26	0.82
1:B:191:GLN:HE21	1:B:195:ARG:HH21	1.27	0.80
1:B:135:ILE:HD11	1:B:174:ILE:HG21	1.64	0.80
1:A:4:ASN:O	1:A:5:LEU:HB2	1.80	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:658:ASP:HB3	1:B:662:LEU:HD12	1.65	0.79
1:C:658:ASP:HB3	1:C:662:LEU:HD12	1.63	0.79
1:A:135:ILE:HD11	1:A:174:ILE:HG21	1.65	0.78
1:C:135:ILE:HD11	1:C:174:ILE:HG21	1.65	0.78
1:B:558:LEU:HD23	1:B:612:ARG:HG2	1.65	0.77
1:C:698:ASN:ND2	1:C:733:ASN:HD22	1.83	0.76
1:C:83:ARG:HG2	1:C:141:MET:HG3	1.67	0.76
1:B:9:LYS:HE2	1:B:55:THR:HG21	1.68	0.76
1:B:619:LEU:HD12	1:B:693:ILE:HG12	1.69	0.75
1:C:9:LYS:HE2	1:C:55:THR:HG21	1.68	0.75
1:A:150:GLN:HE21	1:A:627:GLN:NE2	1.85	0.75
1:A:658:ASP:HB3	1:A:662:LEU:HD12	1.68	0.75
1:B:4:ASN:O	1:B:5:LEU:HB2	1.84	0.75
1:A:558:LEU:HD23	1:A:612:ARG:HG2	1.68	0.74
1:C:558:LEU:HD23	1:C:612:ARG:HG2	1.66	0.74
1:C:4:ASN:O	1:C:5:LEU:HB2	1.87	0.73
1:C:150:GLN:HE21	1:C:627:GLN:NE2	1.87	0.72
1:B:294:GLN:HB2	1:B:298:ARG:HB3	1.71	0.70
1:B:1:MET:H2	1:B:3:GLN:HG3	1.57	0.70
1:B:215:VAL:O	1:B:216:ARG:HB3	1.90	0.70
1:A:9:LYS:HE2	1:A:55:THR:HG21	1.72	0.70
1:B:258:ALA:HB3	1:B:304:LEU:HD21	1.74	0.69
1:A:294:GLN:HB2	1:A:298:ARG:HB3	1.73	0.69
1:B:150:GLN:HE21	1:B:627:GLN:NE2	1.91	0.68
1:A:215:VAL:O	1:A:216:ARG:HB3	1.94	0.67
1:C:294:GLN:HB2	1:C:298:ARG:HB3	1.75	0.67
1:B:279:ILE:HB	1:B:280:PRO:HD3	1.76	0.67
1:C:322:ASN:HA	1:C:331:ARG:NH1	2.10	0.66
1:B:734:THR:O	1:B:735:ARG:HB2	1.96	0.66
1:C:279:ILE:HB	1:C:280:PRO:HD3	1.77	0.65
1:B:698:ASN:HD21	1:B:733:ASN:HD22	1.44	0.65
1:B:519:ASN:ND2	1:B:632:THR:H	1.94	0.65
1:A:279:ILE:HB	1:A:280:PRO:HD3	1.77	0.65
1:B:234:LEU:HG	1:B:272:GLU:HG2	1.78	0.65
1:A:1:MET:H2	1:A:3:GLN:HG3	1.62	0.65
1:B:465:SER:HB2	1:B:489:LEU:HD11	1.78	0.65
1:A:465:SER:HB2	1:A:489:LEU:HD11	1.77	0.64
1:A:489:LEU:HB3	1:A:513:LEU:HD22	1.79	0.64
1:A:619:LEU:HD12	1:A:693:ILE:HG12	1.78	0.64
1:C:1:MET:H2	1:C:3:GLN:HG3	1.63	0.64
1:C:619:LEU:HD12	1:C:693:ILE:HG12	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:734:THR:O	1:C:735:ARG:HB2	1.97	0.64
1:A:234:LEU:HG	1:A:272:GLU:HG2	1.80	0.64
1:A:522:TYR:CE2	1:A:526:LYS:HD3	2.33	0.64
1:C:361:VAL:HG21	1:C:364:LEU:HD12	1.78	0.64
1:B:361:VAL:HG21	1:B:364:LEU:HD12	1.79	0.63
1:B:686:GLN:NE2	1:B:727:LYS:HD2	2.14	0.63
1:A:444:LEU:HD22	1:A:512:THR:HG21	1.82	0.62
1:B:322:ASN:HA	1:B:331:ARG:NH1	2.14	0.62
1:C:215:VAL:O	1:C:216:ARG:HB3	2.00	0.62
1:C:258:ALA:HB3	1:C:304:LEU:HD21	1.80	0.62
1:C:234:LEU:HG	1:C:272:GLU:HG2	1.81	0.62
1:A:361:VAL:HG21	1:A:364:LEU:HD12	1.80	0.62
1:C:465:SER:HB2	1:C:489:LEU:HD11	1.81	0.62
1:A:322:ASN:HA	1:A:331:ARG:NH1	2.15	0.61
1:C:522:TYR:CE2	1:C:526:LYS:HD3	2.35	0.61
1:A:555:SER:HB3	1:A:611:LEU:HD22	1.83	0.61
1:C:94:TYR:OH	1:C:168:SER:HB3	2.01	0.61
1:C:120:LEU:HD13	2:P:1:TYR:HB3	1.83	0.61
1:B:370:ALA:HB1	3:B:786:HOH:O	2.00	0.61
1:B:700:ASP:OD2	1:B:736:ASP:HB3	2.01	0.60
1:B:94:TYR:OH	1:B:168:SER:HB3	2.02	0.60
1:B:106:VAL:O	1:B:110:VAL:HG23	2.01	0.60
