Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 12:52 pm BST

PDB ID	:	1YDE
Title	:	Crystal Structure of Human Retinal Short-Chain Dehydrogenase/Reductase 3
Authors	:	Lukacik, P.; Bunkozci, G.; Kavanagh, K.; Sundstrom, M.; Arrowsmith, C.; Edwards, A.; von Delft, F.; Oppermann, U.; Structural Genomics Consortium (SGC)
Deposited on	:	2004-12-23
Resolution	:	2.40 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 ①) were used in the production of this report:

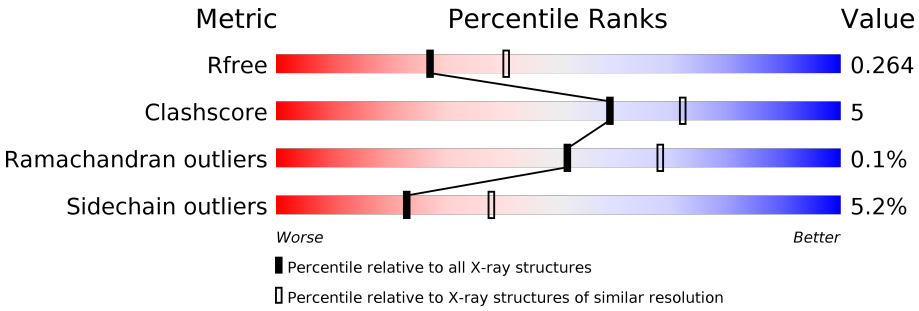
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	270	77% 14% • 7%
1	B	270	78% 12% • 9%
1	C	270	76% 15% • 7%
1	D	270	83% 11% • 6%
1	E	270	78% 13% • 7%
1	F	270	81% 13% • 5%
1	G	270	77% 13% • 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H	270	81% 11% • 6%
1	I	270	81% 9% • 9%
1	J	270	83% 11% 6%
1	K	270	79% 12% • 7%
1	L	270	82% 11% • 6%
1	M	270	77% 13% • 10%
1	N	270	82% 6% • 11%
1	O	270	77% 12% • 9%
1	P	270	81% 11% • 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 30669 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 Retinal dehydrogenase/reductase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	1	0
			1844	1162	324	349	9			
1	B	247	Total	C	N	O	S	0	3	0
			1816	1140	324	342	10			
1	C	250	Total	C	N	O	S	0	0	0
			1847	1162	327	349	9			
1	D	255	Total	C	N	O	S	0	2	0
			1876	1179	330	356	11			
1	E	250	Total	C	N	O	S	0	2	0
			1850	1165	325	350	10			
1	F	256	Total	C	N	O	S	0	2	0
			1896	1191	337	358	10			
1	G	247	Total	C	N	O	S	0	0	0
			1820	1144	323	344	9			
1	H	254	Total	C	N	O	S	0	1	0
			1861	1173	324	354	10			
1	I	247	Total	C	N	O	S	0	0	0
			1825	1150	321	345	9			
1	J	255	Total	C	N	O	S	0	3	0
			1881	1182	331	357	11			
1	K	250	Total	C	N	O	S	0	0	0
			1843	1161	324	349	9			
1	L	255	Total	C	N	O	S	0	1	0
			1870	1177	328	354	11			
1	M	244	Total	C	N	O	S	0	0	0
			1771	1120	303	339	9			
1	N	240	Total	C	N	O	S	0	0	0
			1754	1104	308	333	9			
1	O	247	Total	C	N	O	S	0	0	0
			1806	1140	313	344	9			
1	P	254	Total	C	N	O	S	0	0	0
			1858	1169	327	352	10			

- Molecule 2 is water.

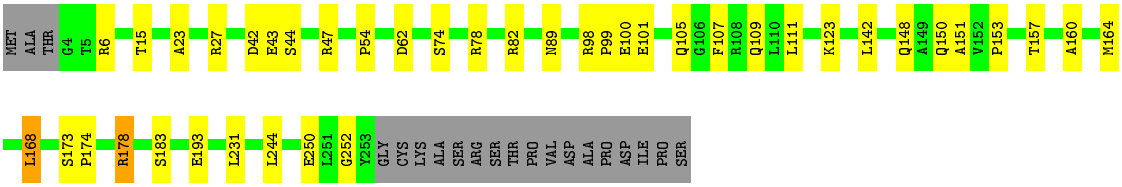
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	133	Total O 133 133	0	0
2	B	121	Total O 121 121	0	0
2	C	123	Total O 123 123	0	0
2	D	130	Total O 130 130	0	0
2	E	116	Total O 116 116	0	0
2	F	113	Total O 113 113	0	0
2	G	86	Total O 86 86	0	0
2	H	78	Total O 78 78	0	0
2	I	54	Total O 54 54	0	0
2	J	68	Total O 68 68	0	0
2	K	89	Total O 89 89	0	0
2	L	78	Total O 78 78	0	0
2	M	22	Total O 22 22	0	0
2	N	13	Total O 13 13	0	0
2	O	9	Total O 9 9	0	0
2	P	18	Total O 18 18	0	0

3 Residue-property plots (i)

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

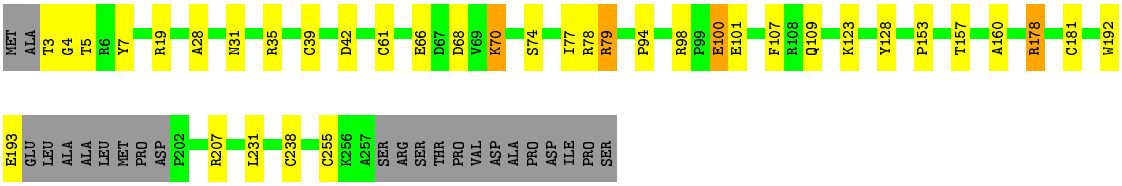
- Molecule 1: Retinal dehydrogenase/reductase 3

Chain A:



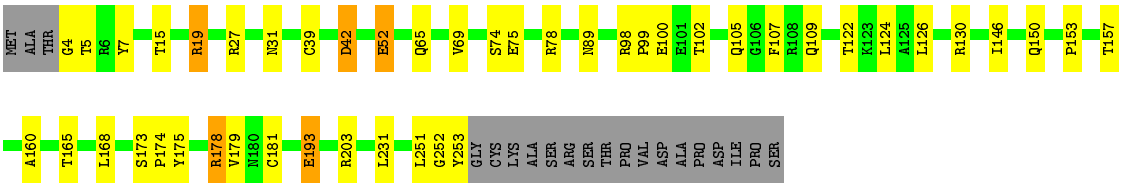
- Molecule 1: Retinal dehydrogenase/reductase 3

Chain B:



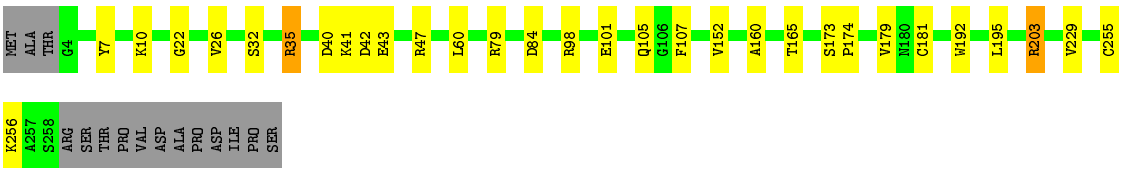
- Molecule 1: Retinal dehydrogenase/reductase 3

