



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 08:53 pm BST

PDB ID : 1TFD
Title : HIGH-RESOLUTION X-RAY STUDIES ON RABBIT SERUM TRANSFER-
RIN: PRELIMINARY STRUCTURE ANALYSIS OF THE N-TERMINAL
HALF-MOLECULE AT 2.3 ANGSTROMS RESOLUTION
Authors : Sarra, R.; Lindley, P.F.
Deposited on : 1990-08-16
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (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) : 2.11

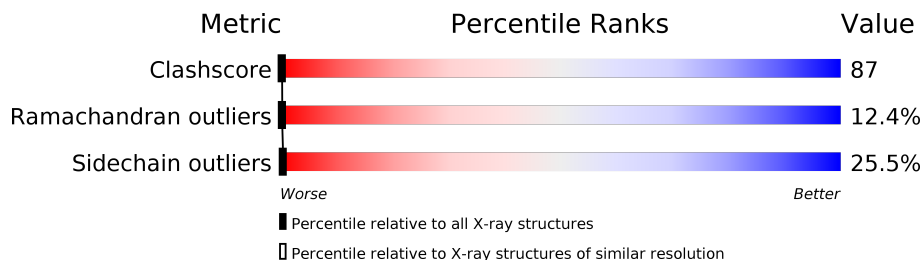
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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 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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	304	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2285 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.

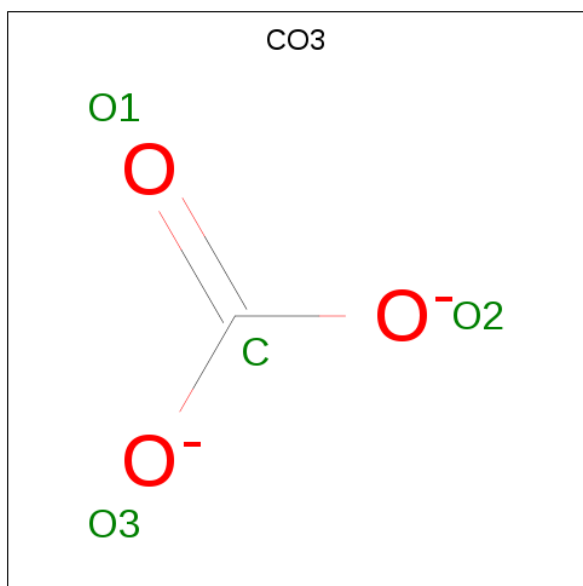
- Molecule 1 is a protein called TRANSFERRIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	294	2280	1447	389	428	16	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	182	SER	VAL	CONFLICT	UNP P19134

- Molecule 2 is CARBONATE ION (three-letter code: CO3) (formula: CO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	4	1	3	0	0

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

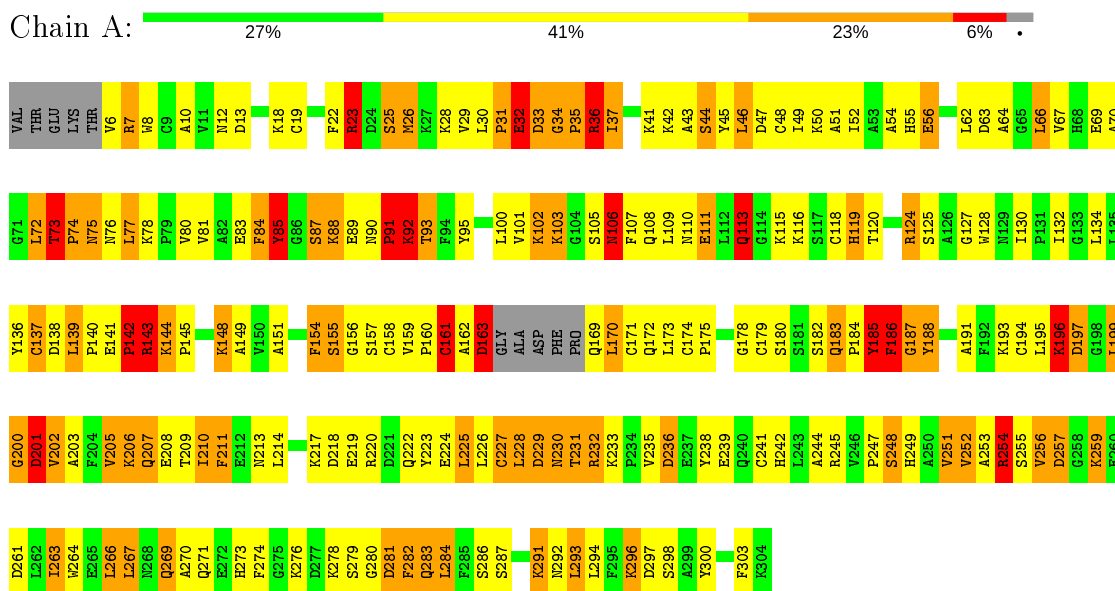
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: TRANSFERRIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	67.06Å 67.06Å 138.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	RESTRAIN	Depositor
R, R_{free}	0.225 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2285	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CO3, FE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.11	3/2334 (0.1%)	1.61	39/3152 (1.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	161	CYS	CA-C	7.20	1.71	1.52
1	A	19	CYS	N-CA	-6.76	1.32	1.46
1	A	142	PRO	N-CD	-5.22	1.40	1.47