1:A:734:THR:O	1:A:735:ARG:HB2	2.01	0.60
1:B:444:LEU:HD22	1:B:512:THR:HG21	1.83	0.60
1:C:172:LEU:O	1:C:176:VAL:HG23	2.02	0.60
1:A:258:ALA:HB3	1:A:304:LEU:HD21	1.82	0.60
1:B:561:GLU:HG2	1:B:562:GLN:HG2	1.83	0.59
1:B:489:LEU:HB3	1:B:513:LEU:HD22	1.85	0.59
1:A:94:TYR:OH	1:A:168:SER:HB3	2.00	0.59
1:A:585:LYS:HD3	1:A:586:ASP:OD1	2.02	0.59
1:C:187:GLU:HB2	3:C:782:HOH:O	2.02	0.59
1:A:272:GLU:HB3	1:A:274:PHE:HE1	1.67	0.59
1:A:698:ASN:HD21	1:A:733:ASN:HD22	1.47	0.59
1:B:555:SER:HB3	1:B:611:LEU:HD22	1.85	0.59
1:C:272:GLU:HB3	1:C:274:PHE:HE1	1.68	0.59
1:B:227:LEU:HB2	1:B:460:ALA:HB3	1.85	0.58
1:A:18:ASN:ND2	1:A:21:LYS:HE3	2.18	0.58
1:C:700:ASP:OD2	1:C:736:ASP:HB3	2.03	0.58
1:A:585:LYS:HD2	1:A:585:LYS:N	2.19	0.58
1:A:519:ASN:ND2	1:A:522:TYR:HB3	2.19	0.58
1:B:585:LYS:HD2	1:B:585:LYS:N	2.17	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:GLN:HG3	1:C:333:MET:HG3	1.84	0.58
1:C:585:LYS:HD3	1:C:586:ASP:OD1	2.03	0.58
1:C:120:LEU:HD13	2:P:1:TYR:CG	2.38	0.58
1:A:369:PHE:CG	1:A:434:ARG:HG2	2.39	0.58
1:C:56:SER:O	1:C:60:GLU:HG2	2.03	0.57
1:C:444:LEU:HD22	1:C:512:THR:HG21	1.85	0.57
1:C:698:ASN:HD21	1:C:733:ASN:HD22	1.52	0.57
1:B:215:VAL:O	1:B:216:ARG:CB	2.52	0.57
1:B:56:SER:O	1:B:60:GLU:HG2	2.04	0.57
1:B:585:LYS:HD3	1:B:586:ASP:OD1	2.05	0.57
1:C:106:VAL:O	1:C:110:VAL:HG23	2.05	0.57
1:B:479:GLU:HB2	1:B:550:TYR:CE1	2.40	0.57
1:A:176:VAL:HG22	3:A:787:HOH:O	2.05	0.57
1:B:522:TYR:CE2	1:B:526:LYS:HD3	2.39	0.57
1:B:541:HIS:NE2	1:B:687:LYS:HE2	2.20	0.56
1:B:272:GLU:HB3	1:B:274:PHE:HE1	1.69	0.56
1:C:489:LEU:HB3	1:C:513:LEU:HD22	1.87	0.56
1:C:548:GLN:HA	1:C:548:GLN:NE2	2.20	0.56
1:A:427:ASP:HB3	1:A:430:ILE:HD12	1.87	0.56
1:A:33:LEU:HB3	1:A:76:ASP:HB3	1.87	0.56
1:B:548:GLN:HA	1:B:548:GLN:NE2	2.21	0.56
1:A:668:LEU:HB2	1:A:671:GLU:HG3	1.88	0.55
1:B:585:LYS:HD2	1:B:585:LYS:H	1.70	0.55
1:B:176:VAL:HG22	3:B:789:HOH:O	2.06	0.55
1:B:215:VAL:HB	3:B:789:HOH:O	2.06	0.55
1:C:686:GLN:NE2	1:C:727:LYS:HD2	2.22	0.55
1:A:56:SER:O	1:A:60:GLU:HG2	2.07	0.55
1:C:150:GLN:NE2	1:C:627:GLN:NE2	2.54	0.55
1:C:176:VAL:HG22	3:C:791:HOH:O	2.05	0.55
1:A:99:PRO:HG2	1:A:137:HIS:CD2	2.42	0.55
1:A:106:VAL:O	1:A:110:VAL:HG23	2.06	0.55
1:A:686:GLN:HE22	1:A:692:SER:HA	1.71	0.55
1:A:187:GLU:HB2	3:C:762:HOH:O	2.06	0.54
1:B:209:THR:N	1:B:210:PRO:HD2	2.21	0.54
1:C:541:HIS:NE2	1:C:687:LYS:HE2	2.21	0.54
1:A:99:PRO:HG2	1:A:137:HIS:CG	2.43	0.54
1:A:150:GLN:NE2	1:A:627:GLN:NE2	2.54	0.54
1:A:561:GLU:HG2	1:A:562:GLN:HG2	1.88	0.54
1:A:272:GLU:HB3	1:A:274:PHE:CE1	2.43	0.54
1:A:479:GLU:HB2	1:A:550:TYR:CE1	2.43	0.54
1:A:558:LEU:CD2	1:A:612:ARG:HG2	2.36	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:LYS:HD2	1:A:585:LYS:H	1.72	0.54
2:D:372:ASN:H	2:D:372:ASN:ND2	2.04	0.54
1:B:30:ALA:HA	1:B:33:LEU:HD12	1.90	0.54
1:B:462:CYS:HB3	1:B:464:LEU:HD21	1.89	0.54
1:B:122:ASP:O	1:B:189:ARG:NH2	2.41	0.54
1:C:49:PHE:CZ	1:C:58:ILE:HG23	2.42	0.54
1:A:522:TYR:CZ	1:A:526:LYS:HD3	2.42	0.54
