



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2016 – 01:04 PM EDT

PDB ID : 5DGY
Title : Crystal structure of rhodopsin bound to visual arrestin
Authors : Zhou, X.E.; Gao, X.; Kang, Y.; He, Y.; de Waal, P.W.; Suino-Powell, K.M.;
Wang, M.; Melcher, K.; Xu, H.E.
Deposited on : 2015-08-28
Resolution : 7.70 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
<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
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027257
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : rb-20027257

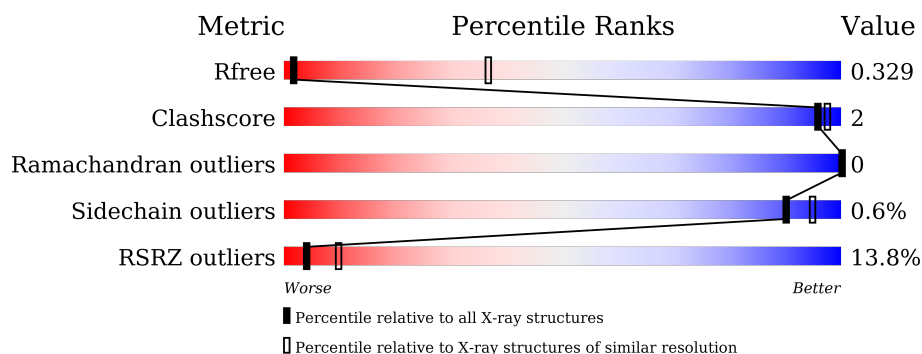
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.70 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}	91344	1015 (11.50-3.66)
Clashscore	102246	1064 (11.50-3.70)
Ramachandran outliers	100387	1036 (11.50-3.66)
Sidechain outliers	100360	1006 (11.50-3.66)
RSRZ outliers	91569	1014 (11.50-3.66)

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	906	<div> <div>9%</div> <div>86%</div> <div>6%</div> <div>8%</div> </div>
1	B	906	<div> <div>7%</div> <div>71%</div> <div>26%</div> </div>
1	C	906	<div> <div>13%</div> <div>82%</div> <div>13%</div> </div>
1	D	906	<div> <div>19%</div> <div>87%</div> <div>5%</div> <div>8%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 24665 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 Endolysin,Rhodopsin,S-arrestin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	833	Total	C	N	O	S	0	0	0
			6565	4264	1076	1187	38			
1	B	673	Total	C	N	O	S	0	0	0
			5296	3463	847	951	35			
1	C	789	Total	C	N	O	S	0	0	0
			6231	4052	1019	1121	39			
1	D	833	Total	C	N	O	S	0	0	0
			6573	4269	1079	1186	39			

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-149	GLY	ARG	engineered mutation	UNP P00720
A	-107	THR	CYS	engineered mutation	UNP P00720
A	-64	ALA	CYS	engineered mutation	UNP P00720
A	-24	ARG	ILE	engineered mutation	UNP P00720
A	2	CYS	ASN	engineered mutation	UNP P08100
A	113	GLN	GLU	engineered mutation	UNP P08100
A	257	TYR	MET	engineered mutation	UNP P08100
A	282	CYS	ASN	engineered mutation	UNP P08100
A	995	ALA	-	linker	UNP P08100
A	996	ALA	-	linker	UNP P08100
A	997	ALA	-	linker	UNP P08100
A	998	GLY	-	linker	UNP P08100
A	999	SER	-	linker	UNP P08100
A	1000	ALA	-	linker	UNP P08100
A	1001	GLY	-	linker	UNP P08100
A	1002	SER	-	linker	UNP P08100
A	1003	ALA	-	linker	UNP P08100
A	1004	GLY	-	linker	UNP P08100
A	1005	SER	-	linker	UNP P08100
A	1006	ALA	-	linker	UNP P08100
A	1007	GLY	-	linker	UNP P08100

