



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2026 – 07:00 AM UTC

PDB ID : 1YDE / pdb_00001yde
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 types of validation reports are described at

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

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

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

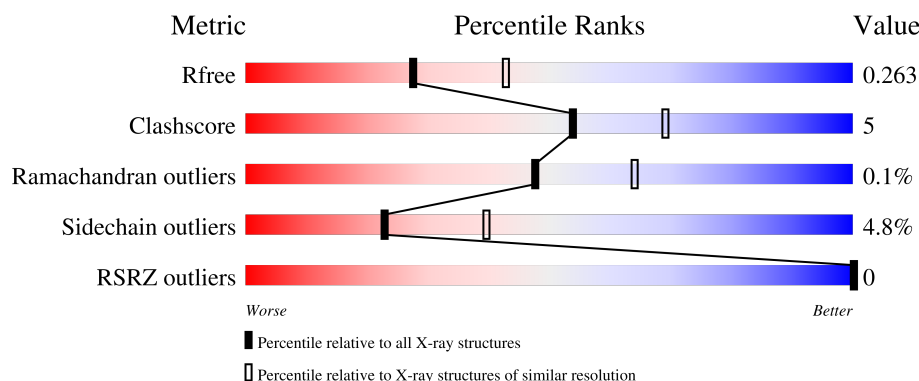
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	270	 78% 14% • 7%
1	B	270	 78% 14% 9%
1	C	270	 75% 16% • 7%
1	D	270	 83% 11% • 6%
1	E	270	 79% 13% • 7%

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Mol	Chain	Length	Quality of chain
1	F	270	 81% 11% • 5%
1	G	270	 77% 13% • 9%
1	H	270	 82% 11% • 6%
1	I	270	 83% 7% • 9%
1	J	270	 81% 13% 6%
1	K	270	 79% 12% • 7%
1	L	270	 83% 10% • 6%
1	M	270	 76% 13% 10%
1	N	270	 81% 7% • 11%
1	O	270	 77% 11% • 9%
1	P	270	 80% 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			

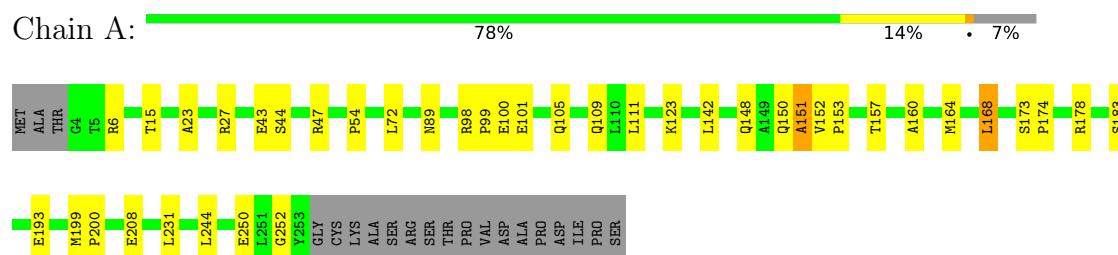
- Molecule 2 is water.

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

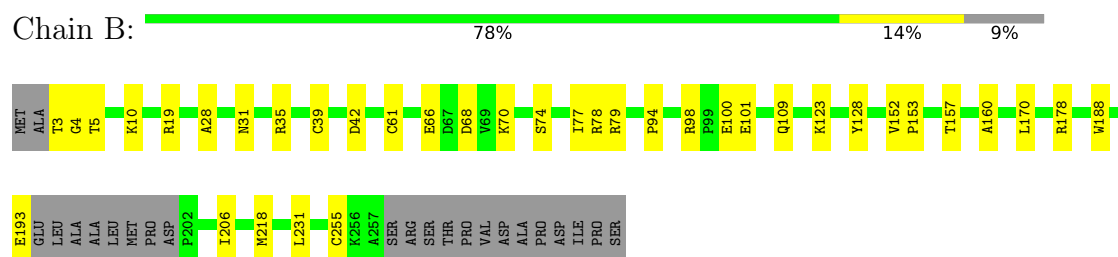
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