1:C:99:PRO:HG2	1:C:137:HIS:CG	2.42	0.54
1:B:427:ASP:HB3	1:B:430:ILE:HD12	1.89	0.54
1:B:294:GLN:HG2	1:B:298:ARG:HD3	1.90	0.53
1:A:172:LEU:O	1:A:176:VAL:HG23	2.09	0.53
1:B:286:GLN:HG3	1:B:333:MET:HG3	1.89	0.53
1:C:561:GLU:HG2	1:C:562:GLN:HG2	1.89	0.53
1:C:548:GLN:HA	1:C:548:GLN:HE21	1.72	0.53
1:C:555:SER:HB3	1:C:611:LEU:HD22	1.90	0.53
1:A:313:VAL:HG22	1:A:317:LEU:HD22	1.91	0.53
1:A:548:GLN:HA	1:A:548:GLN:NE2	2.24	0.53
1:A:700:ASP:OD2	1:A:736:ASP:HB3	2.08	0.53
1:B:99:PRO:HG2	1:B:137:HIS:CD2	2.44	0.53
1:B:99:PRO:HG2	1:B:137:HIS:CG	2.43	0.53
1:B:18:ASN:ND2	1:B:21:LYS:HE3	2.24	0.53
1:C:122:ASP:O	1:C:189:ARG:NH2	2.41	0.53
1:A:30:ALA:HA	1:A:33:LEU:HD12	1.91	0.53
1:A:698:ASN:ND2	1:A:733:ASN:ND2	2.51	0.53
1:C:227:LEU:HB2	1:C:460:ALA:HB3	1.91	0.53
1:C:99:PRO:HG2	1:C:137:HIS:CD2	2.44	0.53
1:B:558:LEU:CD2	1:B:612:ARG:HG2	2.37	0.52
1:C:519:ASN:ND2	1:C:522:TYR:HB3	2.24	0.52
1:B:151:LEU:HA	1:B:155:TYR:HB2	1.91	0.52
1:A:541:HIS:NE2	1:A:687:LYS:HE2	2.23	0.52
1:B:172:LEU:O	1:B:176:VAL:HG23	2.10	0.52
1:C:120:LEU:HD13	2:P:1:TYR:CB	2.40	0.52
1:C:427:ASP:HB3	1:C:430:ILE:HD12	1.90	0.52
1:B:83:ARG:CG	1:B:141:MET:HG3	2.36	0.52
1:A:215:VAL:O	1:A:216:ARG:CB	2.58	0.52
1:C:483:ILE:HG23	1:C:487:ARG:HD2	1.91	0.52
1:C:519:ASN:ND2	1:C:632:THR:H	2.08	0.52
1:A:151:LEU:HA	1:A:155:TYR:HB2	1.92	0.52
1:A:548:GLN:HA	1:A:548:GLN:HE21	1.75	0.52
1:B:272:GLU:HB3	1:B:274:PHE:CE1	2.44	0.52
1:B:520:PHE:HB3	1:B:635:ILE:HA	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:VAL:O	1:C:216:ARG:CB	2.58	0.52
1:A:294:GLN:HG2	1:A:298:ARG:HD3	1.91	0.52
1:A:208:PRO:HG2	1:A:211:ILE:HD12	1.91	0.52
1:B:250:GLN:O	1:B:251:ARG:HB2	2.10	0.52
1:C:272:GLU:HB3	1:C:274:PHE:CE1	2.43	0.52
1:C:522:TYR:CZ	1:C:526:LYS:HD3	2.45	0.51
1:A:49:PHE:CZ	1:A:58:ILE:HG23	2.45	0.51
1:A:522:TYR:CD1	1:A:657:PRO:HB2	2.44	0.51
1:B:698:ASN:ND2	1:B:733:ASN:ND2	2.52	0.51
1:C:585:LYS:HD2	1:C:585:LYS:N	2.24	0.51
1:A:286:GLN:HG3	1:A:333:MET:HG3	1.91	0.51
1:C:444:LEU:HD12	1:C:460:ALA:HB1	1.91	0.51
2:F:372:ASN:ND2	2:F:372:ASN:H	2.08	0.51
1:A:250:GLN:O	1:A:251:ARG:HB2	2.10	0.51
1:C:33:LEU:HB3	1:C:76:ASP:HB3	1.91	0.51
1:B:33:LEU:HB3	1:B:76:ASP:HB3	1.92	0.51
1:A:122:ASP:O	1:A:189:ARG:NH2	2.43	0.51
1:A:209:THR:N	1:A:210:PRO:HD2	2.26	0.51
1:C:522:TYR:CD1	1:C:657:PRO:HB2	2.46	0.51
1:B:49:PHE:CZ	1:B:58:ILE:HG23	2.46	0.51
1:C:209:THR:N	1:C:210:PRO:HD2	2.26	0.51
1:B:263:ALA:HB3	1:B:357:SER:HB2	1.92	0.51
1:B:548:GLN:HA	1:B:548:GLN:HE21	1.75	0.50
1:A:107:VAL:O	1:A:111:GLU:HG3	2.11	0.50
1:C:18:ASN:ND2	1:C:21:LYS:HE3	2.26	0.50
1:B:388:ILE:O	1:B:390:LYS:HE3	2.12	0.50
2:E:372:ASN:H	2:E:372:ASN:ND2	2.08	0.50
1:A:415:GLN:HE22	1:A:435:GLN:HA	1.76	0.50
1:A:150:GLN:HE21	1:A:627:GLN:HE22	1.56	0.49
1:B:171:PHE:HA	1:B:174:ILE:HG22	1.94	0.49
1:B:313:VAL:HG22	1:B:317:LEU:HD22	1.93	0.49
1:B:450:ASN:HB2	1:B:454:ASP:OD2	2.12	0.49
1:B:150:GLN:NE2	1:B:627:GLN:NE2	2.60	0.49
1:B:522:TYR:CZ	1:B:526:LYS:HD3	2.47	0.49
