



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 06:12 am GMT

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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

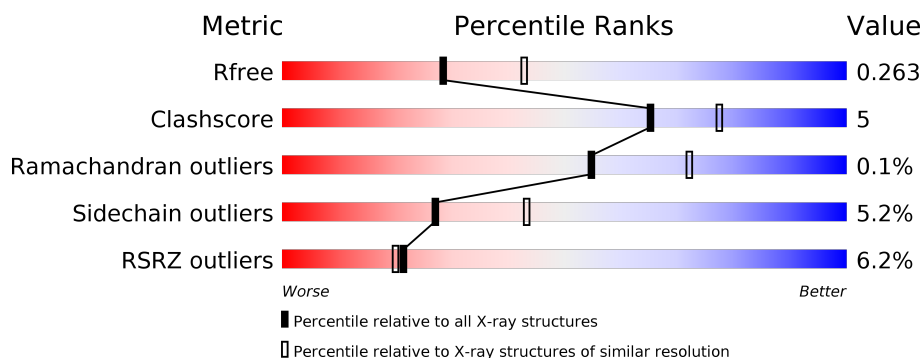
1 Overall quality at a glance

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.











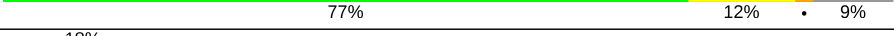

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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. 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	<div> <div>77%</div> <div>14%</div> <div>7%</div> </div>
1	B	270	<div> <div>78%</div> <div>12%</div> <div>9%</div> </div>
1	C	270	<div> <div>76%</div> <div>15%</div> <div>7%</div> </div>
1	D	270	<div> <div>83%</div> <div>11%</div> <div>6%</div> </div>
1	E	270	<div> <div>78%</div> <div>13%</div> <div>7%</div> </div>
1	F	270	<div> <div>81%</div> <div>13%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	270	
1	H	270	
1	I	270	
1	J	270	
1	K	270	
1	L	270	
1	M	270	
1	N	270	
1	O	270	
1	P	270	

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			

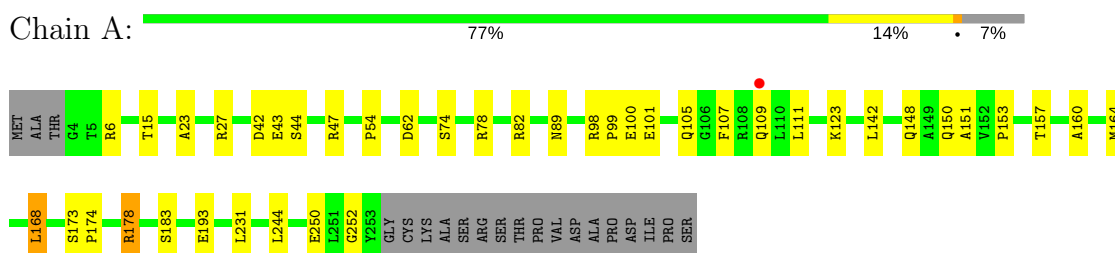
- Molecule 2 is water.

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

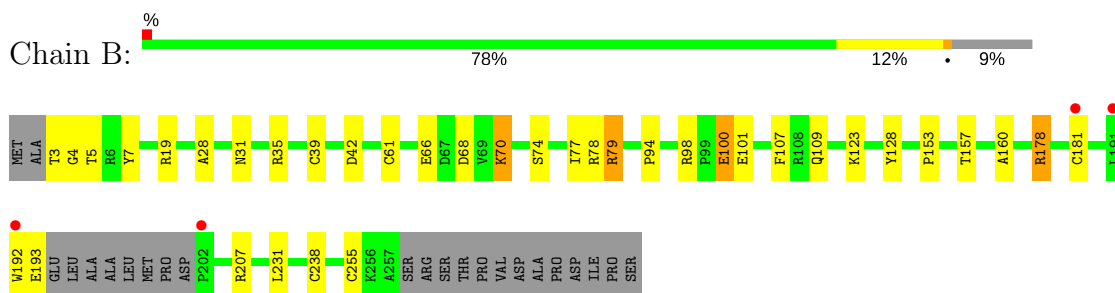
3 Residue-property plots [i](#)

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 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.