Chain C:



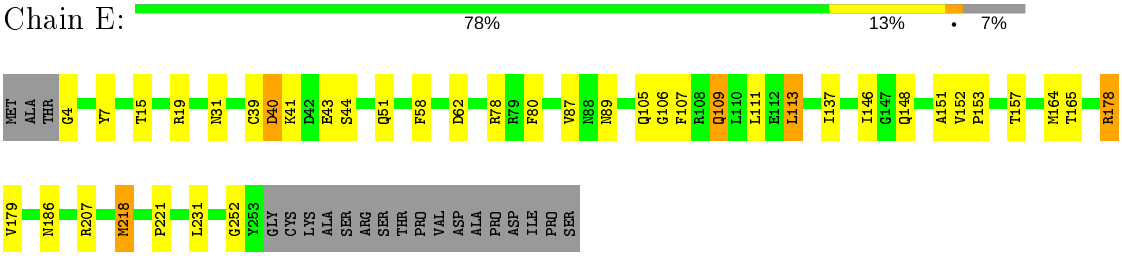
- Molecule 1: Retinal dehydrogenase/reductase 3

Chain D:



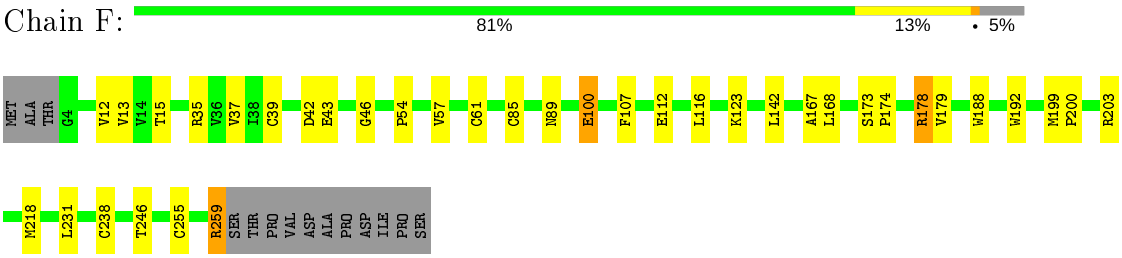
• Molecule 1: Retinal dehydrogenase/reductase 3

Chain E:



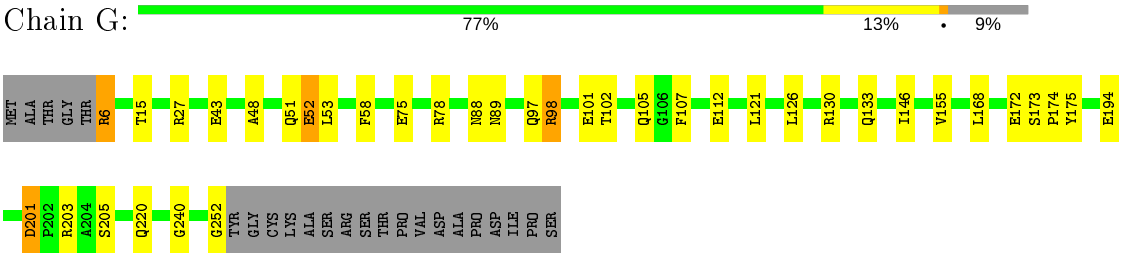
• Molecule 1: Retinal dehydrogenase/reductase 3

Chain F:



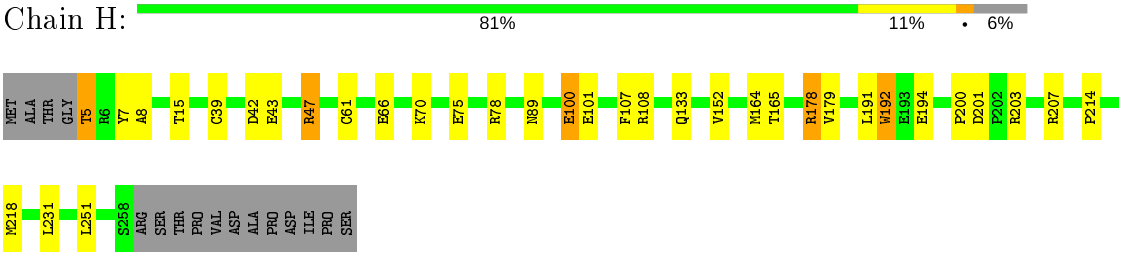
• Molecule 1: Retinal dehydrogenase/reductase 3

Chain G:



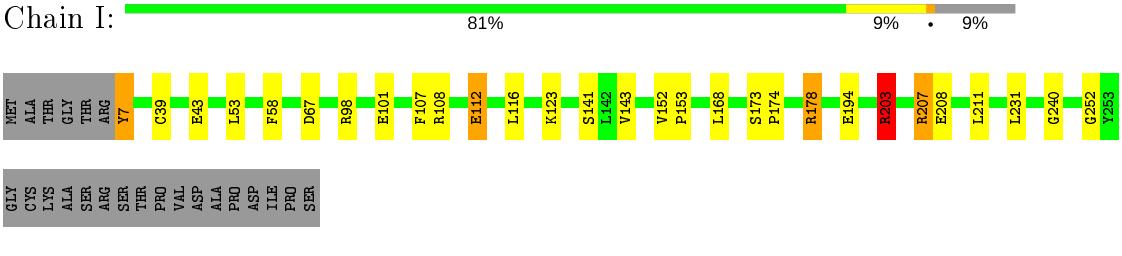
• Molecule 1: Retinal dehydrogenase/reductase 3

Chain H:



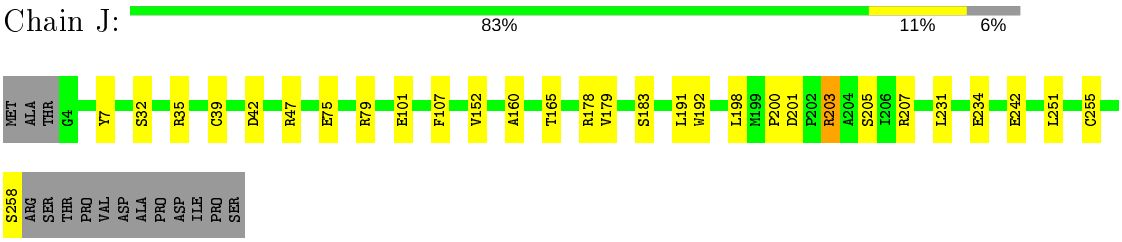
• Molecule 1: Retinal dehydrogenase/reductase 3

Chain I:



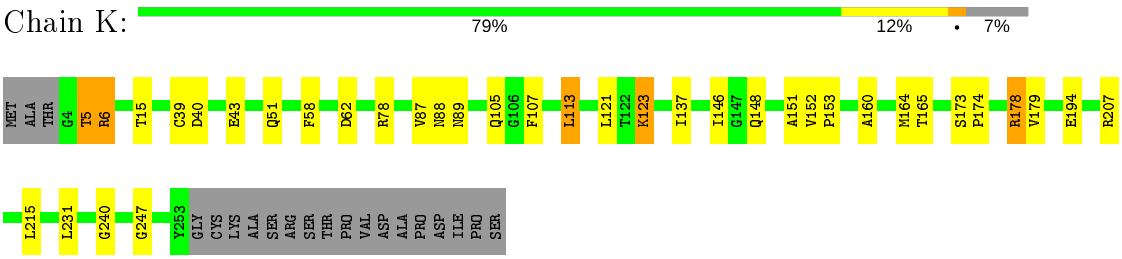
• Molecule 1: Retinal dehydrogenase/reductase 3

Chain J:



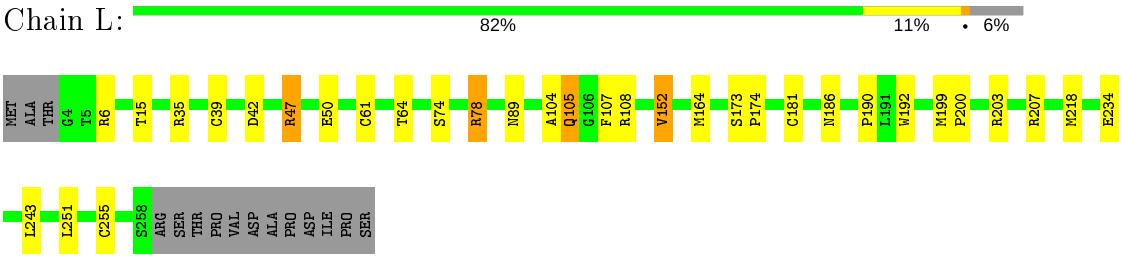
• Molecule 1: Retinal dehydrogenase/reductase 3

Chain K:



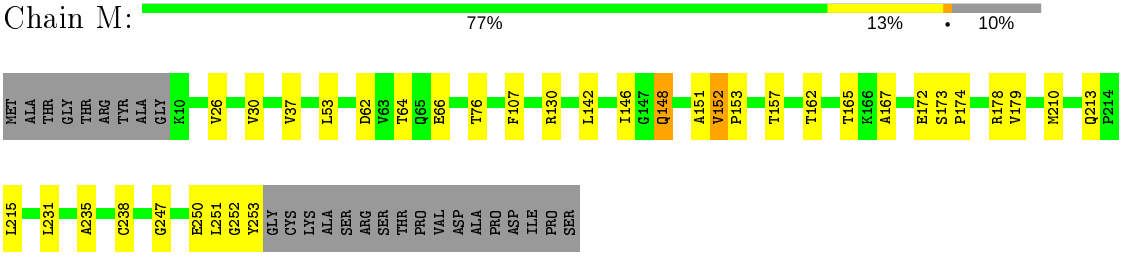
• Molecule 1: Retinal dehydrogenase/reductase 3

Chain L:



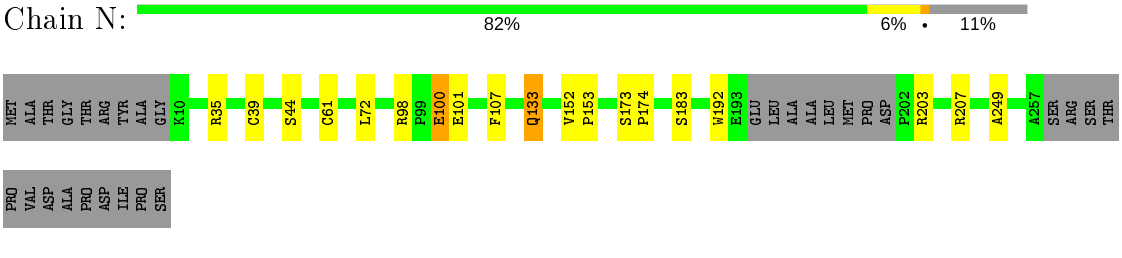
• Molecule 1: Retinal dehydrogenase/reductase 3

Chain M:



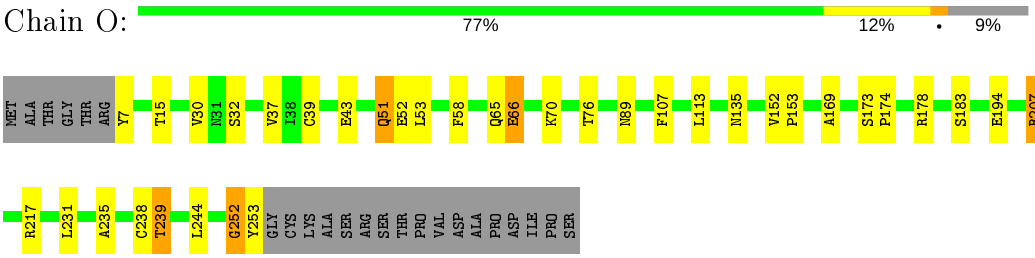
• Molecule 1: Retinal dehydrogenase/reductase 3

Chain N:



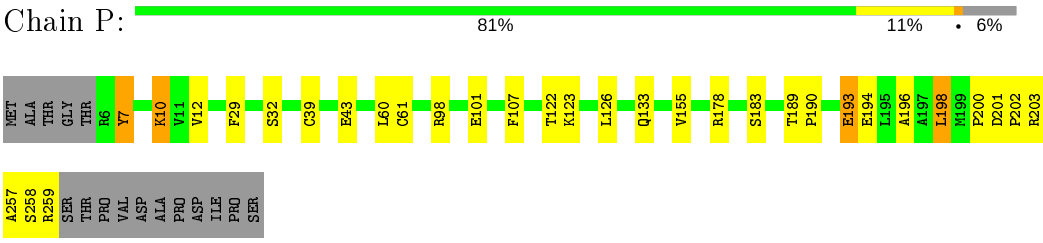
• Molecule 1: Retinal dehydrogenase/reductase 3

Chain O:



• Molecule 1: Retinal dehydrogenase/reductase 3

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	167.12Å 98.82Å 167.46Å 90.00° 115.87° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 75.18 – 2.40	Depositor EDS
% Data completeness (in resolution range)	91.9 (30.00-2.40) 91.4 (75.18-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.181 , 0.229 0.247 , 0.264	Depositor DCC
R_{free} test set	3562 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å^2)	29.1	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 2.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.368 for l,-k,h	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	30669	wwPDB-VP
Average B, all atoms (Å^2)	5.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.97% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.91	0/1879	0.90	7/2555 (0.3%)
1	B	0.94	4/1853 (0.2%)	0.88	3/2517 (0.1%)
1	C	0.94	3/1878 (0.2%)	0.94	5/2553 (0.2%)
1	D	0.85	1/1915 (0.1%)	0.86	3/2602 (0.1%)
1	E	0.89	0/1891	0.92	8/2570 (0.3%)
1	F	0.78	1/1934 (0.1%)	0.80	3/2627 (0.1%)
1	G	0.72	1/1850 (0.1%)	0.81	2/2516 (0.1%)
1	H	0.69	0/1896	0.77	3/2578 (0.1%)
1	I	0.69	0/1856	0.79	3/2524 (0.1%)
1	J	0.71	0/1924	0.77	1/2616 (0.0%)
1	K	0.88	1/1874 (0.1%)	0.89	4/2548 (0.2%)
1	L	0.76	1/1905 (0.1%)	0.75	0/2589
1	M	0.49	0/1801	0.64	0/2455
1	N	0.51	0/1782	0.60	0/2422
1	O	0.51	0/1837	0.63	0/2502
1	P	0.51	0/1889	0.65	0/2569
All	All	0.75	12/29964 (0.0%)	0.80	42/40743 (0.1%)