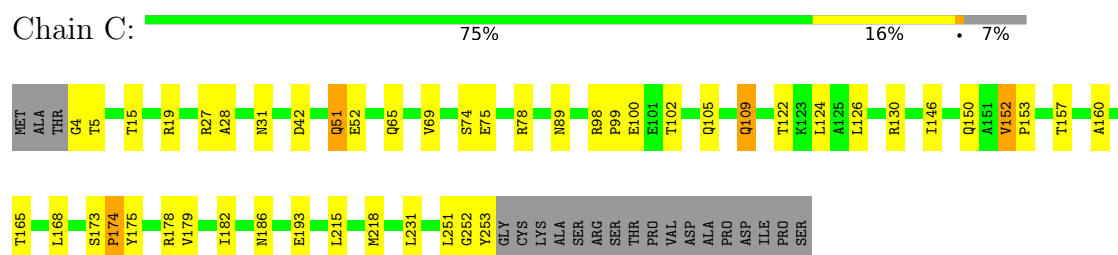
- Molecule 1: Retinal dehydrogenase/reductase 3



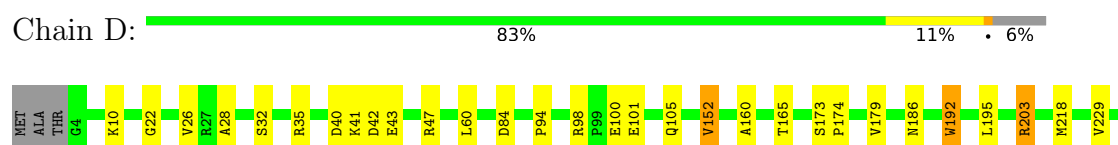
- Molecule 1: Retinal dehydrogenase/reductase 3

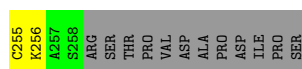


- Molecule 1: Retinal dehydrogenase/reductase 3



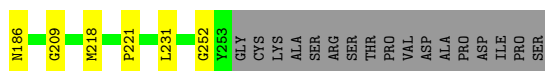
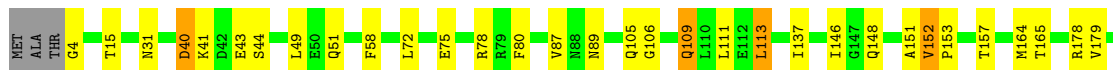
- Molecule 1: Retinal dehydrogenase/reductase 3





• Molecule 1: Retinal dehydrogenase/reductase 3

Chain E: 79% 13% • 7%



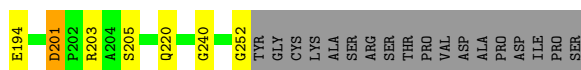
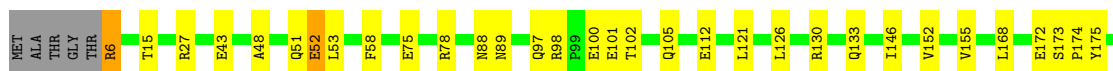
• Molecule 1: Retinal dehydrogenase/reductase 3

Chain F: 81% 11% • 5%



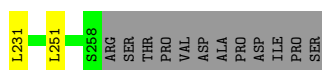
• Molecule 1: Retinal dehydrogenase/reductase 3