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	TYR	O-C-N	-10.08	106.07	123.20
1	A	171	CYS	N-CA-CB	-8.75	94.84	110.60
1	A	229	ASP	O-C-N	8.61	136.48	122.70
1	A	7	ARG	CG-CD-NE	8.49	129.63	111.80
1	A	188	TYR	O-C-N	8.02	135.52	122.70
1	A	85	TYR	CA-C-N	7.99	132.19	116.20
1	A	119	HIS	O-C-N	7.95	135.42	122.70
1	A	185	TYR	CB-CG-CD1	-7.79	116.33	121.00
1	A	36	ARG	NE-CZ-NH2	7.62	124.11	120.30
1	A	254	ARG	NE-CZ-NH2	7.58	124.09	120.30
1	A	205	VAL	O-C-N	7.41	134.56	122.70
1	A	124	ARG	NE-CZ-NH2	7.38	123.99	120.30
1	A	220	ARG	NE-CZ-NH2	7.34	123.97	120.30
1	A	23	ARG	NE-CZ-NH2	7.33	123.96	120.30
1	A	232	ARG	NE-CZ-NH2	7.27	123.94	120.30
1	A	84	PHE	O-C-N	7.25	134.29	122.70
1	A	143	ARG	NE-CZ-NH2	7.19	123.89	120.30
1	A	245	ARG	NE-CZ-NH2	7.17	123.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	SER	CB-CA-C	-6.66	97.44	110.10
1	A	87	SER	O-C-N	6.62	133.29	122.70
1	A	229	ASP	CA-C-N	-6.57	102.74	117.20
1	A	171	CYS	CB-CA-C	-6.51	97.37	110.40
1	A	63	ASP	C-N-CA	-6.34	105.85	121.70
1	A	139	LEU	CB-CA-C	-6.29	98.25	110.20
1	A	188	TYR	CA-C-N	-6.18	103.60	117.20
1	A	252	VAL	O-C-N	6.05	132.38	122.70
1	A	7	ARG	NE-CZ-NH2	6.00	123.30	120.30
1	A	26	MET	CG-SD-CE	6.00	109.80	100.20
1	A	119	HIS	CA-C-N	-5.82	104.39	117.20
1	A	73	THR	O-C-N	5.79	132.10	121.10
1	A	84	PHE	CA-C-N	-5.76	104.53	117.20
1	A	32	GLU	O-C-N	5.66	131.76	122.70
1	A	151	ALA	O-C-N	5.64	131.72	122.70
1	A	256	VAL	O-C-N	5.63	131.72	122.70
1	A	163	ASP	N-CA-C	-5.62	95.83	111.00
1	A	205	VAL	CA-C-N	-5.60	104.89	117.20
1	A	161	CYS	N-CA-CB	-5.42	100.84	110.60
1	A	186	PHE	N-CA-CB	5.31	120.17	110.60
1	A	85	TYR	C-N-CA	-5.14	111.51	122.30

There are no chirality outliers.

There are no planarity outliers.

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	2280	0	2212	393	1
2	A	4	0	0	0	0
3	A	1	0	0	0	0
All	All	2285	0	2212	393	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 87.