1:A:171:PHE:HA	1:A:174:ILE:HG22	1.93	0.49
1:B:312:GLU:O	1:B:316:LEU:HG	2.13	0.49
1:C:479:GLU:HB2	1:C:550:TYR:CE1	2.48	0.49
1:C:10:ARG:O	1:C:11:ASP:C	2.50	0.49
1:C:369:PHE:CG	1:C:434:ARG:HG2	2.47	0.49
1:A:444:LEU:HD12	1:A:460:ALA:HB1	1.94	0.49
1:C:191:GLN:HE21	1:C:195:ARG:NH2	2.00	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ARG:HG3	1:A:331:ARG:NH1	2.27	0.49
1:B:208:PRO:HG2	1:B:211:ILE:HD12	1.94	0.49
1:B:444:LEU:HD12	1:B:460:ALA:HB1	1.94	0.49
1:B:681:LEU:O	1:B:685:MET:HG3	2.12	0.49
1:B:21:LYS:O	1:B:25:VAL:HG23	2.13	0.49
1:C:75:PRO:O	1:C:78:GLN:HG3	2.13	0.49
1:C:263:ALA:HB3	1:C:357:SER:HB2	1.95	0.49
1:C:151:LEU:HA	1:C:155:TYR:HB2	1.94	0.49
1:C:475:LEU:O	1:C:478:LEU:HB2	2.12	0.49
1:C:686:GLN:CD	1:C:727:LYS:HD2	2.34	0.49
1:C:578:LEU:HB3	1:C:579:PRO:HD2	1.95	0.48
1:B:341:LYS:HG2	1:B:722:TYR:OH	2.13	0.48
1:B:686:GLN:CD	1:B:727:LYS:HD2	2.33	0.48
1:C:21:LYS:O	1:C:25:VAL:HG23	2.13	0.48
1:C:700:ASP:CG	1:C:736:ASP:HB3	2.34	0.48
1:B:329:ARG:HG3	1:B:331:ARG:NH1	2.27	0.48
1:A:433:VAL:HG11	1:A:443:ALA:HB1	1.94	0.48
1:B:134:PHE:CE2	1:B:194:LYS:HB2	2.47	0.48
1:C:569:ASN:H	1:C:569:ASN:ND2	2.11	0.48
1:C:28:TRP:O	1:C:31:GLU:HB2	2.14	0.48
1:C:492:LEU:O	1:C:496:GLN:HG2	2.13	0.48
1:A:6:LEU:O	1:A:52:GLY:HA2	2.13	0.48
1:A:34:HIS:O	1:A:35:ASN:HB2	2.12	0.48
1:A:227:LEU:HB2	1:A:460:ALA:HB3	1.95	0.48
1:A:686:GLN:NE2	1:A:727:LYS:HD2	2.28	0.48
1:A:698:ASN:HD22	1:A:733:ASN:HD22	1.60	0.48
1:A:45:SER:CB	1:A:61:THR:HG22	2.43	0.48
1:C:30:ALA:HA	1:C:33:LEU:HD12	1.95	0.47
1:A:263:ALA:HB3	1:A:357:SER:HB2	1.95	0.47
1:B:369:PHE:CG	1:B:434:ARG:HG2	2.49	0.47
1:C:45:SER:CB	1:C:61:THR:HG22	2.45	0.47
1:C:307:PRO:HA	1:C:338:GLN:HB2	1.96	0.47
1:B:187:GLU:HB2	3:B:780:HOH:O	2.14	0.47
1:B:492:LEU:O	1:B:496:GLN:HG2	2.14	0.47
1:A:434:ARG:O	1:A:435:GLN:HB3	2.14	0.47
1:A:532:SER:HA	1:A:677:GLY:HA3	1.95	0.47
1:B:439:CYS:HA	1:B:730:TYR:CE1	2.49	0.47
1:C:462:CYS:HB3	1:C:464:LEU:HD21	1.95	0.47
1:B:222:PHE:HD2	1:B:496:GLN:HB3	1.79	0.47
1:C:171:PHE:HA	1:C:174:ILE:HG22	1.95	0.47
1:C:569:ASN:H	1:C:569:ASN:HD22	1.62	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:617:SER:O	1:B:691:GLN:HG3	2.15	0.47
1:C:341:LYS:HG2	1:C:722:TYR:OH	2.13	0.47
1:C:572:THR:HB	1:C:577:ILE:HB	1.95	0.47
1:A:483:ILE:HG23	1:A:487:ARG:HD2	1.97	0.47
1:B:10:ARG:O	1:B:11:ASP:C	2.53	0.47
1:B:522:TYR:CD1	1:B:657:PRO:HB2	2.49	0.47
1:B:668:LEU:HB2	1:B:671:GLU:HG3	1.97	0.47
1:C:120:LEU:HB3	2:P:1:TYR:CE1	2.50	0.47
1:C:686:GLN:HE22	1:C:692:SER:HA	1.80	0.47
1:A:75:PRO:O	1:A:78:GLN:HG3	2.15	0.47
1:A:519:ASN:ND2	1:A:632:THR:H	2.12	0.47
1:B:686:GLN:HE22	1:B:692:SER:HA	1.80	0.47
1:B:700:ASP:CG	1:B:736:ASP:HB3	2.35	0.47
1:A:21:LYS:O	1:A:25:VAL:HG23	2.15	0.47
1:A:262:ARG:HD2	1:A:274:PHE:HB2	1.97	0.47
1:C:134:PHE:CE2	1:C:194:LYS:HB2	2.49	0.47
1:A:737:GLY:O	1:A:738:ALA:HB3	2.15	0.46
1:B:191:GLN:HE21	1:B:195:ARG:NH2	2.03	0.46
1:C:1:MET:HA	1:C:3:GLN:NE2	2.30	0.46
1:A:83:ARG:CG	1:A:141:MET:HG3	2.36	0.46