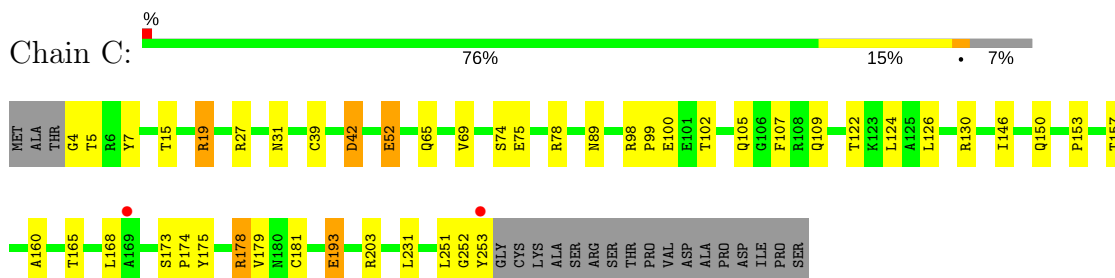
- Molecule 1: Retinal dehydrogenase/reductase 3



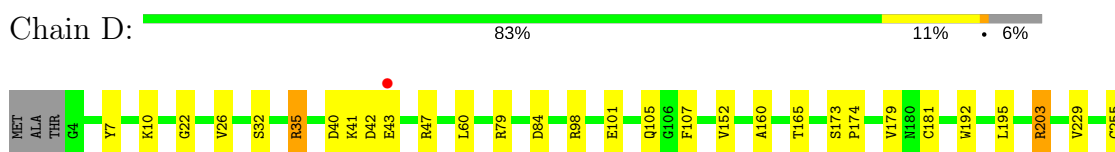
- Molecule 1: Retinal dehydrogenase/reductase 3

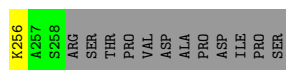


- Molecule 1: Retinal dehydrogenase/reductase 3



- Molecule 1: Retinal dehydrogenase/reductase 3





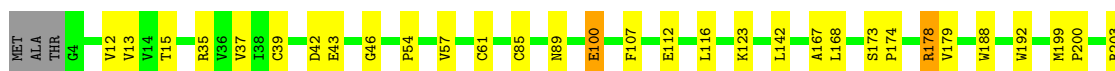
• Molecule 1: Retinal dehydrogenase/reductase 3

Chain E: 78% 13% 7%



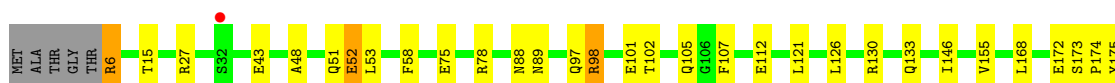
• Molecule 1: Retinal dehydrogenase/reductase 3

Chain F: 81% 13% 5%



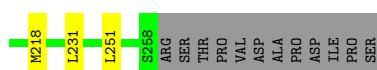
• Molecule 1: Retinal dehydrogenase/reductase 3

Chain G: 77% 13% 9%



• Molecule 1: Retinal dehydrogenase/reductase 3

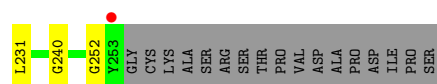
Chain H: 81% 11% 6%



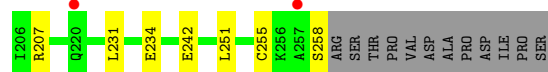
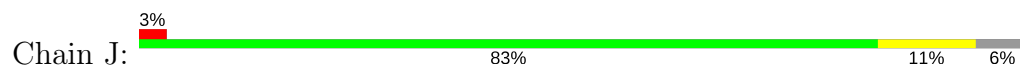
• Molecule 1: Retinal dehydrogenase/reductase 3