Chain G: 77% 13% • 9%



• Molecule 1: Retinal dehydrogenase/reductase 3

Chain H: 82% 11% • 6%



• Molecule 1: Retinal dehydrogenase/reductase 3

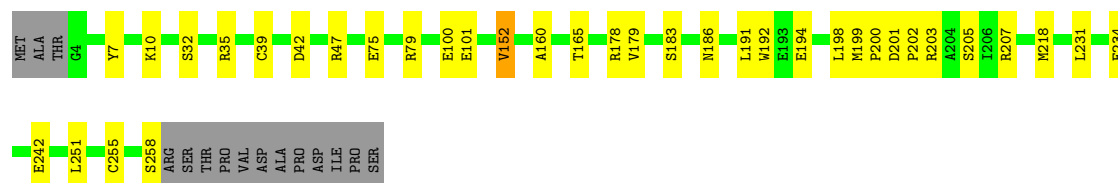
Chain I: 83% 7% • 9%



VAL
ASP
ALA
PRO
ASP
ILE
PRO
SER

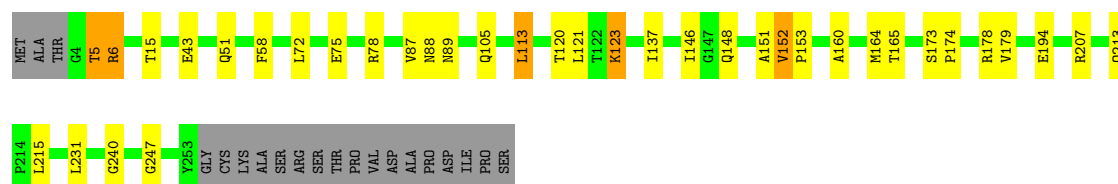
• Molecule 1: Retinal dehydrogenase/reductase 3

Chain J:  81% 13% 6%



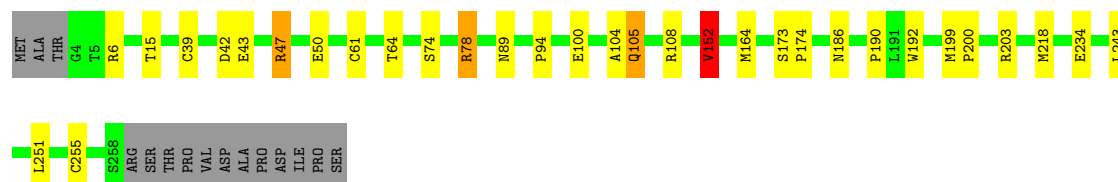
• Molecule 1: Retinal dehydrogenase/reductase 3

Chain K:  79% 12% 7%



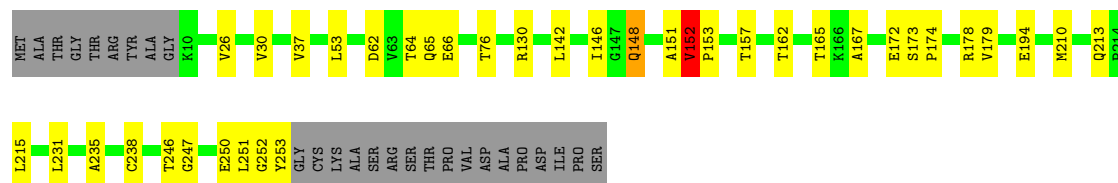
• Molecule 1: Retinal dehydrogenase/reductase 3

Chain L:  83% 10% 6%



• Molecule 1: Retinal dehydrogenase/reductase 3

Chain M:  76% 13% 10%



• Molecule 1: Retinal dehydrogenase/reductase 3

Chain N:  81% 7% 11%



ARG
SER
THR
PRO
VAL
ASP
ALA
PRO
ASP
ILE
PRO
SER

● Molecule 1: Retinal dehydrogenase/reductase 3

Chain O:

77%

11%

•

9%

MET
ALA
THR
GLY
THR
ARG
Y7
T15
V30
N31
S32
V37
E43
Q51
E52
L53
F58
Q65
E66
K70
T76
N89
E100
L113
N135
S140
V152
P153
A169
S173
P174
R178
S183
E194
R207
E208
G209
M210

Q213
R217
L231
A235
C238
T239
L244
G252
Y253
GLY
CYS
LYS
ALA
SER
ARG
SER
THR
PRO
VAL
ASP
ALA
ASP
ILE
PRO
SER

● Molecule 1: Retinal dehydrogenase/reductase 3

Chain P:

80%

11%

•

6%

MET
ALA
THR
GLY
R6
Y7
K10
V11
V12
F29
S32
C39
E43
S44
L60
C61
E100
E101
T122
K123
L126
Q133
V152
V155
R178
S183
T189
P190
E193
E194
L195
A196
A197
L198
R199
P200
D201
P202
R203
L231
I241