1:C:262:ARG:HD2	1:C:274:PHE:HB2	1.97	0.46
1:C:558:LEU:CD2	1:C:612:ARG:HG2	2.41	0.46
1:B:6:LEU:O	1:B:52:GLY:HA2	2.16	0.46
1:C:450:ASN:HB2	1:C:454:ASP:OD2	2.15	0.46
1:A:572:THR:HB	1:A:577:ILE:HB	1.97	0.46
1:C:208:PRO:HG2	1:C:211:ILE:HD12	1.97	0.46
1:C:329:ARG:HG3	1:C:331:ARG:NH1	2.29	0.46
1:A:370:ALA:HB1	3:A:784:HOH:O	2.15	0.46
1:B:415:GLN:HE22	1:B:435:GLN:HA	1.81	0.46
1:A:439:CYS:HA	1:A:730:TYR:CE1	2.51	0.46
1:B:339:ILE:HG22	1:B:340:ASN:N	2.31	0.46
1:C:222:PHE:HD2	1:C:496:GLN:HB3	1.80	0.46
1:C:737:GLY:O	1:C:738:ALA:HB3	2.15	0.46
1:A:686:GLN:CD	1:A:727:LYS:HD2	2.36	0.45
1:B:532:SER:HA	1:B:677:GLY:HA3	1.98	0.45
1:A:191:GLN:HE21	1:A:195:ARG:NH2	2.05	0.45
1:A:341:LYS:HG2	1:A:722:TYR:OH	2.16	0.45
1:B:226:VAL:HG12	1:B:461:LEU:CD2	2.47	0.45
1:A:659:TYR:CE1	1:A:663:HIS:HB3	2.52	0.45
1:B:483:ILE:HG23	1:B:487:ARG:HD2	1.98	0.45
1:B:648:LYS:HE3	1:B:648:LYS:H	1.79	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:353:ILE:HG13	1:C:395:ALA:HB2	1.99	0.45
1:B:45:SER:CB	1:B:61:THR:HG22	2.47	0.45
1:B:117:ASN:H	1:B:117:ASN:ND2	2.13	0.45
1:C:294:GLN:HG2	1:C:298:ARG:HD3	1.98	0.45
1:C:388:ILE:O	1:C:390:LYS:HE3	2.17	0.45
1:A:284:HIS:HA	1:B:287:THR:CB	2.47	0.45
1:A:617:SER:O	1:A:691:GLN:HG3	2.15	0.45
1:B:262:ARG:HD2	1:B:274:PHE:HB2	1.99	0.45
1:C:737:GLY:O	1:C:738:ALA:CB	2.64	0.45
1:A:10:ARG:O	1:A:11:ASP:C	2.55	0.45
1:C:6:LEU:O	1:C:52:GLY:HA2	2.17	0.45
1:C:250:GLN:O	1:C:251:ARG:HB2	2.16	0.45
1:C:532:SER:HA	1:C:677:GLY:HA3	1.98	0.45
1:C:548:GLN:HB2	1:C:688:PHE:HB3	1.99	0.45
1:C:617:SER:O	1:C:691:GLN:HG3	2.17	0.45
1:A:426:PHE:O	1:A:428:PRO:HD3	2.17	0.45
1:B:58:ILE:O	1:B:62:ILE:HG23	2.16	0.45
1:B:737:GLY:O	1:B:738:ALA:HB3	2.16	0.45
1:C:520:PHE:HB3	1:C:635:ILE:HA	1.99	0.45
1:C:633:ASN:O	1:C:634:GLY:C	2.55	0.45
1:A:215:VAL:HB	3:A:787:HOH:O	2.15	0.45
1:A:569:ASN:ND2	1:A:569:ASN:H	2.15	0.45
1:B:262:ARG:HB3	1:B:359:SER:HB3	1.99	0.44
1:C:585:LYS:HD2	1:C:585:LYS:H	1.82	0.44
1:A:58:ILE:O	1:A:62:ILE:HG23	2.18	0.44
1:B:364:LEU:HD22	1:B:375:PHE:CE1	2.52	0.44
1:C:415:GLN:HE22	1:C:435:GLN:HA	1.82	0.44
1:C:434:ARG:O	1:C:435:GLN:HB3	2.18	0.44
1:A:450:ASN:HB2	1:A:454:ASP:OD2	2.17	0.44
1:B:427:ASP:CB	1:B:430:ILE:HD12	2.48	0.44
1:A:681:LEU:O	1:A:685:MET:HG3	2.18	0.44
1:B:179:CYS:SG	1:B:216:ARG:HA	2.57	0.44
1:A:222:PHE:HD2	1:A:496:GLN:HB3	1.82	0.44
1:A:648:LYS:HE3	1:A:648:LYS:H	1.82	0.44
1:A:737:GLY:O	1:A:738:ALA:CB	2.64	0.44
1:B:1:MET:HA	1:B:3:GLN:NE2	2.33	0.44
1:B:307:PRO:HA	1:B:338:GLN:HB2	1.99	0.44
1:C:186:ARG:HG3	3:C:762:HOH:O	2.18	0.44
1:C:425:PRO:HB3	1:C:573:TYR:HE2	1.82	0.44
1:B:433:VAL:HG11	1:B:443:ALA:HB1	2.00	0.44
1:C:107:VAL:O	1:C:111:GLU:HG3	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:GLU:O	1:A:316:LEU:HG	2.18	0.44
1:A:388:ILE:O	1:A:390:LYS:HE3	2.17	0.44
1:B:256:ILE:O	1:B:304:LEU:HA	2.17	0.44
1:B:353:ILE:HG13	1:B:395:ALA:HB2	2.00	0.44
1:A:150:GLN:NE2	1:A:627:GLN:HE22	2.13	0.44