All (393) 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:195:LEU:HD13	1:A:199:LEU:CD2	1.22	1.61
1:A:199:LEU:CD1	1:A:202:VAL:N	1.69	1.50
1:A:195:LEU:CD1	1:A:199:LEU:HD21	1.41	1.48
1:A:183:GLN:N	1:A:185:TYR:CE1	1.85	1.44
1:A:183:GLN:CA	1:A:185:TYR:HE1	1.37	1.37
1:A:199:LEU:HD11	1:A:201:ASP:C	1.43	1.35
1:A:199:LEU:HD12	1:A:200:GLY:C	1.48	1.34
1:A:199:LEU:HD11	1:A:202:VAL:N	1.21	1.34
1:A:195:LEU:CD1	1:A:199:LEU:CD2	1.98	1.32
1:A:184:PRO:CD	1:A:185:TYR:CE1	2.11	1.31
1:A:144:LYS:HB3	1:A:145:PRO:CD	1.56	1.31
1:A:183:GLN:CA	1:A:185:TYR:CE1	2.13	1.31
1:A:113:GLN:NE2	1:A:113:GLN:CA	1.88	1.30
1:A:247:PRO:O	1:A:248:SER:CB	1.79	1.29
1:A:113:GLN:HE21	1:A:113:GLN:CA	1.37	1.28
1:A:199:LEU:HD11	1:A:201:ASP:CA	1.64	1.25
1:A:280:GLY:O	1:A:282:PHE:N	1.71	1.23
1:A:163:ASP:CA	1:A:169:GLN:OE1	1.85	1.22
1:A:174:CYS:HB2	1:A:185:TYR:CD2	1.73	1.22
1:A:183:GLN:C	1:A:185:TYR:CE1	2.13	1.21
1:A:183:GLN:CB	1:A:184:PRO:HD3	1.66	1.21
1:A:141:GLU:O	1:A:143:ARG:N	1.72	1.20
1:A:144:LYS:CB	1:A:145:PRO:HD3	1.68	1.20
1:A:163:ASP:HA	1:A:169:GLN:OE1	1.39	1.20
1:A:199:LEU:HD13	1:A:202:VAL:N	1.55	1.19
1:A:33:ASP:O	1:A:34:GLY:O	1.60	1.18
1:A:183:GLN:HB3	1:A:184:PRO:CD	1.67	1.18
1:A:184:PRO:N	1:A:185:TYR:CE1	2.14	1.15
1:A:170:LEU:CD2	1:A:170:LEU:H	1.58	1.15
1:A:182:SER:OG	1:A:185:TYR:CD2	1.99	1.15
1:A:210:ILE:HD13	1:A:210:ILE:N	1.58	1.15
1:A:88:LYS:HZ1	1:A:89:GLU:HB2	1.06	1.14
1:A:185:TYR:HD1	1:A:185:TYR:N	1.07	1.14
1:A:200:GLY:O	1:A:202:VAL:HG23	1.49	1.13
1:A:88:LYS:NZ	1:A:89:GLU:HB2	1.64	1.12
1:A:199:LEU:CD1	1:A:200:GLY:C	2.17	1.11
1:A:199:LEU:HD12	1:A:199:LEU:C	1.71	1.11
1:A:113:GLN:NE2	1:A:113:GLN:HA	0.99	1.09
1:A:30:LEU:HG	1:A:34:GLY:HA3	1.23	1.09
1:A:163:ASP:HA	1:A:169:GLN:CD	1.73	1.09
1:A:184:PRO:HD2	1:A:185:TYR:CE1	1.76	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:PRO:O	1:A:75:ASN:HB2	1.50	1.09
1:A:141:GLU:HB3	1:A:142:PRO:HD2	1.27	1.07
1:A:174:CYS:HB2	1:A:185:TYR:HD2	0.94	1.07
1:A:36:ARG:HH11	1:A:36:ARG:HG2	0.91	1.05
1:A:183:GLN:C	1:A:185:TYR:HE1	1.51	1.04
1:A:210:ILE:H	1:A:210:ILE:CD1	1.67	1.04
1:A:141:GLU:HB3	1:A:142:PRO:CD	1.85	1.03
1:A:174:CYS:CB	1:A:185:TYR:CD2	2.42	1.03
1:A:163:ASP:HA	1:A:169:GLN:NE2	1.71	1.03
1:A:210:ILE:HD13	1:A:210:ILE:H	0.87	1.02
1:A:247:PRO:O	1:A:248:SER:HB3	1.21	1.02
1:A:130:ILE:HD13	1:A:244:ALA:HB3	1.41	1.02
1:A:106:ASN:HD22	1:A:106:ASN:N	1.55	1.02
1:A:144:LYS:HB3	1:A:145:PRO:HD3	1.01	1.01
1:A:30:LEU:CD1	1:A:269:GLN:NE2	2.25	1.00
1:A:227:CYS:SG	1:A:231:THR:O	2.20	0.99
1:A:170:LEU:H	1:A:170:LEU:HD23	1.24	0.99
1:A:185:TYR:CD1	1:A:185:TYR:N	1.81	0.99
1:A:199:LEU:CD1	1:A:201:ASP:N	2.25	0.98
1:A:195:LEU:HD12	1:A:199:LEU:HG	1.45	0.97
1:A:91:PRO:O	1:A:92:LYS:HB2	1.20	0.97
1:A:36:ARG:HG2	1:A:36:ARG:NH1	1.72	0.97
1:A:199:LEU:HD12	1:A:201:ASP:N	1.77	0.96
1:A:199:LEU:CD1	1:A:201:ASP:CA	2.44	0.96
1:A:74:PRO:O	1:A:75:ASN:CB	2.12	0.96
1:A:184:PRO:N	1:A:185:TYR:CD1	2.33	0.95
1:A:183:GLN:C	1:A:185:TYR:CD1	2.38	0.95
1:A:118:CYS:SG	1:A:199:LEU:CB	2.55	0.95
1:A:136:TYR:O	1:A:137:CYS:HB2	1.64	0.95
1:A:158:CYS:SG	1:A:185:TYR:HB3	2.07	0.94
1:A:199:LEU:HD22	1:A:202:VAL:O	1.67	0.94
1:A:101:VAL:HG13	1:A:201:ASP:O	1.66	0.94
1:A:36:ARG:HH11	1:A:36:ARG:CG	1.81	0.94
1:A:91:PRO:O	1:A:92:LYS:CB	2.10	0.94
1:A:183:GLN:CB	1:A:185:TYR:HE1	1.81	0.94
1:A:195:LEU:CD1	1:A:199:LEU:CG	2.45	0.93
1:A:106:ASN:H	1:A:106:ASN:HD22	1.14	0.93