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1008	SER	-	linker	UNP P08100
A	1009	ALA	-	linker	UNP P08100
A	1374	ALA	LEU	engineered mutation	UNP P20443
A	1375	ALA	VAL	engineered mutation	UNP P20443
A	1376	ALA	PHE	engineered mutation	UNP P20443
B	-149	GLY	ARG	engineered mutation	UNP P00720
B	-107	THR	CYS	engineered mutation	UNP P00720
B	-64	ALA	CYS	engineered mutation	UNP P00720
B	-24	ARG	ILE	engineered mutation	UNP P00720
B	2	CYS	ASN	engineered mutation	UNP P08100
B	113	GLN	GLU	engineered mutation	UNP P08100
B	257	TYR	MET	engineered mutation	UNP P08100
B	282	CYS	ASN	engineered mutation	UNP P08100
B	995	ALA	-	linker	UNP P08100
B	996	ALA	-	linker	UNP P08100
B	997	ALA	-	linker	UNP P08100
B	998	GLY	-	linker	UNP P08100
B	999	SER	-	linker	UNP P08100
B	1000	ALA	-	linker	UNP P08100
B	1001	GLY	-	linker	UNP P08100
B	1002	SER	-	linker	UNP P08100
B	1003	ALA	-	linker	UNP P08100
B	1004	GLY	-	linker	UNP P08100
B	1005	SER	-	linker	UNP P08100
B	1006	ALA	-	linker	UNP P08100
B	1007	GLY	-	linker	UNP P08100
B	1008	SER	-	linker	UNP P08100
B	1009	ALA	-	linker	UNP P08100
B	1374	ALA	LEU	engineered mutation	UNP P20443
B	1375	ALA	VAL	engineered mutation	UNP P20443
B	1376	ALA	PHE	engineered mutation	UNP P20443
C	-149	GLY	ARG	engineered mutation	UNP P00720
C	-107	THR	CYS	engineered mutation	UNP P00720
C	-64	ALA	CYS	engineered mutation	UNP P00720
C	-24	ARG	ILE	engineered mutation	UNP P00720
C	2	CYS	ASN	engineered mutation	UNP P08100
C	113	GLN	GLU	engineered mutation	UNP P08100
C	257	TYR	MET	engineered mutation	UNP P08100
C	282	CYS	ASN	engineered mutation	UNP P08100
C	995	ALA	-	linker	UNP P08100
C	996	ALA	-	linker	UNP P08100
C	997	ALA	-	linker	UNP P08100