1:A:462:CYS:HB3	1:A:464:LEU:HD21	2.00	0.44
1:B:465:SER:O	1:B:515:ILE:HA	2.18	0.44
1:C:111:GLU:O	2:P:4:GLY:HA2	2.18	0.43
1:A:262:ARG:HB3	1:A:359:SER:HB3	2.01	0.43
1:A:520:PHE:HB3	1:A:635:ILE:HA	1.99	0.43
1:B:279:ILE:H	1:B:279:ILE:HG12	1.58	0.43
1:C:179:CYS:SG	1:C:216:ARG:HA	2.58	0.43
1:B:737:GLY:O	1:B:738:ALA:CB	2.66	0.43
1:A:134:PHE:CE2	1:A:194:LYS:HB2	2.53	0.43
1:C:150:GLN:NE2	1:C:627:GLN:HE22	2.15	0.43
1:C:312:GLU:O	1:C:316:LEU:HG	2.17	0.43
1:C:668:LEU:HB2	1:C:671:GLU:HG3	2.01	0.43
1:B:510:ARG:HB2	1:B:512:THR:HG23	2.00	0.43
1:A:109:MET:HB2	1:A:115:TYR:CD2	2.54	0.42
1:B:75:PRO:O	1:B:78:GLN:HG3	2.19	0.42
1:A:179:CYS:SG	1:A:216:ARG:HA	2.59	0.42
1:A:307:PRO:HA	1:A:338:GLN:HB2	2.00	0.42
1:A:466:ALA:HA	1:A:516:GLY:O	2.19	0.42
1:A:569:ASN:H	1:A:569:ASN:HD22	1.66	0.42
1:C:510:ARG:HB2	1:C:512:THR:HG23	2.01	0.42
1:C:734:THR:O	1:C:735:ARG:CB	2.66	0.42
1:A:364:LEU:HD22	1:A:375:PHE:CE1	2.55	0.42
1:A:227:LEU:HD11	1:A:437:ASN:HB3	2.00	0.42
1:B:226:VAL:HG11	1:B:247:TYR:CD2	2.54	0.42
1:C:226:VAL:HG11	1:C:247:TYR:CD2	2.54	0.42
1:A:492:LEU:O	1:A:496:GLN:HG2	2.19	0.42
1:B:107:VAL:O	1:B:111:GLU:HG3	2.19	0.42
1:B:434:ARG:O	1:B:435:GLN:HB3	2.19	0.42
1:B:217:THR:HB	1:B:218:PRO:CD	2.50	0.42
1:C:681:LEU:O	1:C:685:MET:HG3	2.20	0.42
1:A:463:THR:HG22	1:A:489:LEU:HD22	2.02	0.42
1:A:700:ASP:CG	1:A:736:ASP:HB3	2.40	0.42
1:C:34:HIS:O	1:C:35:ASN:HB2	2.20	0.42
1:A:284:HIS:HA	1:B:287:THR:HB	2.00	0.42
1:C:498:TYR:HA	1:C:499:PRO:HD2	1.94	0.42
1:A:28:TRP:O	1:A:31:GLU:HB2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:PHE:O	1:B:288:ALA:HB3	2.20	0.42
1:C:515:ILE:O	1:C:617:SER:HA	2.19	0.42
1:C:105:HIS:O	1:C:109:MET:HG2	2.20	0.41
1:C:339:ILE:HG22	1:C:340:ASN:N	2.35	0.41
1:A:18:ASN:HD22	1:A:21:LYS:HE3	1.85	0.41
1:A:306:TYR:HB2	1:A:307:PRO:HD2	2.02	0.41
1:A:196:PHE:HZ	1:A:207:LEU:HD11	1.85	0.41
2:D:370:LEU:O	2:D:371:SER:C	2.59	0.41
1:C:489:LEU:HD23	1:C:489:LEU:HA	1.88	0.41
1:A:672:MET:HA	1:A:673:PRO:HD3	1.83	0.41
1:B:474:ASN:N	1:B:474:ASN:HD22	2.18	0.41
1:B:519:ASN:HD22	1:B:519:ASN:HA	1.56	0.41
1:B:659:TYR:CE1	1:B:663:HIS:HB3	2.56	0.41
1:C:217:THR:OG1	1:C:219:THR:HG22	2.21	0.41
1:C:433:VAL:HG11	1:C:443:ALA:HB1	2.03	0.41
1:A:45:SER:HB3	1:A:61:THR:HG22	2.01	0.41
1:A:548:GLN:HE21	1:A:548:GLN:CA	2.32	0.41
1:A:1:MET:HA	1:A:3:GLN:NE2	2.36	0.41
1:B:676:ASP:O	1:B:677:GLY:C	2.58	0.41
1:C:227:LEU:HD11	1:C:437:ASN:HB3	2.02	0.41
1:C:442:ILE:HG13	1:C:462:CYS:SG	2.61	0.41
1:B:479:GLU:HB2	1:B:550:TYR:CD1	2.55	0.41
1:C:279:ILE:H	1:C:279:ILE:HG12	1.61	0.41
1:C:221:GLN:HA	1:C:221:GLN:NE2	2.35	0.41
1:C:293:SER:HB2	1:C:298:ARG:O	2.21	0.41
1:C:313:VAL:HG22	1:C:317:LEU:HD22	2.02	0.41
1:C:370:ALA:HB1	3:C:788:HOH:O	2.20	0.41
1:C:426:PHE:O	1:C:428:PRO:HD3	2.21	0.41
1:C:567:TRP:HB3	1:C:570:GLU:HG3	2.03	0.41
1:A:226:VAL:HG11	1:A:247:TYR:CD2	2.55	0.41
1:B:338:GLN:HE21	1:B:415:GLN:NE2	2.19	0.41
1:C:117:ASN:H	1:C:117:ASN:ND2	2.19	0.41
1:A:436:SER:OG	1:A:440:LEU:HA	2.20	0.40