1:A:118:CYS:SG	1:A:199:LEU:HB2	2.09	0.92
1:A:199:LEU:O	1:A:201:ASP:N	2.03	0.92
1:A:195:LEU:CB	1:A:199:LEU:HD23	2.01	0.91
1:A:87:SER:OG	1:A:90:ASN:N	2.03	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ASP:N	1:A:169:GLN:OE1	2.02	0.90
1:A:163:ASP:HA	1:A:169:GLN:HE22	1.37	0.89
1:A:136:TYR:HA	1:A:139:LEU:HG	1.53	0.88
1:A:141:GLU:CB	1:A:142:PRO:HD2	1.94	0.88
1:A:195:LEU:HB2	1:A:199:LEU:HD23	1.55	0.88
1:A:12:ASN:OD1	1:A:13:ASP:N	2.07	0.88
1:A:30:LEU:HD11	1:A:269:GLN:NE2	1.87	0.88
1:A:199:LEU:HD22	1:A:202:VAL:C	1.94	0.87
1:A:199:LEU:O	1:A:199:LEU:HD12	1.75	0.87
1:A:170:LEU:N	1:A:170:LEU:CD2	2.34	0.87
1:A:118:CYS:SG	1:A:199:LEU:HB3	2.15	0.86
1:A:101:VAL:HG13	1:A:201:ASP:HB2	1.57	0.86
1:A:195:LEU:HD12	1:A:199:LEU:CG	2.04	0.85
1:A:144:LYS:CG	1:A:145:PRO:HD3	2.05	0.85
1:A:229:ASP:O	1:A:231:THR:HB	1.78	0.84
1:A:280:GLY:C	1:A:282:PHE:H	1.82	0.84
1:A:170:LEU:HD22	1:A:170:LEU:H	1.42	0.83
1:A:195:LEU:HD13	1:A:199:LEU:CG	2.07	0.83
1:A:199:LEU:CD1	1:A:200:GLY:O	2.24	0.83
1:A:182:SER:OG	1:A:185:TYR:CG	2.32	0.82
1:A:199:LEU:C	1:A:199:LEU:CD1	2.41	0.82
1:A:101:VAL:CG1	1:A:201:ASP:HB2	2.09	0.82
1:A:120:THR:OG1	1:A:127:GLY:HA3	1.78	0.82
1:A:72:LEU:O	1:A:76:ASN:HB2	1.78	0.81
1:A:42:LYS:O	1:A:44:SER:N	2.13	0.81
1:A:169:GLN:HG2	1:A:170:LEU:HD23	1.59	0.81
1:A:8:TRP:HH2	1:A:267:LEU:HD21	1.45	0.81
1:A:188:TYR:HE2	1:A:296:LYS:HD2	1.43	0.81
1:A:183:GLN:N	1:A:185:TYR:CZ	2.24	0.81
1:A:46:LEU:O	1:A:50:LYS:HG3	1.80	0.81
1:A:184:PRO:HD2	1:A:185:TYR:CZ	2.16	0.80
1:A:102:LYS:H	1:A:201:ASP:HB3	1.44	0.80
1:A:199:LEU:O	1:A:199:LEU:CD1	2.30	0.79
1:A:195:LEU:CD1	1:A:201:ASP:HA	2.12	0.79
1:A:119:HIS:CD2	1:A:159:VAL:HG22	2.18	0.79
1:A:195:LEU:HD11	1:A:201:ASP:HA	1.64	0.79
1:A:101:VAL:HG21	1:A:226:LEU:HD13	1.64	0.78
1:A:144:LYS:HB3	1:A:145:PRO:HD2	1.63	0.78
1:A:199:LEU:O	1:A:199:LEU:CG	2.32	0.78
1:A:35:PRO:HB2	1:A:266:LEU:HD13	1.66	0.77
1:A:30:LEU:HB3	1:A:36:ARG:HE	1.47	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:LYS:HD2	1:A:223:TYR:CE2	2.19	0.77
1:A:183:GLN:HB3	1:A:184:PRO:HD3	0.81	0.77
1:A:196:LYS:O	1:A:197:ASP:CB	2.32	0.77
1:A:195:LEU:CD1	1:A:199:LEU:HD23	2.14	0.77
1:A:87:SER:OG	1:A:89:GLU:N	2.17	0.77
1:A:274:PHE:O	1:A:284:LEU:HB2	1.85	0.77
1:A:30:LEU:HB3	1:A:36:ARG:NE	2.01	0.76
1:A:106:ASN:ND2	1:A:106:ASN:N	2.25	0.76
1:A:158:CYS:SG	1:A:185:TYR:CB	2.73	0.76
1:A:196:LYS:O	1:A:197:ASP:HB3	1.85	0.76
1:A:182:SER:OG	1:A:185:TYR:CE2	2.38	0.76
1:A:26:MET:HA	1:A:29:VAL:CG2	2.17	0.75
1:A:88:LYS:NZ	1:A:89:GLU:CB	2.47	0.75
1:A:200:GLY:O	1:A:202:VAL:N	2.20	0.75
1:A:35:PRO:HB2	1:A:266:LEU:CD1	2.16	0.75
1:A:247:PRO:O	1:A:248:SER:HB2	1.84	0.75
1:A:30:LEU:HD11	1:A:269:GLN:HE21	1.51	0.75
1:A:183:GLN:CB	1:A:185:TYR:CE1	2.62	0.74
1:A:233:LYS:HB2	1:A:241:CYS:SG	2.26	0.74
1:A:84:PHE:HE1	1:A:87:SER:O	1.71	0.74
1:A:130:ILE:HD13	1:A:244:ALA:CB	2.16	0.74
1:A:6:VAL:O	1:A:37:ILE:HA	1.88	0.73
1:A:282:PHE:O	1:A:283:GLN:HB2	1.86	0.73
1:A:111:GLU:C	1:A:113:GLN:H	1.91	0.73
1:A:211:PHE:CD1	1:A:211:PHE:N	2.56	0.73
1:A:156:GLY:HA2	1:A:172:GLN:NE2	2.04	0.73
1:A:199:LEU:O	1:A:199:LEU:HG	1.87	0.73
1:A:196:LYS:HG2	1:A:223:TYR:OH	1.87	0.73
1:A:183:GLN:HB3	1:A:185:TYR:CE1	2.23	0.73
1:A:211:PHE:HD1	1:A:211:PHE:N	1.88	0.72
1:A:210:ILE:N	1:A:210:ILE:CD1	2.34	0.72
1:A:200:GLY:O	1:A:202:VAL:CG2	2.33	0.72
1:A:130:ILE:CD1	1:A:244:ALA:HB3	2.19	0.71