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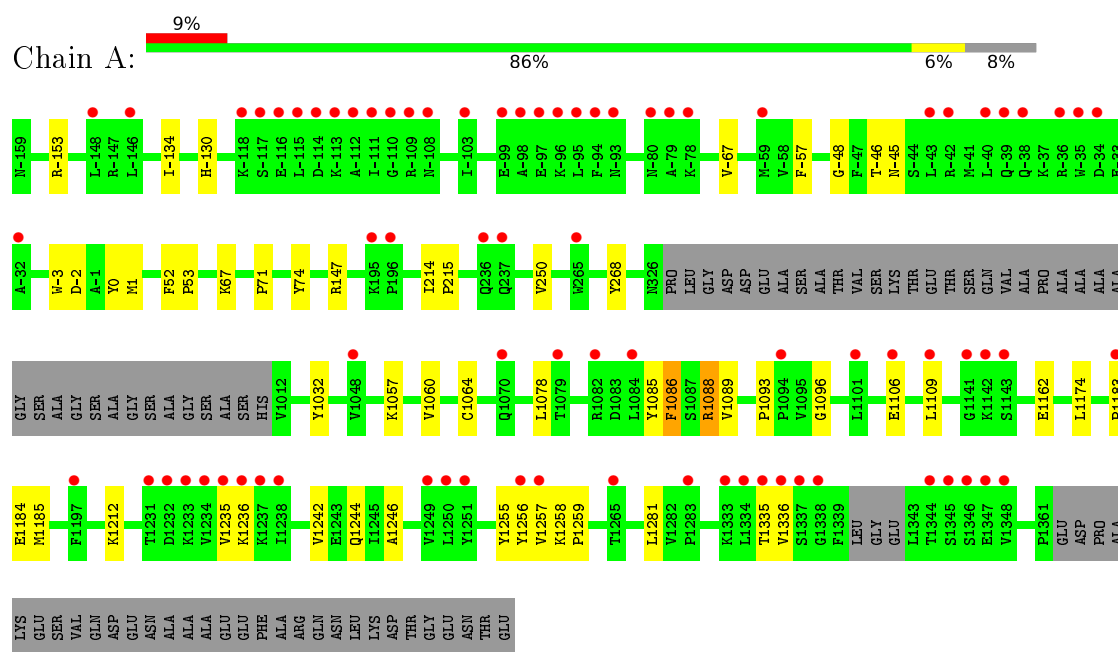
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Chain	Residue	Modelled	Actual	Comment	Reference
C	998	GLY	-	linker	UNP P08100
C	999	SER	-	linker	UNP P08100
C	1000	ALA	-	linker	UNP P08100
C	1001	GLY	-	linker	UNP P08100
C	1002	SER	-	linker	UNP P08100
C	1003	ALA	-	linker	UNP P08100
C	1004	GLY	-	linker	UNP P08100
C	1005	SER	-	linker	UNP P08100
C	1006	ALA	-	linker	UNP P08100
C	1007	GLY	-	linker	UNP P08100
C	1008	SER	-	linker	UNP P08100
C	1009	ALA	-	linker	UNP P08100
C	1374	ALA	LEU	engineered mutation	UNP P20443
C	1375	ALA	VAL	engineered mutation	UNP P20443
C	1376	ALA	PHE	engineered mutation	UNP P20443
D	-149	GLY	ARG	engineered mutation	UNP P00720
D	-107	THR	CYS	engineered mutation	UNP P00720
D	-64	ALA	CYS	engineered mutation	UNP P00720
D	-24	ARG	ILE	engineered mutation	UNP P00720
D	2	CYS	ASN	engineered mutation	UNP P08100
D	113	GLN	GLU	engineered mutation	UNP P08100
D	257	TYR	MET	engineered mutation	UNP P08100
D	282	CYS	ASN	engineered mutation	UNP P08100
D	995	ALA	-	linker	UNP P08100
D	996	ALA	-	linker	UNP P08100
D	997	ALA	-	linker	UNP P08100
D	998	GLY	-	linker	UNP P08100
D	999	SER	-	linker	UNP P08100
D	1000	ALA	-	linker	UNP P08100
D	1001	GLY	-	linker	UNP P08100
D	1002	SER	-	linker	UNP P08100
D	1003	ALA	-	linker	UNP P08100
D	1004	GLY	-	linker	UNP P08100
D	1005	SER	-	linker	UNP P08100
D	1006	ALA	-	linker	UNP P08100
D	1007	GLY	-	linker	UNP P08100
D	1008	SER	-	linker	UNP P08100
D	1009	ALA	-	linker	UNP P08100
D	1374	ALA	LEU	engineered mutation	UNP P20443
D	1375	ALA	VAL	engineered mutation	UNP P20443
D	1376	ALA	PHE	engineered mutation	UNP P20443