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

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

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	123	LYS	CE-NZ	7.37	1.67	1.49
1	B	100	GLU	CB-CG	7.33	1.66	1.52
1	C	181	CYS	CB-SG	-6.85	1.70	1.82
1	D	181	CYS	CB-SG	-6.38	1.71	1.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	181	CYS	CB-SG	-6.18	1.71	1.82
1	F	238	CYS	CB-SG	-5.59	1.72	1.81
1	B	238	CYS	CB-SG	-5.41	1.73	1.81
1	C	193	GLU	CG-CD	5.40	1.60	1.51
1	B	28	ALA	CA-CB	-5.39	1.41	1.52
1	C	52	GLU	CB-CG	-5.38	1.42	1.52
1	L	181	CYS	CB-SG	-5.18	1.73	1.81
1	G	201	ASP	CB-CG	-5.08	1.41	1.51

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	178	ARG	NE-CZ-NH1	10.22	125.41	120.30
1	K	178	ARG	NE-CZ-NH2	-10.10	115.25	120.30
1	D	35	ARG	NE-CZ-NH2	-9.69	115.46	120.30
1	E	178	ARG	NE-CZ-NH1	9.52	125.06	120.30
1	C	178	ARG	NE-CZ-NH2	-8.42	116.09	120.30
1	K	178	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	B	178	ARG	NE-CZ-NH1	7.93	124.27	120.30
1	F	178	ARG	NE-CZ-NH2	-7.83	116.38	120.30
1	E	62	ASP	CB-CG-OD1	7.82	125.34	118.30
1	B	178	ARG	NE-CZ-NH2	-7.81	116.40	120.30
1	E	178	ARG	NE-CZ-NH2	-7.65	116.47	120.30
1	A	178	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	C	42	ASP	CB-CG-OD1	7.37	124.93	118.30
1	A	178	ARG	NE-CZ-NH1	7.33	123.96	120.30
1	D	35	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	F	178	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	E	19	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	C	42	ASP	CB-CG-OD2	-6.54	112.42	118.30
1	E	62	ASP	CB-CG-OD2	-6.47	112.48	118.30
1	K	62	ASP	CB-CG-OD1	6.45	124.11	118.30
1	K	40	ASP	CB-CG-OD2	6.06	123.76	118.30
1	B	79	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	H	108	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	E	218[A]	MET	CG-SD-CE	5.71	109.33	100.20
1	E	218[B]	MET	CG-SD-CE	5.71	109.33	100.20
1	G	201	ASP	CB-CA-C	5.67	121.75	110.40
1	C	19	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	78	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	E	40	ASP	N-CA-CB	5.59	120.66	110.60
1	I	108	ARG	NE-CZ-NH1	5.53	123.06	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	203	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	82	ARG	NE-CZ-NH2	5.39	122.99	120.30
1	A	62	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	H	178	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	H	201	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	D	79	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	A	42	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	I	178	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	G	201	ASP	CB-CG-OD1	-5.06	113.75	118.30
1	J	203	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	A	42	ASP	CB-CG-OD1	5.04	122.84	118.30
1	F	255	CYS	CA-CB-SG	5.00	123.00	114.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	198	LEU	Peptide
1	P	257	ALA	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1844	0	1863	22	0
1	B	1816	0	1828	21	0
1	C	1847	0	1872	29	0
1	D	1876	0	1895	18	1
1	E	1850	0	1870	24	0
1	F	1896	0	1922	18	0
1	G	1820	0	1842	23	0
1	H	1861	0	1874	22	0
1	I	1825	0	1849	14	0
1	J	1881	0	1892	12	0
1	K	1843	0	1865	23	1
1	L	1870	0	1884	20	0
1	M	1771	0	1771	19	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	1754	0	1766	9	0
1	O	1806	0	1812	17	0
1	P	1858	0	1868	19	0
2	A	133	0	0	5	0
2	B	121	0	0	1	0
2	C	123	0	0	4	0
2	D	130	0	0	1	0
2	E	116	0	0	4	0
2	F	113	0	0	3	0
2	G	86	0	0	0	0
2	H	78	0	0	1	0
2	I	54	0	0	3	0
2	J	68	0	0	1	0
2	K	89	0	0	3	0
2	L	78	0	0	3	0
2	M	22	0	0	1	0
2	N	13	0	0	0	0
2	O	9	0	0	0	0
2	P	18	0	0	1	0
All	All	30669	0	29673	277	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 5.