1:B:522:TYR:O	1:B:526:LYS:HG2	2.20	0.40
1:A:442:ILE:HG13	1:A:462:CYS:SG	2.62	0.40
1:B:519:ASN:ND2	1:B:522:TYR:HB3	2.35	0.40
1:B:659:TYR:O	1:B:660:GLU:C	2.60	0.40
1:C:364:LEU:HD22	1:C:375:PHE:CE1	2.56	0.40
1:C:439:CYS:HA	1:C:730:TYR:CE1	2.56	0.40
1:B:640:GLY:HA2	1:B:668:LEU:HD13	2.03	0.40
1:C:215:VAL:HB	3:C:791:HOH:O	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:THR:HB	1:C:218:PRO:CD	2.51	0.40
1:C:306:TYR:HB2	1:C:307:PRO:HD2	2.03	0.40
1:A:425:PRO:HB3	1:A:573:TYR:HE2	1.86	0.40
1:B:475:LEU:O	1:B:478:LEU:HB2	2.22	0.40
1:C:50:TYR:O	1:C:51:ASP:C	2.60	0.40
1:C:325:VAL:HG13	1:C:328:ASN:HB2	2.04	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	736/761 (97%)	681 (92%)	43 (6%)	12 (2%)	9	37
1	B	736/761 (97%)	679 (92%)	43 (6%)	14 (2%)	8	33
1	C	736/761 (97%)	683 (93%)	40 (5%)	13 (2%)	8	34
2	D	16/20 (80%)	14 (88%)	1 (6%)	1 (6%)	1	8
2	E	16/20 (80%)	13 (81%)	2 (12%)	1 (6%)	1	8
2	F	16/20 (80%)	14 (88%)	1 (6%)	1 (6%)	1	8
2	P	2/20 (10%)	0	1 (50%)	1 (50%)	0	0
All	All	2258/2363 (96%)	2084 (92%)	131 (6%)	43 (2%)	8	33

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	51	ASP
1	A	216	ARG
1	A	294	GLN
1	A	735	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	14	THR
1	B	51	ASP
1	B	294	GLN
1	B	735	ARG
1	C	14	THR
1	C	51	ASP
1	C	294	GLN
1	C	735	ARG
1	A	5	LEU
1	A	11	ASP
1	B	5	LEU
1	B	11	ASP
1	B	13	SER
1	B	216	ARG
1	C	5	LEU
1	C	11	ASP
1	C	216	ARG
1	A	2	ASN
1	A	13	SER
1	B	2	ASN
1	C	2	ASN
1	C	13	SER
1	A	15	GLU
2	D	371	SER
1	B	15	GLU
1	B	622	SER
2	E	371	SER
2	F	371	SER
2	P	3	VAL
1	A	10	ARG
1	B	10	ARG
1	C	10	ARG
1	C	15	GLU
1	B	12	GLY
1	A	12	GLY
1	C	12	GLY
1	B	737	GLY
1	C	737	GLY

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	631/650 (97%)	562 (89%)	69 (11%)	6	25
1	B	631/650 (97%)	560 (89%)	71 (11%)	6	23
1	C	631/650 (97%)	560 (89%)	71 (11%)	6	23
2	D	17/19 (90%)	15 (88%)	2 (12%)	5	21
2	E	17/19 (90%)	15 (88%)	2 (12%)	5	21
2	F	17/19 (90%)	15 (88%)	2 (12%)	5	21
2	P	3/19 (16%)	2 (67%)	1 (33%)	0	0
All	All	1947/2026 (96%)	1729 (89%)	218 (11%)	6	24

All (218) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	GLN
1	A	8	THR
1	A	9	LYS
1	A	14	THR
1	A	16	ARG
1	A	17	ILE
1	A	21	LYS
1	A	31	GLU
1	A	40	GLN
1	A	44	ARG
1	A	48	GLN
1	A	54	LYS
1	A	64	LYS
1	A	72	ARG
1	A	73	ASP
1	A	78	GLN
1	A	96	GLN
1	A	139	ARG
1	A	141	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	149	LYS
1	A	154	LYS
1	A	161	VAL
1	A	165	ILE
1	A	168	SER
1	A	189	ARG
1	A	204	LYS
1	A	206	SER
1	A	225	CYS
1	A	249	SER
1	A	260	ARG
1	A	264	LEU
1	A	279	ILE
1	A	283	LYS
1	A	290	LYS
1	A	297	VAL
1	A	317	LEU
1	A	320	LYS
1	A	323	ARG
1	A	364	LEU
1	A	380	THR
1	A	384	LYS
1	A	386	ASP
1	A	387	SER
1	A	390	LYS
1	A	394	LYS
1	A	408	SER
1	A	424	SER
1	A	440	LEU
1	A	465	SER
1	A	474	ASN
1	A	484	LEU
1	A	505	ARG
1	A	510	ARG
1	A	519	ASN
1	A	530	ARG
1	A	542	LYS
1	A	555	SER
1	A	585	LYS
1	A	605	SER
1	A	607	LYS
1	A	616	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	629	SER