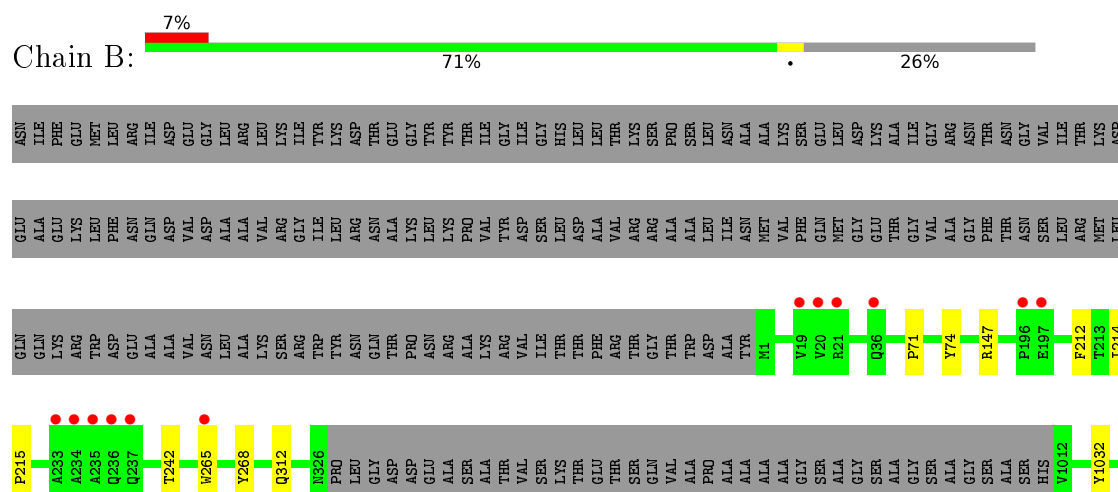
3 Residue-property plots

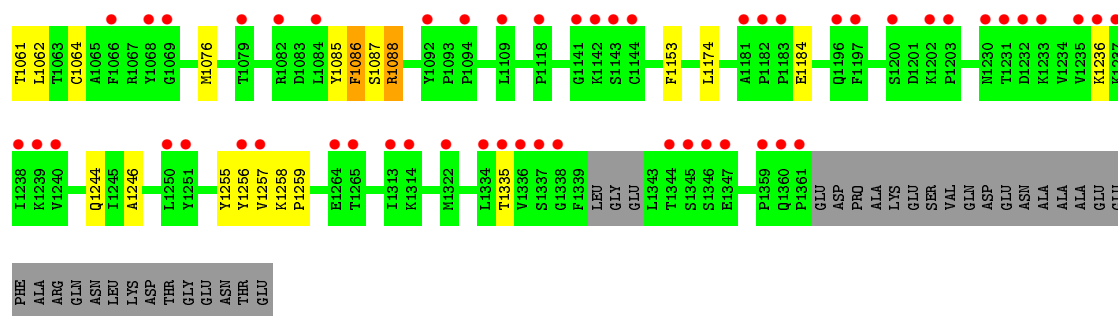
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Endolysin,Rhodopsin,S-arrestin

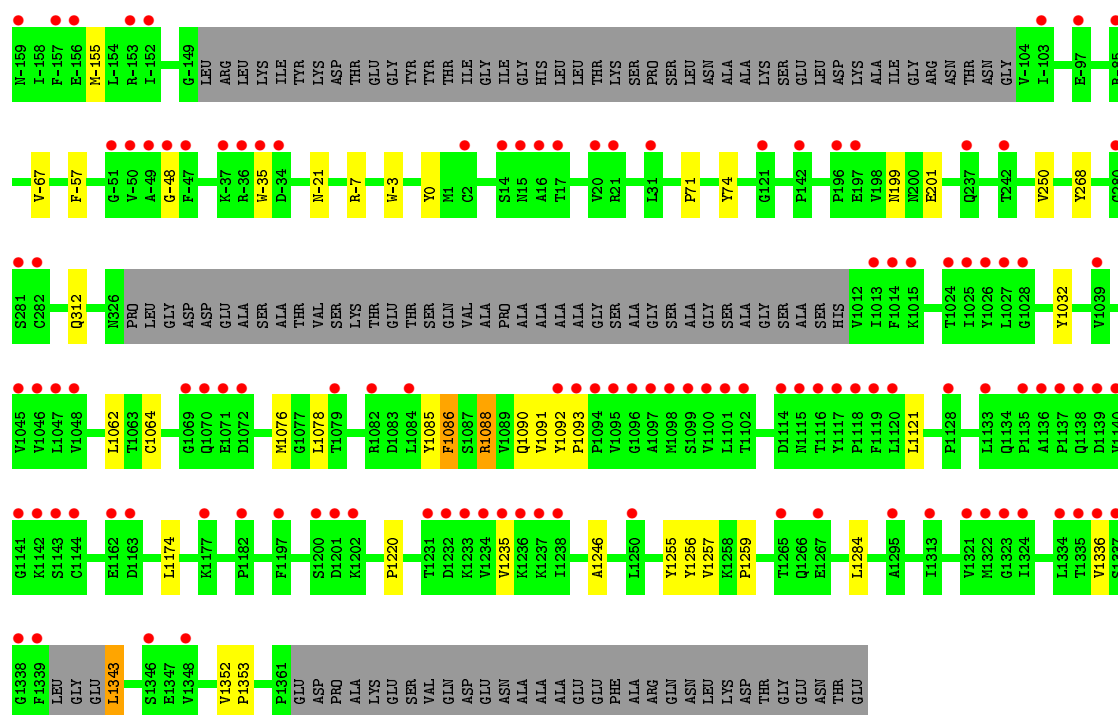
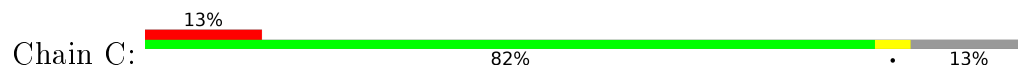