C255
K256
A257
S258
R259
SER
THR
PRO
VAL
ASP
ALA
PRO
ASP
ILE
PRO
SER

4 Data and refinement statistics

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 30.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	91.9 (30.00-2.40) 91.4 (30.00-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.181 , 0.229 0.247 , 0.263	Depositor DCC
R_{free} test set	3562 reflections (1.86%)	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 , 27.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.368 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

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	1.13	2/1879 (0.1%)	1.07	0/2555
1	B	1.17	4/1853 (0.2%)	1.08	0/2517
1	C	1.20	4/1878 (0.2%)	1.10	2/2553 (0.1%)
1	D	1.10	2/1915 (0.1%)	1.03	2/2602 (0.1%)
1	E	1.12	1/1891 (0.1%)	1.07	1/2570 (0.0%)
1	F	1.00	3/1934 (0.2%)	1.03	5/2627 (0.2%)
1	G	0.93	1/1850 (0.1%)	1.00	1/2516 (0.0%)
1	H	0.88	0/1896	0.96	1/2578 (0.0%)
1	I	0.87	1/1856 (0.1%)	0.98	0/2524
1	J	0.90	1/1924 (0.1%)	0.97	3/2616 (0.1%)
1	K	1.14	3/1874 (0.2%)	1.10	3/2548 (0.1%)
1	L	0.95	1/1905 (0.1%)	1.03	3/2589 (0.1%)
1	M	0.69	1/1801 (0.1%)	0.91	1/2455 (0.0%)
1	N	0.65	1/1782 (0.1%)	0.86	1/2422 (0.0%)
1	O	0.67	1/1837 (0.1%)	0.92	4/2502 (0.2%)
1	P	0.65	0/1889	0.97	2/2569 (0.1%)
All	All	0.96	26/29964 (0.1%)	1.01	29/40743 (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 (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	152	VAL	CA-CB	16.27	1.63	1.54
1	C	152	VAL	CA-CB	12.62	1.61	1.54
1	L	152	VAL	CA-CB	11.45	1.60	1.54
1	B	152	VAL	CA-CB	11.26	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	152	VAL	CA-CB	10.10	1.59	1.54
1	F	152	VAL	CA-CB	9.88	1.59	1.54
1	G	152	VAL	CA-CB	8.13	1.58	1.54
1	D	152	VAL	CA-CB	8.02	1.58	1.54
1	N	152	VAL	CA-CB	8.00	1.58	1.54
1	B	28	ALA	CA-CB	-7.88	1.41	1.53
1	E	152	VAL	CA-CB	7.23	1.58	1.54
1	B	206	ILE	CA-CB	6.17	1.61	1.54
1	I	152	VAL	CA-CB	6.14	1.57	1.54
1	K	123	LYS	CE-NZ	6.04	1.67	1.49
1	J	152	VAL	CA-CB	5.99	1.57	1.54
1	D	28	ALA	CA-CB	-5.74	1.44	1.53
1	B	170	LEU	C-O	-5.69	1.17	1.24
1	A	151	ALA	C-O	5.59	1.28	1.24
1	O	152	VAL	CA-CB	5.57	1.57	1.53
1	F	157	THR	CA-CB	5.54	1.61	1.53
1	C	182	ILE	CA-C	-5.42	1.46	1.52
1	K	120	THR	CA-CB	5.31	1.61	1.53
1	F	231	LEU	C-O	-5.20	1.18	1.24
1	C	28	ALA	CA-CB	-5.18	1.45	1.53
1	A	152	VAL	CA-CB	5.09	1.57	1.54
1	C	215	LEU	C-O	-5.01	1.17	1.24