All (277) 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:K:123:LYS:CE	1:K:123:LYS:NZ	1.67	1.53
1:B:109:GLN:NE2	1:P:200:PRO:O	1.93	1.02
1:B:255[B]:CYS:HB3	1:D:255[B]:CYS:SG	2.06	0.95
1:B:255[B]:CYS:CB	1:D:255[B]:CYS:SG	2.56	0.94
1:C:193:GLU:HG3	2:C:368:HOH:O	1.71	0.88
1:L:78:ARG:HD2	2:L:337:HOH:O	1.76	0.84
1:I:203:ARG:HG2	1:I:203:ARG:HH11	1.45	0.81
1:B:255[B]:CYS:HB2	1:D:255[B]:CYS:SG	2.20	0.81
1:M:162:THR:HB	2:M:274:HOH:O	1.82	0.80
1:K:6:ARG:H	1:K:6:ARG:HD2	1.46	0.79
1:P:193:GLU:O	1:P:196:ALA:N	2.15	0.79
1:C:105:GLN:O	1:C:109:GLN:HG3	1.84	0.78
1:C:193:GLU:CG	2:C:368:HOH:O	2.29	0.77
1:C:130:ARG:NH1	1:C:175:TYR:CE1	2.54	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:113:LEU:HD23	2:K:353:HOH:O	1.91	0.70
1:L:6:ARG:HD3	1:L:234:GLU:OE2	1.91	0.70
1:F:39:CYS:SG	1:F:61:CYS:HB3	2.31	0.70
1:E:113:LEU:O	2:E:382:HOH:O	2.10	0.69
1:B:193:GLU:HG2	2:B:283:HOH:O	1.92	0.69
1:C:4:GLY:HA2	2:C:380:HOH:O	1.93	0.68
1:E:178:ARG:NH2	1:E:231:LEU:O	2.25	0.68
1:K:152:VAL:HG22	1:K:153:PRO:HD3	1.76	0.68
1:G:130:ARG:NH1	1:G:172:GLU:OE2	2.28	0.66
1:G:130:ARG:NH1	1:G:175:TYR:CD1	2.64	0.65
1:E:4:GLY:HA3	2:E:366:HOH:O	1.97	0.64
1:C:19:ARG:HD2	1:C:42:ASP:OD2	1.98	0.64
1:A:168:LEU:CD1	2:A:399:HOH:O	2.46	0.64
1:N:39:CYS:SG	1:N:61:CYS:HB3	2.39	0.63
1:G:27:ARG:NH2	1:G:52:GLU:OE1	2.30	0.63
1:B:255[B]:CYS:CB	1:D:255[B]:CYS:HG	2.11	0.62
1:E:186:ASN:HB3	1:E:218[B]:MET:CE	2.29	0.62
1:M:210:MET:O	1:M:213:GLN:NE2	2.33	0.62
1:C:27:ARG:NH2	1:C:52:GLU:OE1	2.32	0.62
1:A:193:GLU:HG2	2:A:395:HOH:O	2.00	0.62
1:K:178:ARG:NH2	1:K:231:LEU:O	2.28	0.61
1:L:39:CYS:SG	1:L:61:CYS:HB3	2.40	0.61
1:H:5:THR:HG23	1:H:8:ALA:HB2	1.81	0.61
1:E:164:MET:HG3	1:H:152:VAL:HG13	1.83	0.61
1:E:146:ILE:HD12	1:G:252:GLY:HA2	1.83	0.60
1:A:98:ARG:HG3	1:A:150:GLN:HE21	1.66	0.60
1:A:168:LEU:HD11	2:A:399:HOH:O	2.02	0.59
1:B:178:ARG:NH2	1:B:231:LEU:O	2.34	0.59
1:J:258:SER:C	2:J:277:HOH:O	2.40	0.59
1:M:146:ILE:HD12	1:O:252:GLY:HA2	1.83	0.59
1:G:6:ARG:HG3	1:G:6:ARG:HH11	1.67	0.59
1:D:40:ASP:O	1:D:60:LEU:HD12	2.03	0.58
1:H:192:TRP:NE1	1:H:218:MET:HE3	2.19	0.58
1:P:178:ARG:NH2	1:P:231:LEU:O	2.36	0.58
1:G:52:GLU:HG2	1:G:53:LEU:HG	1.84	0.58
1:C:251:LEU:O	1:C:253:TYR:N	2.37	0.57
1:E:252:GLY:HA2	1:G:146:ILE:HD12	1.87	0.57
1:A:160:ALA:HB2	1:D:160:ALA:HB2	1.85	0.57
1:D:203:ARG:HB2	1:D:203:ARG:CZ	2.33	0.57
1:N:152:VAL:HG23	1:N:153:PRO:HD3	1.85	0.57
1:J:152:VAL:HG13	1:K:164:MET:HG3	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:ARG:NH2	1:C:231:LEU:O	2.29	0.57
1:L:105:GLN:H	1:L:105:GLN:CD	2.08	0.56
1:G:98:ARG:HB2	1:G:101:GLU:HG3	1.88	0.56
1:E:113:LEU:HD23	2:E:292:HOH:O	2.06	0.56
1:P:193:GLU:HG3	1:P:194:GLU:N	2.21	0.56
1:M:215:LEU:HD12	1:M:247:GLY:HA2	1.87	0.55
1:O:178:ARG:NH2	1:O:231:LEU:O	2.39	0.55
1:A:111:LEU:HD23	1:A:157:THR:HG22	1.89	0.55
1:E:186:ASN:HB3	1:E:218[B]:MET:HE1	1.89	0.55
1:H:100:GLU:HG3	2:H:281:HOH:O	2.05	0.55
1:L:47:ARG:HH11	1:L:47:ARG:HG3	1.72	0.55
1:C:173:SER:N	1:C:174:PRO:CD	2.69	0.54
1:K:15:THR:O	1:K:89:ASN:HB3	2.06	0.54
1:O:30:VAL:HG21	1:O:53:LEU:HD13	1.89	0.54
1:H:178:ARG:NH2	1:H:231:LEU:O	2.39	0.54
1:K:215:LEU:HD12	1:K:247:GLY:HA2	1.90	0.54
1:M:178:ARG:NH2	1:M:231:LEU:O	2.41	0.54
1:K:113:LEU:O	2:K:356:HOH:O	2.17	0.54
1:E:106:GLY:HA2	1:E:109[A]:GLN:HG3	1.91	0.53
1:I:7:TYR:N	2:I:324:HOH:O	2.42	0.53
1:M:30:VAL:HG21	1:M:53:LEU:HD13	1.91	0.53
1:A:15:THR:O	1:A:89:ASN:HB3	2.10	0.52
1:O:183:SER:HB2	1:O:244:LEU:HD23	1.90	0.52
1:C:75:GLU:OE1	1:C:78:ARG:HD3	2.09	0.52
1:E:152:VAL:HG13	1:H:164:MET:HG3	1.90	0.52
1:B:4:GLY:HA3	1:B:31:ASN:O	2.09	0.52
1:B:255[B]:CYS:HB2	1:D:255[B]:CYS:HG	1.73	0.52
1:K:5:THR:HG22	1:K:6:ARG:NH1	2.25	0.52
1:I:152:VAL:HG13	1:L:164:MET:HG3	1.92	0.52
1:G:98:ARG:HH11	1:G:98:ARG:HG2	1.74	0.52
1:H:5:THR:CG2	1:H:5:THR:O	2.58	0.52
1:P:258:SER:O	1:P:259:ARG:C	2.49	0.52
1:H:43:GLU:O	1:H:47:ARG:HB2	2.10	0.51
1:C:165:THR:HG23	1:C:179:VAL:HG12	1.92	0.51
1:C:251:LEU:C	1:C:253:TYR:H	2.13	0.51
1:E:165:THR:HG23	1:E:179:VAL:HG12	1.91	0.51
1:O:15:THR:O	1:O:89:ASN:HB3	2.10	0.51
1:M:152:VAL:HG22	1:M:153:PRO:HD3	1.93	0.51
1:I:252:GLY:HA2	1:K:146:ILE:HD12	1.91	0.51
1:M:142:LEU:HD11	1:M:250:GLU:HB3	1.93	0.51
1:P:39:CYS:SG	1:P:61:CYS:HB3	2.51	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:43:GLU:HA	1:O:58:PHE:CZ	2.45	0.51
1:C:4:GLY:N	1:C:31:ASN:O	2.43	0.51
1:I:152:VAL:HB	1:I:153:PRO:HD3	1.92	0.51
1:O:51:GLN:HA	1:O:51:GLN:HE21	1.75	0.51
1:D:22:GLY:O	1:D:26:VAL:HG23	2.11	0.50
1:F:142:LEU:HD13	1:F:246:THR:HG21	1.93	0.50
1:P:200:PRO:O	2:P:272:HOH:O	2.19	0.50
1:F:15:THR:O	1:F:89:ASN:HB3	2.11	0.50
1:P:122:THR:O	1:P:126:LEU:HG	2.11	0.50
2:I:313:HOH:O	1:L:152:VAL:HG13	2.10	0.50
1:F:178:ARG:NH2	1:F:231:LEU:O	2.40	0.50
1:E:186:ASN:HB3	1:E:218[B]:MET:HE2	1.92	0.50
1:M:130:ARG:NH2	1:M:172:GLU:OE1	2.44	0.50
1:M:62:ASP:OD1	1:M:64:THR:OG1	2.18	0.50
1:A:43:GLU:O	1:A:47:ARG:HG3	2.11	0.49
1:K:152:VAL:HG13	2:K:322:HOH:O	2.12	0.49
1:O:173:SER:N	1:O:174:PRO:HD2	2.27	0.49
1:O:169:ALA:HB1	1:O:239:THR:HG23	1.94	0.49
1:O:210:MET:HG2	1:O:217:ARG:HA	1.94	0.49
1:O:207:ARG:N	1:O:207:ARG:HD2	2.28	0.49
1:K:152:VAL:CG2	1:K:153:PRO:HD3	2.42	0.49
1:C:69:VAL:HG12	1:C:124:LEU:HD12	1.94	0.49
1:B:98:ARG:O	1:B:101:GLU:HG2	2.13	0.49
1:P:7:TYR:CD1	1:P:10:LYS:HG3	2.48	0.49
1:C:27:ARG:NH1	1:C:52:GLU:OE1	2.46	0.48
1:C:75:GLU:HA	1:C:78:ARG:HG2	1.95	0.48
1:M:165:THR:HG23	1:M:179:VAL:HG12	1.96	0.48
1:P:39:CYS:HG	1:P:61:CYS:HB3	1.78	0.48
1:G:98:ARG:CG	1:G:98:ARG:HH11	2.26	0.48
1:A:164:MET:HG3	1:D:152:VAL:HG13	1.95	0.48
1:G:75:GLU:HA	1:G:78:ARG:HG2	1.95	0.48
1:F:100:GLU:HG3	1:F:100:GLU:H	1.29	0.48
1:L:104:ALA:O	1:L:108:ARG:HG3	2.14	0.48
1:P:189:THR:HB	1:P:190:PRO:HD2	1.95	0.48
1:D:173:SER:N	1:D:174:PRO:CD	2.77	0.48
1:A:153:PRO:O	1:A:157:THR:HG23	2.13	0.48
1:I:178:ARG:NH2	1:I:231:LEU:O	2.33	0.48
1:O:66:GLU:OE1	1:O:70:LYS:HE2	2.14	0.48
1:K:88:ASN:OD1	1:K:121:LEU:HD23	2.13	0.47
1:A:98:ARG:CG	1:A:150:GLN:HE21	2.26	0.47
1:F:12:VAL:HG13	1:F:85:CYS:HB3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:GLN:HE22	1:P:201:ASP:HA	1.79	0.47