1:A:35:PRO:CB	1:A:266:LEU:HD13	2.20	0.71
1:A:31:PRO:O	1:A:33:ASP:N	2.22	0.71
1:A:199:LEU:HD11	1:A:201:ASP:N	1.98	0.71
1:A:169:GLN:HG2	1:A:170:LEU:CD2	2.20	0.70
1:A:259:LYS:O	1:A:263:ILE:HG13	1.92	0.70
1:A:30:LEU:HD12	1:A:269:GLN:NE2	2.05	0.70
1:A:80:VAL:HG12	1:A:81:VAL:HG23	1.71	0.70
1:A:30:LEU:CD1	1:A:269:GLN:HE22	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:LEU:HD12	1:A:200:GLY:N	2.05	0.70
1:A:30:LEU:CD1	1:A:269:GLN:HE21	2.04	0.70
1:A:141:GLU:C	1:A:143:ARG:N	2.40	0.69
1:A:211:PHE:H	1:A:211:PHE:HD1	1.40	0.69
1:A:32:GLU:OE1	1:A:32:GLU:HA	1.92	0.69
1:A:170:LEU:N	1:A:170:LEU:HD23	2.01	0.69
1:A:34:GLY:O	1:A:36:ARG:HD3	1.93	0.69
1:A:46:LEU:HA	1:A:49:ILE:CG1	2.24	0.67
1:A:103:LYS:HG2	1:A:224:GLU:HG3	1.77	0.66
1:A:45:TYR:O	1:A:48:CYS:HB2	1.96	0.66
1:A:274:PHE:CD1	1:A:282:PHE:HB3	2.30	0.66
1:A:95:TYR:CG	1:A:206:LYS:HE3	2.31	0.66
1:A:219:GLU:O	1:A:222:GLN:HB2	1.95	0.66
1:A:85:TYR:OH	1:A:296:LYS:HE2	1.95	0.66
1:A:33:ASP:O	1:A:34:GLY:C	2.34	0.66
1:A:136:TYR:CB	1:A:139:LEU:HG	2.26	0.65
1:A:30:LEU:CB	1:A:36:ARG:HE	2.10	0.65
1:A:174:CYS:HB3	1:A:185:TYR:CD2	2.30	0.65
1:A:264:TRP:O	1:A:264:TRP:CG	2.50	0.64
1:A:105:SER:O	1:A:107:PHE:N	2.31	0.64
1:A:8:TRP:CH2	1:A:267:LEU:HD21	2.30	0.64
1:A:144:LYS:HG2	1:A:145:PRO:HD3	1.80	0.64
1:A:46:LEU:HD12	1:A:50:LYS:HE3	1.79	0.64
1:A:207:GLN:NE2	1:A:207:GLN:H	1.95	0.64
1:A:270:ALA:O	1:A:284:LEU:HD22	1.97	0.64
1:A:26:MET:HA	1:A:29:VAL:HG22	1.78	0.64
1:A:34:GLY:O	1:A:35:PRO:C	2.35	0.64
1:A:87:SER:CB	1:A:90:ASN:H	2.09	0.64
1:A:88:LYS:HZ1	1:A:89:GLU:CB	1.98	0.64
1:A:105:SER:OG	1:A:232:ARG:NH2	2.28	0.63
1:A:276:LYS:HG2	1:A:300:TYR:CD2	2.32	0.63
1:A:46:LEU:HA	1:A:49:ILE:HG13	1.79	0.63
1:A:70:ALA:O	1:A:76:ASN:HB3	1.98	0.63
1:A:208:GLU:O	1:A:208:GLU:CG	2.46	0.63
1:A:292:ASN:HD22	1:A:297:ASP:H	1.44	0.62
1:A:111:GLU:C	1:A:113:GLN:N	2.52	0.62
1:A:83:GLU:HG3	1:A:85:TYR:CZ	2.34	0.62
1:A:87:SER:OG	1:A:88:LYS:N	2.25	0.62
1:A:77:LEU:HD23	1:A:252:VAL:HG23	1.80	0.62
1:A:136:TYR:O	1:A:137:CYS:CB	2.43	0.62
1:A:136:TYR:CA	1:A:139:LEU:HG	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:LEU:CG	1:A:34:GLY:HA3	2.15	0.62
1:A:186:PHE:CD2	1:A:187:GLY:N	2.68	0.61
1:A:188:TYR:CE2	1:A:296:LYS:HD2	2.30	0.61
1:A:256:VAL:O	1:A:257:ASP:HB2	1.99	0.61
1:A:233:LYS:HD3	1:A:241:CYS:SG	2.41	0.61
1:A:73:THR:HG23	1:A:74:PRO:CG	2.31	0.61
1:A:195:LEU:CA	1:A:199:LEU:HD23	2.31	0.61
1:A:184:PRO:CD	1:A:185:TYR:HE1	1.81	0.61
1:A:282:PHE:O	1:A:283:GLN:CB	2.49	0.61
1:A:64:ALA:HA	1:A:67:VAL:HG13	1.81	0.60
1:A:199:LEU:HD12	1:A:200:GLY:CA	2.28	0.60
1:A:33:ASP:C	1:A:34:GLY:O	2.39	0.60
1:A:199:LEU:CD2	1:A:202:VAL:C	2.70	0.59
1:A:54:ALA:O	1:A:55:HIS:HB2	2.02	0.59
1:A:183:GLN:HB3	1:A:185:TYR:HE1	1.59	0.59
1:A:169:GLN:HG2	1:A:170:LEU:H	1.68	0.59
1:A:233:LYS:CD	1:A:241:CYS:SG	2.92	0.58
1:A:73:THR:HG23	1:A:74:PRO:CD	2.34	0.58
1:A:191:ALA:O	1:A:194:CYS:HB3	2.02	0.58
1:A:30:LEU:HD12	1:A:269:GLN:HE22	1.64	0.58
1:A:73:THR:HG23	1:A:74:PRO:HG2	1.85	0.58
1:A:33:ASP:O	1:A:36:ARG:HD3	2.04	0.58
1:A:195:LEU:HB2	1:A:203:ALA:HB2	1.85	0.57
1:A:45:TYR:CD1	1:A:46:LEU:N	2.72	0.57
1:A:184:PRO:HD3	1:A:185:TYR:CE1	2.32	0.57
1:A:170:LEU:N	1:A:170:LEU:HD22	2.08	0.57
1:A:69:GLU:O	1:A:72:LEU:HB2	2.03	0.57
1:A:195:LEU:CG	1:A:199:LEU:CD2	2.79	0.57
1:A:157:SER:C	1:A:173:LEU:HD12	2.24	0.57
1:A:160:PRO:O	1:A:161:CYS:HB2	2.04	0.56
1:A:101:VAL:CG1	1:A:201:ASP:CB	2.83	0.56