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	201	ASP	CA-C-N	13.80	137.09	119.84
1	P	201	ASP	C-N-CA	13.80	137.09	119.84
1	L	152	VAL	N-CA-CB	13.13	120.69	110.45
1	K	152	VAL	N-CA-CB	12.64	120.31	110.45
1	O	152	VAL	N-CA-CB	11.04	117.45	110.50
1	M	152	VAL	N-CA-CB	10.21	118.42	110.45
1	N	152	VAL	N-CA-CB	9.51	117.87	110.45
1	G	201	ASP	CB-CA-C	7.01	121.75	111.02
1	F	199	MET	CA-C-N	6.70	126.49	119.05
1	F	199	MET	C-N-CA	6.70	126.49	119.05
1	F	94	PRO	CA-C-N	-5.82	114.39	120.38
1	F	94	PRO	C-N-CA	-5.82	114.39	120.38
1	H	202	PRO	N-CA-C	5.81	121.78	113.47
1	O	213	GLN	CA-C-N	5.63	125.74	119.32
1	O	213	GLN	C-N-CA	5.63	125.74	119.32
1	K	213	GLN	CA-C-N	5.46	125.54	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	213	GLN	C-N-CA	5.46	125.54	119.32
1	O	140	SER	CA-C-O	5.43	121.09	117.94
1	D	94	PRO	CA-C-N	-5.42	114.80	120.38
1	D	94	PRO	C-N-CA	-5.42	114.80	120.38
1	F	255	CYS	CB-CA-C	-5.41	102.14	111.23
1	E	40	ASP	N-CA-CB	5.41	120.66	111.57
1	J	202	PRO	N-CA-C	5.34	121.10	113.47
1	C	51	GLN	N-CA-CB	5.29	118.47	110.28
1	J	199	MET	CA-C-N	5.25	124.88	119.05
1	J	199	MET	C-N-CA	5.25	124.88	119.05
1	C	174	PRO	CB-CA-C	-5.21	104.44	111.85
1	L	94	PRO	CA-C-N	-5.04	115.19	120.38
1	L	94	PRO	C-N-CA	-5.04	115.19	120.38