Chain I: 2% 81% 9% 9%

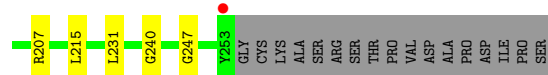
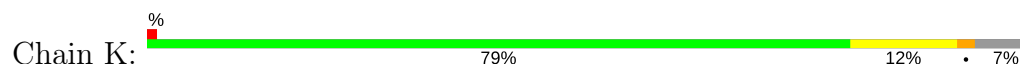




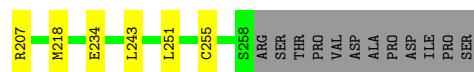
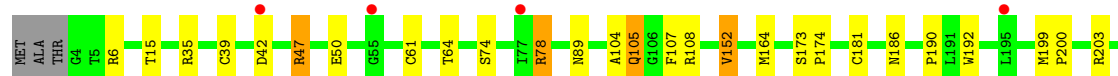
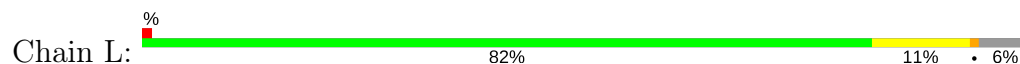
- Molecule 1: Retinal dehydrogenase/reductase 3



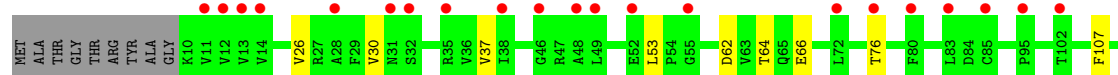
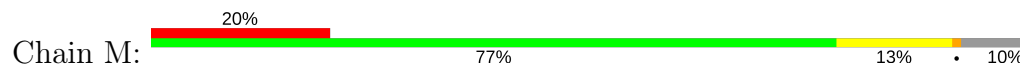
- Molecule 1: Retinal dehydrogenase/reductase 3



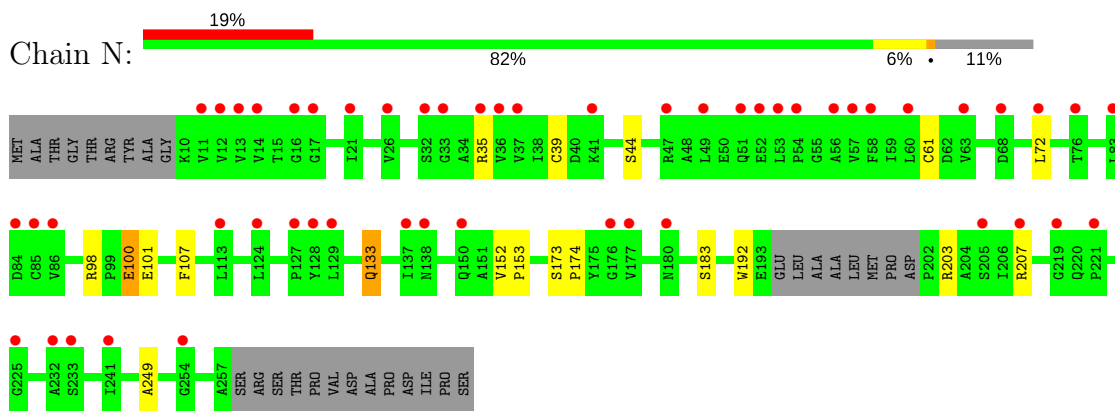
- Molecule 1: Retinal dehydrogenase/reductase 3