1:G:6:ARG:CG	1:G:6:ARG:HH11	2.26	0.47
1:H:39:CYS:SG	1:H:61:CYS:HB3	2.54	0.47
1:G:173:SER:N	1:G:174:PRO:CD	2.77	0.47
1:A:23:ALA:O	1:A:27:ARG:HG3	2.14	0.47
1:M:173:SER:N	1:M:174:PRO:HD2	2.30	0.47
1:D:43:GLU:OE2	1:D:47:ARG:HD2	2.15	0.47
1:J:201:ASP:OD1	1:J:203:ARG:NH2	2.48	0.47
1:G:173:SER:OG	1:G:174:PRO:HD3	2.13	0.47
1:B:61:CYS:SG	1:B:68:ASP:HB3	2.55	0.47
1:A:148:GLN:HG3	1:A:151:ALA:HB3	1.97	0.46
1:L:190:PRO:HD2	2:L:332:HOH:O	2.15	0.46
1:E:106:GLY:O	1:E:109[A]:GLN:OE1	2.32	0.46
1:H:191:LEU:HA	1:H:194:GLU:HG2	1.98	0.46
1:A:142:LEU:HD11	1:A:250:GLU:HB3	1.96	0.46
1:B:39:CYS:SG	1:B:61:CYS:HB3	2.55	0.46
1:E:40:ASP:HB2	2:E:302:HOH:O	2.15	0.46
1:K:240:GLY:HA3	1:L:251:LEU:HD11	1.97	0.46
1:C:15:THR:O	1:C:89:ASN:HB3	2.14	0.46
1:G:43:GLU:HA	1:G:58:PHE:CZ	2.51	0.46
1:L:47:ARG:NH1	1:L:47:ARG:HG3	2.30	0.46
1:C:251:LEU:C	1:C:253:TYR:N	2.70	0.46
1:N:98:ARG:O	1:N:101:GLU:HG2	2.16	0.46
1:D:98:ARG:O	1:D:101:GLU:HG2	2.16	0.46
1:D:32[A]:SER:OG	1:D:229:VAL:HG11	2.16	0.46
1:J:183:SER:OG	1:J:242:GLU:OE2	2.30	0.46
1:B:123:LYS:NZ	1:C:102:THR:O	2.48	0.45
1:A:173:SER:N	1:A:174:PRO:CD	2.80	0.45
1:P:7:TYR:N	1:P:32:SER:O	2.50	0.45
1:P:43:GLU:HG2	1:P:60:LEU:HD13	1.98	0.45
1:C:193:GLU:HG2	2:C:368:HOH:O	2.08	0.45
1:H:15:THR:O	1:H:89:ASN:HB3	2.16	0.45
1:F:46:GLY:N	2:F:381:HOH:O	2.33	0.45
1:F:123:LYS:NZ	1:G:102:THR:O	2.41	0.45
1:I:112:GLU:OE1	1:I:116:LEU:HD12	2.16	0.45
1:M:235:ALA:HB1	1:M:238:CYS:SG	2.56	0.45
1:E:106:GLY:O	1:E:109[A]:GLN:HG3	2.17	0.45
1:H:200:PRO:HG3	1:J:101:GLU:HA	1.99	0.45
1:I:141:SER:OG	1:I:143:VAL:HG22	2.16	0.45
1:P:12:VAL:HG21	1:P:29:PHE:CD1	2.52	0.45
1:I:207:ARG:HD3	1:I:211:LEU:CD1	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:213:GLN:NE2	1:O:217:ARG:O	2.45	0.45
1:N:249:ALA:O	1:P:256:LYS:NZ	2.43	0.44
1:B:160:ALA:HB2	1:C:160:ALA:HB2	1.99	0.44
1:J:165:THR:HG23	1:J:179:VAL:HG12	1.97	0.44
1:L:243:LEU:C	1:L:243:LEU:HD23	2.38	0.44
1:O:37:VAL:HG21	1:O:76:THR:HG23	2.00	0.44
1:H:66:GLU:HG2	1:H:70:LYS:HZ2	1.81	0.44
1:G:88:ASN:OD1	1:G:121:LEU:HD23	2.18	0.44
1:M:148:GLN:HG2	1:M:151:ALA:HB3	2.00	0.44
1:G:48:ALA:O	1:G:51:GLN:HG2	2.17	0.44
1:M:251:LEU:O	1:M:253:TYR:N	2.51	0.44
1:C:153:PRO:O	1:C:157:THR:HG23	2.18	0.44
1:D:165:THR:HG23	1:D:179:VAL:HG12	1.99	0.44
1:H:66:GLU:HG2	1:H:70:LYS:NZ	2.33	0.44
1:I:53:LEU:O	2:I:322:HOH:O	2.21	0.44
1:O:7:TYR:HB3	1:O:32:SER:HB3	1.99	0.44
1:C:27:ARG:CZ	1:C:52:GLU:OE1	2.66	0.44
1:H:101:GLU:HA	1:J:200:PRO:HG3	1.99	0.43
1:D:105:GLN:NE2	2:D:363:HOH:O	2.50	0.43
1:L:15:THR:O	1:L:89:ASN:HB3	2.18	0.43
1:E:111:LEU:HD23	1:E:157:THR:HG22	2.01	0.43
1:E:87:VAL:HA	1:E:137:ILE:O	2.18	0.43
1:H:192:TRP:CE2	1:H:218:MET:HE3	2.54	0.43
1:A:183:SER:HB2	1:A:244:LEU:HD23	2.01	0.43
1:E:43:GLU:HA	1:E:58:PHE:CZ	2.54	0.43
1:F:259:ARG:NH2	1:H:214:PRO:O	2.52	0.43
1:G:126:LEU:HD11	1:G:168:LEU:HD21	2.00	0.43
1:K:43:GLU:HA	1:K:58:PHE:CZ	2.53	0.43
1:M:167:ALA:HB2	1:P:155:VAL:HG11	1.99	0.43
1:C:99:PRO:HD2	1:C:100:GLU:OE2	2.18	0.43
1:N:173:SER:N	1:N:174:PRO:CD	2.82	0.43
1:P:196:ALA:HA	1:P:202:PRO:HB3	2.00	0.43
1:J:160:ALA:HB2	1:K:160:ALA:HB2	2.00	0.43
1:M:153:PRO:O	1:M:157:THR:HG23	2.18	0.43
1:B:77:ILE:HG13	1:B:128:TYR:CE2	2.54	0.43
1:J:75:GLU:HG3	1:J:79:ARG:HH11	1.84	0.43
1:D:10:LYS:HD3	1:D:84:ASP:CG	2.40	0.43
1:F:167:ALA:HB2	1:G:155:VAL:HG11	2.01	0.43
1:B:79:ARG:HD3	1:E:80:PHE:O	2.19	0.43
1:E:4:GLY:HA2	1:E:31:ASN:O	2.19	0.42
1:H:165:THR:HG23	1:H:179:VAL:HG12	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:133:GLN:HA	1:N:133:GLN:HE21	1.84	0.42
1:A:178:ARG:NH2	1:A:231:LEU:O	2.41	0.42
1:F:188:TRP:N	1:F:218:MET:HE2	2.34	0.42
1:L:186:ASN:HB3	1:L:218:MET:HE3	2.01	0.42
1:E:148:GLN:HG2	1:E:151:ALA:HB3	2.01	0.42
1:K:173:SER:N	1:K:174:PRO:CD	2.82	0.42
1:A:252:GLY:HA2	1:C:146:ILE:HD12	2.01	0.42
1:K:148:GLN:HG2	1:K:151:ALA:HB3	2.00	0.42
1:L:218:MET:HB3	1:L:218:MET:HE2	1.70	0.42
1:L:64:THR:HA	2:L:326:HOH:O	2.18	0.42
1:E:15:THR:O	1:E:89:ASN:HB3	2.19	0.42
1:F:112:GLU:OE1	1:F:116:LEU:HD12	2.18	0.42
1:I:173:SER:N	1:I:174:PRO:CD	2.82	0.42
1:J:178:ARG:NH2	1:J:231:LEU:O	2.53	0.42
1:O:152:VAL:HG22	1:O:153:PRO:HD3	2.00	0.42
1:B:94:PRO:HB3	1:P:200:PRO:HD3	2.02	0.42
1:K:87:VAL:HA	1:K:137:ILE:O	2.20	0.42
1:D:41:LYS:O	1:D:60:LEU:HD11	2.20	0.41
1:N:152:VAL:CG2	1:N:153:PRO:HD3	2.48	0.41
1:O:235:ALA:HB1	1:O:238:CYS:HB2	2.02	0.41
1:A:98:ARG:O	1:A:101:GLU:HG2	2.20	0.41
1:F:54:PRO:HA	2:F:303:HOH:O	2.20	0.41
1:H:207:ARG:HB2	1:H:207:ARG:HE	1.78	0.41
1:F:13:VAL:HG22	1:F:37:VAL:HB	2.02	0.41
1:G:240:GLY:HA3	1:H:251:LEU:HD11	2.01	0.41
1:K:165:THR:HG23	1:K:179:VAL:HG12	2.03	0.41
1:K:5:THR:HG22	1:K:6:ARG:HH11	1.84	0.41
1:L:47:ARG:HH11	1:L:47:ARG:CG	2.33	0.41
1:C:98:ARG:HG3	1:C:150:GLN:HE21	1.86	0.41
1:M:26:VAL:O	1:M:30:VAL:HG22	2.20	0.41
1:B:3:THR:O	1:B:31:ASN:O	2.39	0.41
1:E:152:VAL:HB	1:E:153:PRO:HD3	2.02	0.41
1:L:199:MET:HA	1:L:200:PRO:HD3	1.94	0.41
1:I:98:ARG:HB2	1:I:101:GLU:HG2	2.03	0.41
1:A:54:PRO:HD2	2:A:400:HOH:O	2.21	0.41
1:F:57:VAL:HG13	2:F:318:HOH:O	2.21	0.41
1:H:5:THR:HG22	1:H:5:THR:O	2.21	0.41
1:C:122:THR:O	1:C:126:LEU:HG	2.20	0.41
1:C:130:ARG:NH1	1:C:175:TYR:CD1	2.79	0.41
1:N:39:CYS:SG	1:N:72:LEU:HD22	2.61	0.41
1:A:6:ARG:HD3	2:A:383:HOH:O	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:PRO:HD2	1:A:100:GLU:OE2	2.21	0.40
1:H:133:GLN:HA	1:H:133:GLN:HE21	1.85	0.40
1:I:240:GLY:HA3	1:J:251:LEU:HD11	2.03	0.40
1:K:215:LEU:HD23	1:K:215:LEU:HA	1.91	0.40
1:B:153:PRO:O	1:B:157:THR:HG23	2.20	0.40
1:G:133:GLN:NE2	1:G:175:TYR:O	2.54	0.40
1:I:43:GLU:HA	1:I:58:PHE:CZ	2.57	0.40
1:N:98:ARG:HB3	1:N:100:GLU:OE2	2.21	0.40
1:B:66:GLU:HG2	1:B:70:LYS:HE3	2.03	0.40
1:F:168:LEU:HB3	1:F:179:VAL:HG11	2.04	0.40
1:F:199:MET:HA	1:F:200:PRO:HD3	1.92	0.40
1:G:15:THR:O	1:G:89:ASN:HB3	2.21	0.40
1:M:37:VAL:HG21	1:M:76:THR:HG23	2.03	0.40
1:F:173:SER:N	1:F:174:PRO:CD	2.85	0.40
1:L:173:SER:OG	1:L:174:PRO:HD3	2.22	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:D:35:ARG:NH2	1:K:78:ARG:O[2_444]	2.11	0.09