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

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	23	0
1	B	1816	0	1828	22	0
1	C	1847	0	1872	30	0
1	D	1876	0	1895	21	1
1	E	1850	0	1870	25	0
1	F	1896	0	1922	18	0
1	G	1820	0	1842	23	0
1	H	1861	0	1874	23	0
1	I	1825	0	1849	14	0
1	J	1881	0	1892	13	0
1	K	1843	0	1865	23	1
1	L	1870	0	1884	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	1771	0	1771	19	0
1	N	1754	0	1766	10	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	287	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 (287) 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:E:186:ASN:HB3	1:E:218[B]:MET:HE2	1.41	1.00
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:HH11	1:I:203:ARG:HG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:J:258:SER:C	2:J:277:HOH:O	2.40	0.63
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:H:192:TRP:CD1	1:H:218:MET:HE1	2.34	0.63
1:B:255[B]:CYS:CB	1:D:255[B]:CYS:HG	2.11	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:H:186:ASN:HB3	1:H:218:MET:HE3	1.81	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:L:105:GLN:CD	1:L:105:GLN:H	2.08	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:209:GLY:O	1:E:218[B]:MET:HE3	2.01	0.60
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: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:D:186:ASN:HB3	1:D:218:MET:HE3	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:178:ARG:NH2	1:C:231:LEU:O	2.29	0.57
1:P:258:SER:O	1:P:259:ARG:C	2.49	0.56
1:C:251:LEU:C	1:C:253:TYR:H	2.13	0.56
1:D:192:TRP:CD1	1:D:218:MET:HE1	2.40	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:H:100:GLU:HG3	2:H:281:HOH:O	2.05	0.55
1:L:47:ARG:HG3	1:L:47:ARG:HH11	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:I:152:VAL:HG13	1:L:164:MET:HG3	1.92	0.52
1:K:5:THR:HG22	1:K:6:ARG:NH1	2.25	0.52
1:G:98:ARG:HG2	1:G:98:ARG:HH11	1.74	0.52
1:H:5:THR:O	1:H:5:THR:CG2	2.58	0.52
1:F:123:LYS:NZ	1:G:102:THR:O	2.41	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:E:165:THR:HG23	1:E:179:VAL:HG12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:186:ASN:HB3	1:E:218[B]:MET:CE	2.29	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
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:A:199:MET:HE3	1:A:200:PRO:HD2	1.94	0.50
1:M:62:ASP:OD1	1:M:64:THR:OG1	2.18	0.50
1:M:130:ARG:NH2	1:M:172:GLU:OE1	2.44	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:169:ALA:HB1	1:O:239:THR:HG23	1.94	0.49
1:O:173:SER:N	1:O:174:PRO:HD2	2.27	0.49
1:O:210:MET:HG2	1:O:217:ARG:HA	1.94	0.49
1:O:207:ARG:HD2	1:O:207:ARG:N	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:G:98:ARG:HH11	1:G:98:ARG:CG	2.26	0.48
1:A:164:MET:HG3	1:D:152:VAL:HG13	1.95	0.48
1:C:251:LEU:C	1:C:253:TYR:N	2.70	0.48
1:G:75:GLU:HA	1:G:78:ARG:HG2	1.95	0.48
1:F:100:GLU:H	1:F:100:GLU:HG3	1.29	0.48
1:L:243:LEU:C	1:L:243:LEU:HD23	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:10:LYS:HD3	1:D:84:ASP:CG	2.40	0.47
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:B:109:GLN:HE22	1:P:201:ASP:HA	1.79	0.47
1:F:12:VAL:HG13	1:F:85:CYS:HB3	1.96	0.47
1:G:6:ARG:HH11	1:G:6:ARG:CG	2.26	0.47
1:H:39:CYS:SG	1:H:61:CYS:HB3	2.54	0.47
1:H:192:TRP:CG	1:H:218:MET:HE1	2.50	0.47
1:A:23:ALA:O	1:A:27:ARG:HG3	2.14	0.47
1:G:173:SER:N	1:G:174:PRO:CD	2.77	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:C:186:ASN:HB3	1:C:218:MET:HE3	1.98	0.46
1:L:192:TRP:CD1	1:L:218:MET:HE1	2.51	0.46
1:G:43:GLU:HA	1:G:58:PHE:CZ	2.51	0.46
1:L:47:ARG:HG3	1:L:47:ARG:NH1	2.30	0.46
1:N:98:ARG:O	1:N:101:GLU:HG2	2.16	0.46
1:D:32[A]:SER:OG	1:D:229:VAL:HG11	2.16	0.46
1:D:98:ARG:O	1:D:101:GLU:HG2	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:H:66:GLU:HG2	1:H:70:LYS:HZ2	1.80	0.45
1:A:173:SER:N	1:A:174:PRO:CD	2.80	0.45
1:E:186:ASN:CB	1:E:218[B]:MET:HE2	2.30	0.45
1:N:192:TRP:CG	1:N:218:MET:HE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:186:ASN:HB3	1:L:218:MET:HE3	2.00	0.44
1:O:37:VAL:HG21	1:O:76:THR:HG23	2.00	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:F:188:TRP:N	1:F:218:MET:HE2	2.33	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:N:133:GLN:HE21	1:N:133:GLN:HA	1.84	0.42
1:A:178:ARG:NH2	1:A:231:LEU:O	2.41	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: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:B:188:TRP:CA	1:B:218:MET:HE2	2.50	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:D:192:TRP:CG	1:D:218:MET:HE1	2.55	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:HE	1:H:207:ARG:HB2	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:5:THR:HG22	1:K:6:ARG:HH11	1.84	0.41
1:K:165:THR:HG23	1:K:179:VAL:HG12	2.03	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:J:186:ASN:HB3	1:J:218:MET:HE3	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:O	1:H:5:THR:HG22	2.21	0.41
1:I:98:ARG:HB2	1:I:101:GLU:HG2	2.03	0.41
1:P:193:GLU:O	1:P:194:GLU:C	2.63	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
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%)	30	43
1	D	255/270 (94%)	252 (99%)	3 (1%)	0	100	100
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%)	30	43
1	N	236/270 (87%)	233 (99%)	3 (1%)	0	100	100
1	O	245/270 (91%)	240 (98%)	4 (2%)	1 (0%)	30	43
1	P	252/270 (93%)	243 (96%)	8 (3%)	1 (0%)	30	43
All	All	3980/4320 (92%)	3901 (98%)	75 (2%)	4 (0%)	48	64