1:A:30:LEU:O	1:A:36:ARG:NH2	2.37	0.56
1:A:144:LYS:CB	1:A:145:PRO:CD	2.34	0.56
1:A:73:THR:HG22	1:A:76:ASN:ND2	2.20	0.56
1:A:148:LYS:O	1:A:148:LYS:HG3	2.05	0.56
1:A:183:GLN:CG	1:A:184:PRO:HD3	2.32	0.56
1:A:186:PHE:CG	1:A:187:GLY:N	2.71	0.56
1:A:77:LEU:CD1	1:A:77:LEU:N	2.68	0.56
1:A:46:LEU:HD11	1:A:50:LYS:NZ	2.21	0.55
1:A:113:GLN:C	1:A:113:GLN:NE2	2.58	0.55
1:A:101:VAL:CG1	1:A:201:ASP:O	2.49	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:SER:CA	1:A:173:LEU:HD12	2.36	0.55
1:A:280:GLY:C	1:A:282:PHE:N	2.42	0.54
1:A:183:GLN:C	1:A:185:TYR:H	2.10	0.54
1:A:169:GLN:CG	1:A:170:LEU:CD2	2.85	0.54
1:A:292:ASN:ND2	1:A:297:ASP:H	2.05	0.54
1:A:30:LEU:O	1:A:31:PRO:O	2.25	0.54
1:A:77:LEU:HD12	1:A:77:LEU:N	2.23	0.53
1:A:179:CYS:HA	1:A:186:PHE:CD1	2.43	0.53
1:A:174:CYS:HB3	1:A:185:TYR:HB3	1.89	0.53
1:A:184:PRO:N	1:A:185:TYR:HE1	1.71	0.53
1:A:73:THR:CB	1:A:74:PRO:HD2	2.27	0.53
1:A:174:CYS:HB3	1:A:185:TYR:CG	2.44	0.52
1:A:88:LYS:HZ3	1:A:89:GLU:CB	2.19	0.52
1:A:101:VAL:HG13	1:A:201:ASP:CB	2.36	0.52
1:A:18:LYS:NZ	1:A:284:LEU:O	2.39	0.52
1:A:163:ASP:CA	1:A:169:GLN:HE22	2.17	0.52
1:A:32:GLU:CA	1:A:32:GLU:OE1	2.57	0.52
1:A:199:LEU:HD11	1:A:201:ASP:HA	1.77	0.52
1:A:238:TYR:O	1:A:242:HIS:HB3	2.10	0.52
1:A:10:ALA:O	1:A:41:LYS:HA	2.10	0.52
1:A:205:VAL:HG23	1:A:206:LYS:O	2.10	0.52
1:A:73:THR:C	1:A:75:ASN:H	2.10	0.52
1:A:184:PRO:C	1:A:185:TYR:CD1	2.73	0.51
1:A:95:TYR:HB2	1:A:207:GLN:HE22	1.74	0.51
1:A:195:LEU:HA	1:A:199:LEU:HD23	1.91	0.51
1:A:23:ARG:HA	1:A:37:ILE:HD12	1.92	0.51
1:A:101:VAL:HG12	1:A:201:ASP:HB2	1.90	0.51
1:A:281:ASP:O	1:A:281:ASP:OD1	2.28	0.51
1:A:45:TYR:CG	1:A:46:LEU:N	2.78	0.51
1:A:116:LYS:HA	1:A:156:GLY:O	2.10	0.51
1:A:199:LEU:HD13	1:A:202:VAL:CA	2.36	0.51
1:A:184:PRO:CD	1:A:185:TYR:CD1	2.82	0.50
1:A:46:LEU:HA	1:A:49:ILE:HD12	1.93	0.50
1:A:85:TYR:HH	1:A:296:LYS:HE2	1.75	0.50
1:A:93:THR:OG1	1:A:93:THR:O	2.23	0.50
1:A:46:LEU:HA	1:A:49:ILE:CD1	2.42	0.50
1:A:52:ILE:HG22	1:A:254:ARG:HG3	1.92	0.50
1:A:158:CYS:HB2	1:A:173:LEU:HB2	1.94	0.50
1:A:283:GLN:OE1	1:A:286:SER:OG	2.28	0.50
1:A:77:LEU:HD23	1:A:252:VAL:CG2	2.41	0.50
1:A:102:LYS:N	1:A:201:ASP:HB3	2.22	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:HIS:HB2	1:A:274:PHE:CD2	2.46	0.50
1:A:278:LYS:HG2	1:A:279:SER:N	2.27	0.50
1:A:242:HIS:CD2	1:A:242:HIS:O	2.65	0.49
1:A:195:LEU:CG	1:A:199:LEU:HD23	2.42	0.49
1:A:91:PRO:HB3	1:A:303:PHE:HE2	1.77	0.49
1:A:36:ARG:NH1	1:A:36:ARG:CG	2.50	0.49
1:A:143:ARG:HA	1:A:149:ALA:HB2	1.94	0.49
1:A:51:ALA:O	1:A:56:GLU:N	2.37	0.49
1:A:108:GLN:H	1:A:111:GLU:HG3	1.77	0.49
1:A:195:LEU:HD12	1:A:199:LEU:CD2	2.15	0.48
1:A:225:LEU:O	1:A:232:ARG:HA	2.13	0.48
1:A:101:VAL:HA	1:A:201:ASP:O	2.14	0.48
1:A:22:PHE:HA	1:A:282:PHE:CZ	2.49	0.48
1:A:276:LYS:HG2	1:A:300:TYR:CE2	2.48	0.48
1:A:101:VAL:CG2	1:A:226:LEU:HD13	2.39	0.48
1:A:162:ALA:O	1:A:163:ASP:HB3	2.12	0.48
1:A:34:GLY:O	1:A:36:ARG:N	2.46	0.48
1:A:48:CYS:O	1:A:52:ILE:HG13	2.13	0.48
1:A:72:LEU:N	1:A:72:LEU:HD23	2.29	0.48
1:A:84:PHE:CE1	1:A:87:SER:O	2.60	0.48
1:A:108:GLN:C	1:A:110:ASN:H	2.15	0.47
1:A:261:ASP:OD1	1:A:261:ASP:O	2.32	0.47
1:A:90:ASN:O	1:A:91:PRO:O	2.33	0.47
1:A:184:PRO:CD	1:A:185:TYR:CZ	2.83	0.47
1:A:72:LEU:O	1:A:76:ASN:CB	2.56	0.47
1:A:108:GLN:H	1:A:111:GLU:CG	2.28	0.47
1:A:111:GLU:HG2	1:A:111:GLU:H	1.36	0.47
1:A:31:PRO:C	1:A:33:ASP:N	2.68	0.47
1:A:62:LEU:HB3	1:A:66:LEU:HB3	1.95	0.47