1	A	639	ARG
1	A	643	SER
1	A	648	LYS
1	A	708	LYS
1	A	735	ARG
1	A	736	ASP
2	D	361	ILE
2	D	372	ASN
1	B	3	GLN
1	B	8	THR
1	B	9	LYS
1	B	14	THR
1	B	16	ARG
1	B	17	ILE
1	B	21	LYS
1	B	31	GLU
1	B	40	GLN
1	B	44	ARG
1	B	48	GLN
1	B	54	LYS
1	B	64	LYS
1	B	72	ARG
1	B	73	ASP
1	B	78	GLN
1	B	96	GLN
1	B	139	ARG
1	B	141	MET
1	B	149	LYS
1	B	154	LYS
1	B	161	VAL
1	B	165	ILE
1	B	168	SER
1	B	189	ARG
1	B	204	LYS
1	B	206	SER
1	B	225	CYS
1	B	249	SER
1	B	260	ARG
1	B	264	LEU
1	B	279	ILE
1	B	283	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	290	LYS
1	B	297	VAL
1	B	317	LEU
1	B	320	LYS
1	B	323	ARG
1	B	364	LEU
1	B	380	THR
1	B	384	LYS
1	B	386	ASP
1	B	387	SER
1	B	390	LYS
1	B	394	LYS
1	B	408	SER
1	B	424	SER
1	B	440	LEU
1	B	464	LEU
1	B	465	SER
1	B	474	ASN
1	B	484	LEU
1	B	505	ARG
1	B	510	ARG
1	B	512	THR
1	B	519	ASN
1	B	530	ARG
1	B	542	LYS
1	B	555	SER
1	B	570	GLU
1	B	585	LYS
1	B	605	SER
1	B	607	LYS
1	B	616	LEU
1	B	629	SER
1	B	639	ARG
1	B	643	SER
1	B	648	LYS
1	B	708	LYS
1	B	735	ARG
1	B	736	ASP
2	E	361	ILE
2	E	372	ASN
1	C	3	GLN
1	C	8	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	9	LYS
1	C	14	THR
1	C	16	ARG
1	C	17	ILE
1	C	21	LYS
1	C	31	GLU
1	C	40	GLN
1	C	44	ARG
1	C	48	GLN
1	C	54	LYS
1	C	64	LYS
1	C	72	ARG
1	C	73	ASP
1	C	78	GLN
1	C	96	GLN
1	C	139	ARG
1	C	141	MET
1	C	149	LYS
1	C	154	LYS
1	C	161	VAL
1	C	165	ILE
1	C	168	SER
1	C	189	ARG
1	C	204	LYS
1	C	206	SER
1	C	225	CYS
1	C	249	SER
1	C	260	ARG
1	C	264	LEU
1	C	279	ILE
1	C	283	LYS
1	C	290	LYS
1	C	297	VAL
1	C	317	LEU
1	C	320	LYS
1	C	323	ARG
1	C	364	LEU
1	C	380	THR
1	C	384	LYS
1	C	386	ASP
1	C	387	SER
1	C	390	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	394	LYS
1	C	408	SER
1	C	424	SER
1	C	440	LEU
1	C	464	LEU
1	C	465	SER
1	C	474	ASN
1	C	484	LEU
1	C	505	ARG
1	C	510	ARG
1	C	512	THR
1	C	519	ASN
1	C	526	LYS
1	C	530	ARG
1	C	542	LYS
1	C	570	GLU
1	C	585	LYS
1	C	605	SER
1	C	607	LYS
1	C	616	LEU
1	C	629	SER
1	C	639	ARG
1	C	643	SER
1	C	648	LYS
1	C	708	LYS
1	C	735	ARG
1	C	736	ASP
2	F	361	ILE
2	F	372	ASN
2	P	2	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	46	HIS
1	A	117	ASN
1	A	191	GLN
1	A	221	GLN
1	A	328	ASN
1	A	415	GLN
1	A	496	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	519	ASN
1	A	548	GLN
1	A	569	ASN
1	A	627	GLN
1	A	633	ASN
1	A	686	GLN
1	A	698	ASN
2	D	360	GLN
2	D	372	ASN
1	B	3	GLN
1	B	40	GLN
1	B	46	HIS
1	B	117	ASN
1	B	191	GLN
1	B	221	GLN
1	B	328	ASN
1	B	415	GLN
1	B	496	GLN
1	B	519	ASN
1	B	527	HIS
1	B	548	GLN
1	B	569	ASN
1	B	627	GLN
1	B	633	ASN
1	B	686	GLN
1	B	698	ASN
2	E	360	GLN
2	E	372	ASN
1	C	3	GLN
1	C	18	ASN
1	C	46	HIS
1	C	117	ASN
1	C	191	GLN
1	C	221	GLN
1	C	328	ASN
1	C	415	GLN
1	C	496	GLN
1	C	519	ASN
1	C	548	GLN
1	C	569	ASN
1	C	627	GLN
1	C	633	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	686	GLN
1	C	698	ASN
2	F	360	GLN
2	F	372	ASN

5.3.3 RNA (i)

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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.