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 ⓘ

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%)	26	45
1	B	188/208 (90%)	180 (96%)	8 (4%)	26	44
1	C	192/208 (92%)	185 (96%)	7 (4%)	31	52
1	D	196/208 (94%)	190 (97%)	6 (3%)	35	57
1	E	193/208 (93%)	181 (94%)	12 (6%)	16	29
1	F	197/208 (95%)	191 (97%)	6 (3%)	36	58
1	G	189/208 (91%)	178 (94%)	11 (6%)	18	32
1	H	192/208 (92%)	184 (96%)	8 (4%)	26	45
1	I	190/208 (91%)	183 (96%)	7 (4%)	30	51
1	J	196/208 (94%)	181 (92%)	15 (8%)	12	20
1	K	191/208 (92%)	182 (95%)	9 (5%)	23	41
1	L	193/208 (93%)	183 (95%)	10 (5%)	21	36
1	M	182/208 (88%)	176 (97%)	6 (3%)	33	55
1	N	182/208 (88%)	173 (95%)	9 (5%)	22	39
1	O	186/208 (89%)	174 (94%)	12 (6%)	15	27
1	P	191/208 (92%)	177 (93%)	14 (7%)	13	22
All	All	3049/3328 (92%)	2901 (95%)	148 (5%)	23	39

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	SER
1	A	72	LEU
1	A	105	GLN
1	A	109[A]	GLN
1	A	109[B]	GLN
1	A	123	LYS
1	A	168	LEU
1	A	208	GLU
1	B	5	THR
1	B	10	LYS
1	B	19	ARG
1	B	35	ARG
1	B	42	ASP
1	B	74	SER
1	B	78	ARG
1	B	100	GLU

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Mol	Chain	Res	Type
1	C	5	THR
1	C	51	GLN
1	C	65	GLN
1	C	74	SER
1	C	109	GLN
1	C	152	VAL
1	C	168	LEU
1	D	42	ASP
1	D	100	GLU
1	D	192	TRP
1	D	195	LEU
1	D	203	ARG
1	D	256	LYS
1	E	41	LYS
1	E	44	SER
1	E	49	LEU
1	E	51	GLN
1	E	72	LEU
1	E	75	GLU
1	E	78	ARG
1	E	105	GLN
1	E	109[A]	GLN
1	E	109[B]	GLN
1	E	113	LEU
1	E	221	PRO
1	F	42	ASP
1	F	43	GLU
1	F	100	GLU
1	F	152	VAL
1	F	192	TRP
1	F	259	ARG
1	G	6	ARG
1	G	52	GLU
1	G	97	GLN
1	G	100	GLU
1	G	105	GLN
1	G	112	GLU
1	G	194	GLU
1	G	201	ASP
1	G	203	ARG
1	G	205	SER
1	G	220	GLN

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Mol	Chain	Res	Type
1	H	5	THR
1	H	42	ASP
1	H	47	ARG
1	H	75	GLU
1	H	78	ARG
1	H	100	GLU
1	H	192	TRP
1	H	203	ARG
1	I	101	GLU
1	I	112	GLU
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	10	LYS
1	J	32	SER
1	J	35	ARG
1	J	39	CYS
1	J	42	ASP
1	J	47	ARG
1	J	100	GLU
1	J	191	LEU
1	J	192	TRP
1	J	194	GLU
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	51	GLN
1	K	72	LEU
1	K	75	GLU
1	K	105	GLN
1	K	113	LEU
1	K	194	GLU
1	K	207	ARG
1	L	42	ASP
1	L	43	GLU
1	L	47	ARG