1:A:195:LEU:CB	1:A:199:LEU:CD2	2.82	0.46
1:A:136:TYR:HB2	1:A:143:ARG:HD3	1.97	0.46
1:A:108:GLN:C	1:A:110:ASN:N	2.69	0.46
1:A:102:LYS:HE2	1:A:195:LEU:O	2.16	0.46
1:A:213:ASN:O	1:A:214:LEU:HD23	2.15	0.46
1:A:88:LYS:HZ3	1:A:89:GLU:HB2	1.65	0.46
1:A:111:GLU:O	1:A:113:GLN:N	2.49	0.46
1:A:101:VAL:HG12	1:A:201:ASP:CB	2.46	0.46
1:A:136:TYR:HB3	1:A:139:LEU:CD1	2.45	0.46
1:A:141:GLU:O	1:A:143:ARG:HB2	2.15	0.46
1:A:251:VAL:CG2	1:A:251:VAL:O	2.64	0.46
1:A:183:GLN:H	1:A:185:TYR:CE1	1.60	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LEU:HD11	1:A:201:ASP:CA	2.38	0.46
1:A:207:GLN:HE21	1:A:207:GLN:H	1.60	0.46
1:A:25:SER:O	1:A:28:LYS:HB2	2.16	0.45
1:A:6:VAL:O	1:A:37:ILE:CG2	2.64	0.45
1:A:205:VAL:HG11	1:A:209:THR:HG21	1.98	0.45
1:A:160:PRO:CG	1:A:186:PHE:HA	2.46	0.45
1:A:208:GLU:HG3	1:A:208:GLU:O	2.16	0.45
1:A:136:TYR:HB2	1:A:139:LEU:HG	1.97	0.45
1:A:208:GLU:HG2	1:A:208:GLU:O	2.17	0.45
1:A:174:CYS:HB3	1:A:185:TYR:CB	2.46	0.45
1:A:184:PRO:O	1:A:194:CYS:HB2	2.16	0.45
1:A:136:TYR:CB	1:A:139:LEU:CG	2.94	0.45
1:A:293:LEU:O	1:A:294:LEU:HB2	2.17	0.44
1:A:141:GLU:O	1:A:143:ARG:CB	2.66	0.44
1:A:141:GLU:CB	1:A:142:PRO:CD	2.60	0.44
1:A:154:PHE:O	1:A:155:SER:HB3	2.18	0.44
1:A:169:GLN:HG2	1:A:170:LEU:N	2.32	0.44
1:A:95:TYR:CD2	1:A:206:LYS:HE3	2.53	0.44
1:A:267:LEU:HD12	1:A:267:LEU:HA	1.71	0.43
1:A:296:LYS:HB3	1:A:296:LYS:HE3	1.85	0.43
1:A:196:LYS:O	1:A:197:ASP:HB2	2.17	0.43
1:A:293:LEU:N	1:A:293:LEU:HD13	2.33	0.43
1:A:32:GLU:O	1:A:33:ASP:HB2	2.18	0.43
1:A:184:PRO:CA	1:A:185:TYR:CD1	3.01	0.43
1:A:239:GLU:HA	1:A:242:HIS:HD1	1.83	0.43
1:A:30:LEU:HA	1:A:30:LEU:HD12	1.80	0.43
1:A:178:GLY:C	1:A:179:CYS:SG	2.96	0.43
1:A:183:GLN:CB	1:A:184:PRO:CD	2.44	0.43
1:A:30:LEU:O	1:A:31:PRO:C	2.57	0.43
1:A:136:TYR:C	1:A:138:ASP:H	2.22	0.43
1:A:90:ASN:O	1:A:91:PRO:C	2.56	0.43
1:A:101:VAL:HG21	1:A:226:LEU:CD1	2.42	0.43
1:A:158:CYS:SG	1:A:185:TYR:HB2	2.57	0.43
1:A:66:LEU:HA	1:A:66:LEU:HD12	1.82	0.43
1:A:87:SER:CB	1:A:89:GLU:H	2.31	0.43
1:A:31:PRO:C	1:A:33:ASP:H	2.16	0.42
1:A:37:ILE:H	1:A:37:ILE:HG13	1.36	0.42
1:A:206:LYS:HG3	1:A:207:GLN:N	2.34	0.42
1:A:109:LEU:CD2	1:A:228:LEU:HD12	2.50	0.42
1:A:76:ASN:HB3	1:A:77:LEU:H	1.73	0.42
1:A:103:LYS:HB2	1:A:222:GLN:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:LYS:O	1:A:42:LYS:HG2	2.20	0.41
1:A:73:THR:HA	1:A:74:PRO:HD2	1.42	0.41
1:A:103:LYS:HG2	1:A:224:GLU:CG	2.49	0.41
1:A:85:TYR:CZ	1:A:296:LYS:HE2	2.54	0.41
1:A:105:SER:CB	1:A:201:ASP:OD2	2.68	0.41
1:A:128:TRP:O	1:A:132:ILE:HG12	2.21	0.41
1:A:25:SER:O	1:A:29:VAL:HG22	2.20	0.41
1:A:249:HIS:CE1	1:A:296:LYS:HD3	2.56	0.41
1:A:73:THR:HG23	1:A:74:PRO:HD2	2.02	0.41
1:A:91:PRO:HB3	1:A:303:PHE:CE2	2.55	0.41
1:A:281:ASP:C	1:A:281:ASP:OD1	2.59	0.41
1:A:46:LEU:O	1:A:49:ILE:HB	2.20	0.41
1:A:18:LYS:HD3	1:A:293:LEU:HB2	2.03	0.41
1:A:30:LEU:C	1:A:31:PRO:O	2.59	0.41
1:A:73:THR:CG2	1:A:74:PRO:CD	2.98	0.41
1:A:101:VAL:HG21	1:A:226:LEU:HD22	2.01	0.41
1:A:183:GLN:C	1:A:185:TYR:HD1	2.05	0.41
1:A:108:GLN:O	1:A:110:ASN:N	2.54	0.40
1:A:225:LEU:HD22	1:A:235:VAL:HA	2.01	0.40
1:A:29:VAL:HG23	1:A:30:LEU:H	1.85	0.40
1:A:18:LYS:HD2	1:A:287:SER:HB2	2.03	0.40
1:A:253:ALA:HB2	1:A:263:ILE:HD12	2.03	0.40
1:A:100:LEU:HD13	1:A:210:ILE:CD1	2.51	0.40
1:A:22:PHE:O	1:A:26:MET:HG2	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ASP:OD2	1:A:236:ASP:OD2[4_467]	2.05	0.15