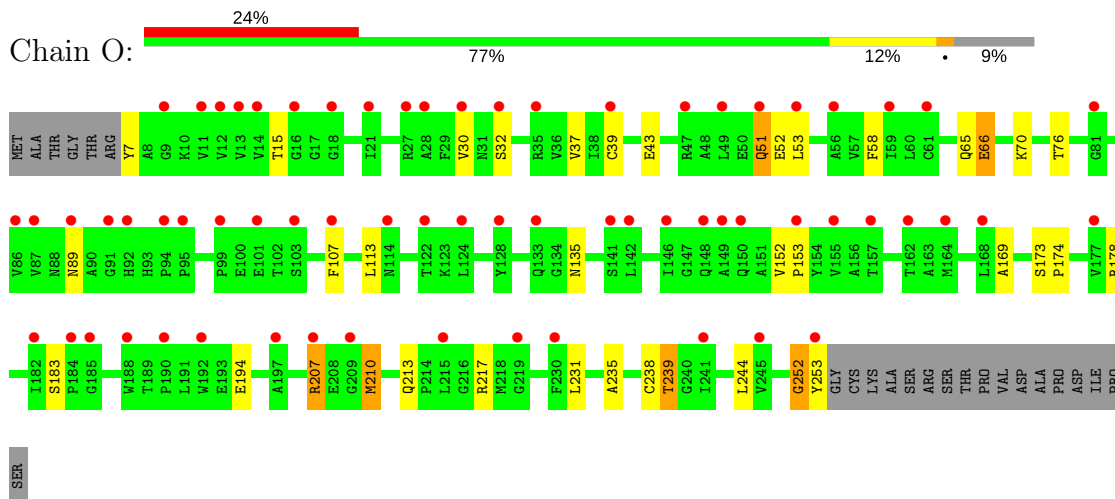
- Molecule 1: Retinal dehydrogenase/reductase 3



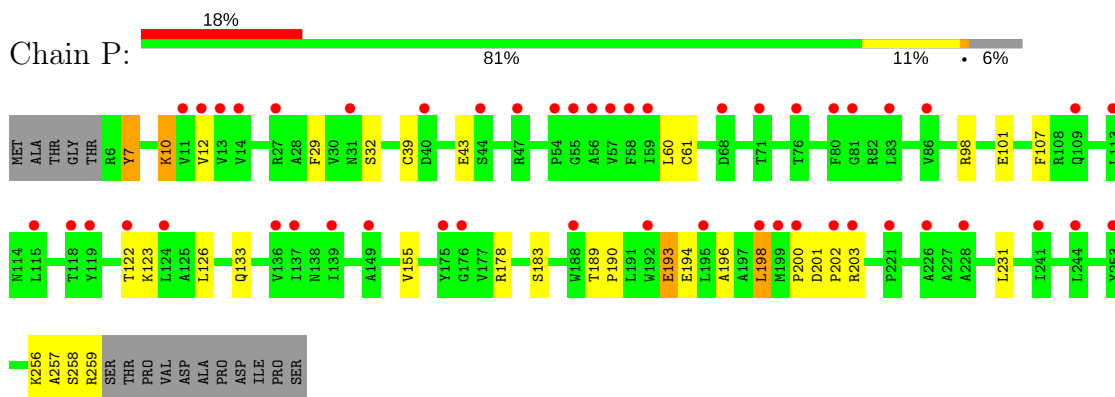
- Molecule 1: Retinal dehydrogenase/reductase 3



- Molecule 1: Retinal dehydrogenase/reductase 3



- Molecule 1: Retinal dehydrogenase/reductase 3



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 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
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.181 , 0.229 0.248 , 0.263	Depositor DCC
R_{free} test set	3560 reflections (2.02%)	DCC
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	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.368 for l,-k,h	Xtriage
F_o, F_c correlation	0.89	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.*

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	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

The worst 5 of 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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	181	CYS	CB-SG	-6.18	1.71	1.82

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

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
1	N	1754	0	1766	9	0
1	O	1806	0	1812	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