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Mol	Chain	Res	Type
1	L	50	GLU
1	L	74	SER
1	L	78	ARG
1	L	100	GLU
1	L	105	GLN
1	L	152	VAL
1	L	203	ARG
1	M	65	GLN
1	M	66	GLU
1	M	148	GLN
1	M	152	VAL
1	M	194	GLU
1	M	246	THR
1	N	35	ARG
1	N	44	SER
1	N	100	GLU
1	N	133	GLN
1	N	183	SER
1	N	203	ARG
1	N	206	ILE
1	N	207	ARG
1	N	255	CYS
1	O	51	GLN
1	O	52	GLU
1	O	65	GLN
1	O	66	GLU
1	O	100	GLU
1	O	113	LEU
1	O	135	ASN
1	O	194	GLU
1	O	207	ARG
1	O	208	GLU
1	O	210	MET
1	O	239	THR
1	P	10	LYS
1	P	32	SER
1	P	44	SER
1	P	100	GLU
1	P	101	GLU
1	P	123	LYS
1	P	133	GLN
1	P	152	VAL

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Mol	Chain	Res	Type
1	P	183	SER
1	P	193	GLU
1	P	198	LEU
1	P	203	ARG
1	P	241	ILE
1	P	255	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	105	GLN
1	A	150	GLN
1	A	220	GLN
1	B	109	GLN
1	B	186	ASN
1	B	213	GLN
1	C	97	GLN
1	C	133	GLN
1	C	135	ASN
1	C	150	GLN
1	C	220	GLN
1	D	92	HIS
1	D	97	GLN
1	D	105	GLN
1	D	150	GLN
1	D	186	ASN
1	D	213	GLN
1	D	236	ASN
1	E	97	GLN
1	E	150	GLN
1	F	92	HIS
1	F	135	ASN
1	G	31	ASN
1	G	97	GLN
1	G	109	GLN
1	G	133	GLN
1	H	65	GLN
1	H	89	ASN
1	H	105	GLN
1	H	133	GLN
1	H	148	GLN

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Mol	Chain	Res	Type
1	H	150	GLN
1	I	92	HIS
1	I	133	GLN
1	I	135	ASN
1	J	109	GLN
1	J	133	GLN
1	J	135	ASN
1	J	148	GLN
1	K	92	HIS
1	K	97	GLN
1	K	150	GLN
1	L	88	ASN
1	L	97	GLN
1	L	105	GLN
1	L	236	ASN
1	M	88	ASN
1	M	97	GLN
1	M	213	GLN
1	M	220	GLN
1	N	92	HIS
1	N	97	GLN
1	N	133	GLN
1	N	236	ASN
1	O	51	GLN
1	O	89	ASN
1	O	92	HIS
1	P	133	GLN
1	P	135	ASN
1	P	150	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/270 (92%)	-1.46	0 100 100	2, 3, 13, 26	1 (0%)
1	B	247/270 (91%)	-1.39	0 100 100	2, 3, 18, 36	3 (1%)
1	C	250/270 (92%)	-1.44	0 100 100	2, 3, 13, 31	0
1	D	255/270 (94%)	-1.43	0 100 100	2, 3, 16, 36	2 (0%)
1	E	250/270 (92%)	-1.44	0 100 100	2, 4, 13, 29	2 (0%)
1	F	256/270 (94%)	-1.41	0 100 100	1, 4, 15, 25	2 (0%)
1	G	247/270 (91%)	-1.39	0 100 100	2, 4, 12, 22	0
1	H	254/270 (94%)	-1.41	0 100 100	2, 4, 13, 25	1 (0%)
1	I	247/270 (91%)	-1.30	0 100 100	2, 5, 13, 24	0
1	J	255/270 (94%)	-1.36	0 100 100	1, 4, 15, 27	3 (1%)
1	K	250/270 (92%)	-1.42	0 100 100	2, 4, 14, 31	0
1	L	255/270 (94%)	-1.34	0 100 100	2, 4, 15, 25	1 (0%)
1	M	244/270 (90%)	-0.98	0 100 100	2, 5, 11, 25	0
1	N	240/270 (88%)	-0.96	0 100 100	2, 5, 12, 18	0
1	O	247/270 (91%)	-0.98	0 100 100	2, 5, 11, 17	0
1	P	254/270 (94%)	-1.04	0 100 100	2, 5, 13, 22	0
All	All	4001/4320 (92%)	-1.30	0 100 100	1, 4, 14, 36	15 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.