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	290/304 (95%)	206 (71%)	48 (17%)	36 (12%)	0 0

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	ASP
1	A	34	GLY
1	A	35	PRO
1	A	43	ALA
1	A	74	PRO
1	A	75	ASN
1	A	91	PRO
1	A	92	LYS
1	A	106	ASN
1	A	113	GLN
1	A	142	PRO
1	A	144	LYS
1	A	183	GLN
1	A	186	PHE
1	A	197	ASP
1	A	201	ASP
1	A	230	ASN
1	A	248	SER
1	A	281	ASP
1	A	32	GLU
1	A	85	TYR
1	A	155	SER
1	A	187	GLY
1	A	200	GLY
1	A	31	PRO
1	A	180	SER
1	A	257	ASP
1	A	266	LEU
1	A	154	PHE
1	A	125	SER
1	A	140	PRO
1	A	196	LYS
1	A	291	LYS
1	A	254	ARG
1	A	282	PHE
1	A	175	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	247/255 (97%)	184 (74%)	63 (26%)	0 0

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	23	ARG
1	A	25	SER
1	A	36	ARG
1	A	37	ILE
1	A	44	SER
1	A	46	LEU
1	A	47	ASP
1	A	56	GLU
1	A	66	LEU
1	A	72	LEU
1	A	73	THR
1	A	77	LEU
1	A	78	LYS
1	A	88	LYS
1	A	91	PRO
1	A	92	LYS
1	A	93	THR
1	A	102	LYS
1	A	103	LYS
1	A	106	ASN
1	A	111	GLU
1	A	113	GLN
1	A	115	LYS
1	A	124	ARG
1	A	134	LEU
1	A	137	CYS
1	A	143	ARG
1	A	148	LYS
1	A	161	CYS

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Mol	Chain	Res	Type
1	A	163	ASP
1	A	170	LEU
1	A	185	TYR
1	A	193	LYS
1	A	196	LYS
1	A	199	LEU
1	A	201	ASP
1	A	202	VAL
1	A	206	LYS
1	A	207	GLN
1	A	210	ILE
1	A	211	PHE
1	A	217	LYS
1	A	218	ASP
1	A	225	LEU
1	A	227	CYS
1	A	228	LEU
1	A	230	ASN
1	A	231	THR
1	A	236	ASP
1	A	251	VAL
1	A	255	SER
1	A	259	LYS
1	A	263	ILE
1	A	267	LEU
1	A	269	GLN
1	A	271	GLN
1	A	283	GLN
1	A	284	LEU
1	A	291	LYS
1	A	293	LEU
1	A	296	LYS
1	A	298	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	106	ASN
1	A	113	GLN
1	A	172	GLN
1	A	183	GLN

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Mol	Chain	Res	Type
1	A	207	GLN
1	A	213	ASN
1	A	269	GLN
1	A	289	HIS
1	A	292	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	CO3	A	900	3	0,3,3	0.00	-	0,3,3	0.00	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.