• Molecule 1: Endolysin,Rhodopsin,S-arrestin

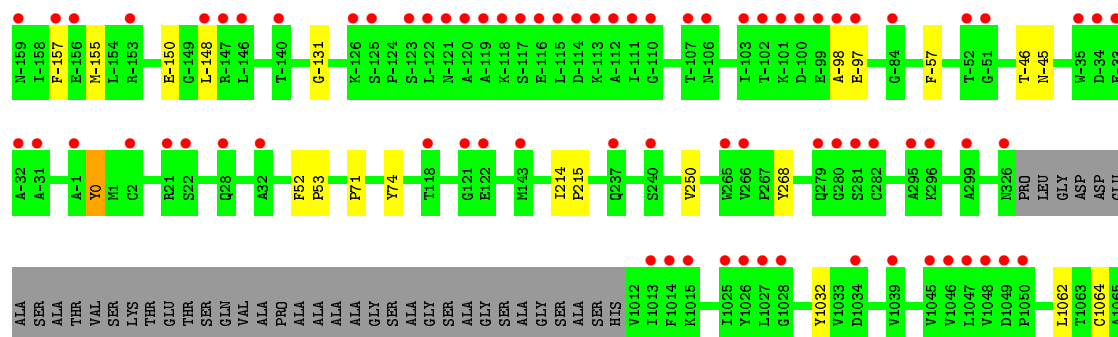
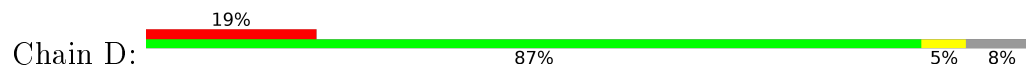




• Molecule 1: Endolysin,Rhodopsin,S-arrestin



• Molecule 1: Endolysin,Rhodopsin,S-arrestin





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.48Å 107.26Å 460.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 7.70 29.98 – 7.25	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.98-7.70) 98.8 (29.98-7.25)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 7.23Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.285 , 0.335 0.281 , 0.329	Depositor DCC
R_{free} test set	466 reflections (7.03%)	DCC
Wilson B-factor (Å ²)	312.8	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 289.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.31$, $\langle L^2 \rangle = 0.14$	Xtriage
Estimated twinning fraction	0.266 for k,h,-l	Xtriage
Reported twinning fraction	0.390 for k,h,-l	Depositor
Outliers	3 of 7833 reflections (0.038%)	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	24665	wwPDB-VP
Average B, all atoms (Å ²)	420.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.58% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.42	1/6723 (0.0%)	0.52	1/9138 (0.0%)
1	B	0.44	2/5433 (0.0%)	0.54	1/7395 (0.0%)
1	C	0.42	1/6383 (0.0%)	0.54	2/8676 (0.0%)
1	D	0.42	3/6731 (0.0%)	0.53	1/9146 (0.0%)
All	All	0.42	7/25270 (0.0%)	0.53	5/34355 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	3
1	C	0	6
1	D	0	4
All	All	0	19

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1086	PHE	C-O	-7.99	1.08	1.23
1	B	1086	PHE	C-O	-7.42	1.09	1.23
1	A	1086	PHE	C-O	-6.99	1.10	1.23
1	B	1088	ARG	C-O	-6.78	1.10	1.23
1	C	1086	PHE	C-O	-6.34	1.11	1.23
1	D	1088	ARG	C-O	-5.83	1.12	1.23
1	D	1255	TYR	C-O	-5.39	1.13	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1088	ARG	NE-CZ-NH1	-8.23	116.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1032	TYR	O-C-N	5.05	130.78	122.70
1	D	1032	TYR	O-C-N	5.04	130.77	122.70
1	C	1032	TYR	O-C-N	5.04	130.77	122.70
1	B	1032	TYR	O-C-N	5.00	130.71	122.70

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	0	TYR	Mainchain
1	A	1088	ARG	Mainchain
1	A	1096	GLY	Mainchain
1	A	1255	TYR	Mainchain
1	A	1257	VAL	Mainchain
1	A	1259	PRO	Mainchain
1	B	1255	TYR	Mainchain
1	B	1257	VAL	Mainchain
1	B	1259	PRO	Mainchain
1	C	1086	PHE	Mainchain
1	C	1088	ARG	Mainchain
1	C	1090	GLN	Mainchain
1	C	1255	TYR	Mainchain
1	C	1257	VAL	Mainchain
1	C	1259	PRO	Mainchain
1	D	0	TYR	Mainchain
1	D	1096	GLY	Mainchain
1	D	1257	VAL	Mainchain
1	D	1259	PRO	Mainchain

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	6565	0	6626	27	13
1	B	5296	0	5340	14	6
1	C	6231	0	6287	21	7
1	D	6573	0	6647	17	22

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	24665	0	24900	76	24

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 2.