The worst 5 of 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

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

5.3.1 Protein backbone

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%)	38	54
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%)	38	54
1	N	236/270 (87%)	233 (99%)	3 (1%)	0	100	100
1	O	245/270 (91%)	240 (98%)	4 (2%)	1 (0%)	38	54
1	P	252/270 (93%)	243 (96%)	8 (3%)	1 (0%)	38	54
All	All	3980/4320 (92%)	3901 (98%)	75 (2%)	4 (0%)	55	72

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%)	34	53
1	B	188/208 (90%)	176 (94%)	12 (6%)	20	32
1	C	192/208 (92%)	184 (96%)	8 (4%)	34	53
1	D	196/208 (94%)	189 (96%)	7 (4%)	40	60
1	E	193/208 (93%)	180 (93%)	13 (7%)	19	30
1	F	197/208 (95%)	189 (96%)	8 (4%)	35	54
1	G	189/208 (91%)	177 (94%)	12 (6%)	21	33
1	H	192/208 (92%)	182 (95%)	10 (5%)	27	43
1	I	190/208 (91%)	179 (94%)	11 (6%)	23	37
1	J	196/208 (94%)	183 (93%)	13 (7%)	19	30
1	K	191/208 (92%)	182 (95%)	9 (5%)	30	48
1	L	193/208 (93%)	181 (94%)	12 (6%)	21	34
1	M	182/208 (88%)	178 (98%)	4 (2%)	57	76
1	N	182/208 (88%)	173 (95%)	9 (5%)	29	46
1	O	186/208 (89%)	173 (93%)	13 (7%)	18	28
1	P	191/208 (92%)	181 (95%)	10 (5%)	27	43
All	All	3049/3328 (92%)	2890 (95%)	159 (5%)	27	43

5 of 159 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	47	ARG
1	J	7	TYR
1	O	210	MET
1	H	100	GLU
1	I	67	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	148	GLN
1	K	150	GLN
1	P	133	GLN
1	H	150	GLN
1	J	109	GLN

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/270 (92%)	0.30	1 (0%) 92 91	2, 3, 13, 26	0
1	B	247/270 (91%)	0.51	4 (1%) 72 70	2, 3, 18, 36	0
1	C	250/270 (92%)	0.29	2 (0%) 86 84	2, 3, 13, 31	0
1	D	255/270 (94%)	0.28	1 (0%) 92 91	2, 3, 16, 36	0
1	E	250/270 (92%)	0.31	0 100 100	2, 4, 13, 29	0
1	F	256/270 (94%)	0.27	0 100 100	2, 4, 15, 25	0
1	G	247/270 (91%)	0.13	1 (0%) 92 91	2, 4, 12, 22	0
1	H	254/270 (94%)	0.13	1 (0%) 92 91	2, 4, 13, 25	0
1	I	247/270 (91%)	0.27	5 (2%) 65 63	2, 5, 13, 24	0
1	J	255/270 (94%)	0.25	9 (3%) 44 43	2, 4, 15, 27	0
1	K	250/270 (92%)	0.07	2 (0%) 86 84	2, 4, 14, 31	0
1	L	255/270 (94%)	0.21	4 (1%) 72 70	2, 4, 15, 25	0
1	M	244/270 (90%)	1.14	53 (21%) 1 1	2, 5, 11, 25	0
1	N	240/270 (88%)	1.31	52 (21%) 1 1	2, 5, 12, 18	0
1	O	247/270 (91%)	1.35	66 (26%) 1 1	2, 5, 11, 17	0
1	P	254/270 (94%)	1.14	49 (19%) 1 1	2, 5, 13, 22	0
All	All	4001/4320 (92%)	0.49	250 (6%) 21 20	2, 4, 14, 36	0

The worst 5 of 250 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	191	LEU	6.7
1	O	49	LEU	6.6
1	L	55	GLY	6.2
1	O	14	VAL	5.9
1	N	13	VAL	5.5

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 carbohydrates 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.