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	249/270 (92%)	244 (98%)	5 (2%)	0	100	100
1	B	246/270 (91%)	241 (98%)	5 (2%)	0	100	100
1	C	248/270 (92%)	242 (98%)	5 (2%)	1 (0%)	34	48
1	D	255/270 (94%)	252 (99%)	3 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	250/270 (93%)	245 (98%)	5 (2%)	0	100	100
1	F	256/270 (95%)	252 (98%)	4 (2%)	0	100	100
1	G	245/270 (91%)	239 (98%)	6 (2%)	0	100	100
1	H	253/270 (94%)	249 (98%)	4 (2%)	0	100	100
1	I	245/270 (91%)	240 (98%)	5 (2%)	0	100	100
1	J	256/270 (95%)	251 (98%)	5 (2%)	0	100	100
1	K	248/270 (92%)	243 (98%)	5 (2%)	0	100	100
1	L	254/270 (94%)	250 (98%)	4 (2%)	0	100	100
1	M	242/270 (90%)	237 (98%)	4 (2%)	1 (0%)	34	48
1	N	236/270 (87%)	233 (99%)	3 (1%)	0	100	100
1	O	245/270 (91%)	240 (98%)	4 (2%)	1 (0%)	34	48
1	P	252/270 (93%)	243 (96%)	8 (3%)	1 (0%)	34	48
All	All	3980/4320 (92%)	3901 (98%)	75 (2%)	4 (0%)	51	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	252	GLY
1	P	7	TYR
1	C	252	GLY
1	O	252	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	191/208 (92%)	183 (96%)	8 (4%)	30	47
1	B	188/208 (90%)	176 (94%)	12 (6%)	17	28
1	C	192/208 (92%)	184 (96%)	8 (4%)	30	47
1	D	196/208 (94%)	189 (96%)	7 (4%)	35	54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	193/208 (93%)	180 (93%)	13 (7%)	16 26
1	F	197/208 (95%)	189 (96%)	8 (4%)	30 48
1	G	189/208 (91%)	177 (94%)	12 (6%)	18 28
1	H	192/208 (92%)	182 (95%)	10 (5%)	23 38
1	I	190/208 (91%)	179 (94%)	11 (6%)	20 32
1	J	196/208 (94%)	183 (93%)	13 (7%)	16 26
1	K	191/208 (92%)	182 (95%)	9 (5%)	26 42
1	L	193/208 (93%)	181 (94%)	12 (6%)	18 29
1	M	182/208 (88%)	178 (98%)	4 (2%)	52 71
1	N	182/208 (88%)	173 (95%)	9 (5%)	25 40
1	O	186/208 (89%)	173 (93%)	13 (7%)	15 24
1	P	191/208 (92%)	181 (95%)	10 (5%)	23 38
All	All	3049/3328 (92%)	2890 (95%)	159 (5%)	23 38