All (76) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1184:GLU:N	1:A:1184:GLU:OE1	1.99	0.94
1:A:1246:ALA:O	1:A:1256:TYR:N	2.29	0.66
1:A:1064:CYS:N	1:A:1085:TYR:O	2.33	0.61
1:A:1183:PRO:HG2	1:A:1184:GLU:OE1	2.00	0.61
1:A:1246:ALA:N	1:A:1256:TYR:O	2.31	0.59
1:C:-155:MET:HG3	1:C:0:TYR:HE1	1.68	0.58
1:B:1246:ALA:O	1:B:1256:TYR:N	2.36	0.58
1:C:1246:ALA:N	1:C:1256:TYR:O	2.34	0.57
1:A:1244:GLN:N	1:A:1258:LYS:O	2.39	0.56
1:B:1246:ALA:N	1:B:1256:TYR:O	2.37	0.55
1:D:1246:ALA:N	1:D:1256:TYR:O	2.34	0.55
1:A:1106:GLU:CD	1:C:1284:LEU:CD1	2.74	0.55
1:B:1086:PHE:CZ	1:B:1088:ARG:HB3	2.44	0.53
1:D:1086:PHE:CZ	1:D:1162:GLU:HG3	2.45	0.51
1:C:312:GLN:HB2	1:C:1076:MET:CB	2.41	0.51
1:B:1064:CYS:N	1:B:1085:TYR:O	2.43	0.50
1:C:1246:ALA:O	1:C:1256:TYR:N	2.44	0.50
1:A:250:VAL:HG22	1:A:1078:LEU:HG	1.92	0.50
1:D:1245:ILE:HA	1:D:1257:VAL:HA	1.93	0.50
1:C:1062:LEU:HB2	1:C:1121:LEU:HD13	1.93	0.50
1:D:1062:LEU:HB2	1:D:1121:LEU:HD13	1.93	0.50
1:D:250:VAL:HG22	1:D:1078:LEU:HG	1.95	0.49
1:A:1106:GLU:CD	1:C:1284:LEU:HD11	2.32	0.49
1:D:1064:CYS:N	1:D:1085:TYR:O	2.43	0.49
1:A:71:PRO:O	1:A:74:TYR:HB2	2.12	0.49
1:C:-35:TRP:HB3	1:C:-7:ARG:HA	1.93	0.49
1:C:-3:TRP:HE3	1:C:0:TYR:CD2	2.30	0.49
1:A:1109:LEU:HD13	1:C:1220:PRO:HG3	1.95	0.49
1:A:1235:VAL:HA	1:A:1336:VAL:HA	1.94	0.48
1:C:250:VAL:HG22	1:C:1078:LEU:HG	1.95	0.48
1:C:1343:LEU:HD22	1:C:1343:LEU:N	2.28	0.48
1:A:1057:LYS:NZ	1:A:1093:PRO:O	2.48	0.47
1:B:1244:GLN:N	1:B:1258:LYS:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1185:MET:SD	1:A:1212:LYS:HB3	2.56	0.46
1:B:214:ILE:HB	1:B:215:PRO:HD3	1.97	0.46
1:A:214:ILE:HB	1:A:215:PRO:HD3	1.98	0.46
1:A:1086:PHE:CZ	1:A:1162:GLU:HG3	2.51	0.45
1:A:1086:PHE:HZ	1:A:1162:GLU:HG3	1.81	0.45
1:D:-150:GLU:HG2	1:D:-131:GLY:N	2.32	0.45
1:D:1236:LYS:N	1:D:1335:THR:O	2.46	0.45
1:D:1235:VAL:HA	1:D:1336:VAL:HA	1.97	0.45
1:A:1086:PHE:CZ	1:A:1088:ARG:HB3	2.51	0.44
1:B:1061:THR:HG21	1:B:1153:PHE:CE2	2.52	0.44
1:B:1062:LEU:N	1:B:1087:SER:O	2.44	0.44
1:D:214:ILE:HB	1:D:215:PRO:HD3	2.00	0.44
1:B:312:GLN:HB2	1:B:1076:MET:CB	2.47	0.44
1:C:-67:VAL:HG22	1:C:-3:TRP:NE1	2.33	0.44
1:C:71:PRO:O	1:C:74:TYR:HB2	2.18	0.44
1:D:1086:PHE:CZ	1:D:1088:ARG:HB3	2.53	0.43
1:A:1236:LYS:N	1:A:1335:THR:O	2.48	0.43
1:B:1236:LYS:N	1:B:1335:THR:O	2.48	0.43
1:B:71:PRO:O	1:B:74:TYR:HB2	2.18	0.43
1:B:1061:THR:HA	1:B:1088:ARG:HA	2.01	0.43
1:A:1060:VAL:O	1:A:1089:VAL:O	2.37	0.43
1:C:-3:TRP:CE3	1:C:0:TYR:CE2	3.07	0.43
1:D:-157:PHE:CE1	1:D:-97:GLU:HG3	2.55	0.42
1:A:-153:ARG:HD3	1:A:-153:ARG:HH11	1.72	0.42
1:A:-2:ASP:HA	1:A:1:MET:HG3	2.01	0.42
1:C:1352:VAL:HA	1:C:1353:PRO:HD3	1.94	0.42
1:A:-67:VAL:HG22	1:A:-3:TRP:CZ2	2.54	0.42
1:D:-155:MET:HG3	1:D:0:TYR:CE1	2.55	0.42
1:C:1235:VAL:HA	1:C:1336:VAL:HA	2.02	0.42
1:A:1184:GLU:H	1:A:1184:GLU:CD	2.08	0.41
1:D:71:PRO:O	1:D:74:TYR:HB2	2.20	0.41
1:B:147:ARG:HA	1:B:147:ARG:HD3	1.73	0.41
1:C:1092:TYR:HA	1:C:1093:PRO:HA	1.90	0.41
1:A:-134:ILE:O	1:A:-130:HIS:HB3	2.21	0.41
1:C:1091:VAL:HG13	1:C:1092:TYR:N	2.35	0.41
1:D:1157:ILE:HG22	1:D:1158:THR:N	2.36	0.41
1:B:212:PHE:HE1	1:B:265:TRP:HB3	1.86	0.41
1:C:1064:CYS:N	1:C:1085:TYR:O	2.46	0.41
1:C:-67:VAL:HG22	1:C:-3:TRP:CE2	2.55	0.41
1:D:-148:LEU:HD21	1:D:-98:ALA:HB3	2.03	0.41
1:A:1242:VAL:HG23	1:A:1281:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:PHE:HB3	1:A:53:PRO:HD3	2.04	0.40
1:D:52:PHE:HB3	1:D:53:PRO:HD3	2.03	0.40

All (24) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-45:ASN:N	1:D:1184:GLU:OE2[3_545]	1.15	1.05
1:C:199:ASN:ND2	1:D:1343:LEU:CA[4_446]	1.63	0.57
1:B:1184:GLU:OE2	1:D:-46:THR:N[4_456]	1.67	0.53
1:A:-45:ASN:N	1:D:1184:GLU:CD[3_545]	1.73	0.47
1:B:1184:GLU:OE1	1:D:-46:THR:CB[4_456]	1.74	0.46
1:C:201:GLU:OE1	1:D:1339:PHE:CE1[4_446]	1.75	0.45
1:A:-46:THR:N	1:D:1184:GLU:CD[3_545]	1.77	0.43
1:C:199:ASN:OD1	1:D:1343:LEU:N[4_446]	1.79	0.41
1:B:1184:GLU:OE1	1:D:-46:THR:N[4_456]	1.80	0.40
1:A:-48:GLY:CA	1:D:1183:PRO:CG[3_545]	1.85	0.35
1:C:199:ASN:ND2	1:D:1343:LEU:CB[4_446]	1.86	0.34
1:A:-46:THR:CA	1:D:1184:GLU:CD[3_545]	1.89	0.31
1:A:-46:THR:N	1:D:1184:GLU:OE2[3_545]	1.94	0.26
1:A:-46:THR:CA	1:D:1184:GLU:OE2[3_545]	1.96	0.24
1:A:-46:THR:CA	1:D:1184:GLU:OE1[3_545]	1.98	0.22
1:B:1184:GLU:OE1	1:D:-46:THR:CA[4_456]	2.00	0.20
1:A:-46:THR:N	1:D:1184:GLU:CG[3_545]	2.03	0.17
1:A:-46:THR:C	1:D:1184:GLU:CD[3_545]	2.09	0.11
1:A:1183:PRO:CG	1:C:-48:GLY:C[4_446]	2.09	0.11
1:B:1184:GLU:OE2	1:D:-45:