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	SER
1	A	74	SER
1	A	105	GLN
1	A	107	PHE
1	A	109[A]	GLN
1	A	109[B]	GLN
1	A	123	LYS
1	A	168	LEU
1	B	5	THR
1	B	7	TYR
1	B	19	ARG
1	B	35	ARG
1	B	42	ASP
1	B	70	LYS
1	B	74	SER
1	B	78	ARG
1	B	100	GLU
1	B	107	PHE
1	B	192	TRP
1	B	207	ARG
1	C	5	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	7	TYR
1	C	39	CYS
1	C	65	GLN
1	C	74	SER
1	C	107	PHE
1	C	168	LEU
1	C	203	ARG
1	D	7	TYR
1	D	42	ASP
1	D	107	PHE
1	D	192	TRP
1	D	195	LEU
1	D	203	ARG
1	D	256	LYS
1	E	7	TYR
1	E	39	CYS
1	E	41	LYS
1	E	44	SER
1	E	51	GLN
1	E	78	ARG
1	E	105	GLN
1	E	107	PHE
1	E	109[A]	GLN
1	E	109[B]	GLN
1	E	113	LEU
1	E	207	ARG
1	E	221	PRO
1	F	35	ARG
1	F	42	ASP
1	F	43	GLU
1	F	100	GLU
1	F	107	PHE
1	F	192	TRP
1	F	203	ARG
1	F	259	ARG
1	G	6	ARG
1	G	52	GLU
1	G	97	GLN
1	G	98	ARG
1	G	105	GLN
1	G	107	PHE
1	G	112	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	194	GLU
1	G	201	ASP
1	G	203	ARG
1	G	205	SER
1	G	220	GLN
1	H	5	THR
1	H	7	TYR
1	H	42	ASP
1	H	47	ARG
1	H	75	GLU
1	H	78	ARG
1	H	100	GLU
1	H	107	PHE
1	H	192	TRP
1	H	203	ARG
1	I	7	TYR
1	I	39	CYS
1	I	67	ASP
1	I	107	PHE
1	I	112	GLU
1	I	123	LYS
1	I	168	LEU
1	I	194	GLU
1	I	203	ARG
1	I	207	ARG
1	I	208	GLU
1	J	7	TYR
1	J	32	SER
1	J	35	ARG
1	J	39	CYS
1	J	42	ASP
1	J	47	ARG
1	J	107	PHE
1	J	191	LEU
1	J	192	TRP
1	J	198	LEU
1	J	205	SER
1	J	207	ARG
1	J	234	GLU
1	K	5	THR
1	K	6	ARG
1	K	39	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	51	GLN
1	K	105	GLN
1	K	107	PHE
1	K	113	LEU
1	K	194	GLU
1	K	207	ARG
1	L	35	ARG
1	L	42	ASP
1	L	47	ARG
1	L	50	GLU
1	L	74	SER
1	L	78	ARG
1	L	105	GLN
1	L	107	PHE
1	L	152	VAL
1	L	192	TRP
1	L	203	ARG
1	L	207	ARG
1	M	66	GLU
1	M	107	PHE
1	M	148	GLN
1	M	152	VAL
1	N	35	ARG
1	N	44	SER
1	N	100	GLU
1	N	107	PHE
1	N	133	GLN
1	N	183	SER
1	N	192	TRP
1	N	203	ARG
1	N	207	ARG
1	O	39	CYS
1	O	51	GLN
1	O	52	GLU
1	O	65	GLN
1	O	66	GLU
1	O	107	PHE
1	O	113	LEU
1	O	135	ASN
1	O	194	GLU
1	O	207	ARG
1	O	210	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	239	THR
1	O	253	TYR
1	P	10	LYS
1	P	98	ARG
1	P	101	GLU
1	P	107	PHE
1	P	123	LYS
1	P	133	GLN
1	P	183	SER
1	P	193	GLU
1	P	198	LEU
1	P	203	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	GLN
1	C	97	GLN
1	C	133	GLN
1	C	148	GLN
1	C	150	GLN
1	D	65	GLN
1	D	97	GLN
1	D	133	GLN
1	D	150	GLN
1	E	97	GLN
1	G	31	ASN
1	G	133	GLN
1	G	148	GLN
1	H	150	GLN
1	J	109	GLN
1	K	150	GLN
1	M	97	GLN
1	M	213	GLN
1	M	220	GLN
1	N	97	GLN
1	N	133	GLN
1	N	150	GLN
1	O	51	GLN
1	O	65	GLN
1	O	89	ASN
1	P	133	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	P	150	GLN
1	P	236	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.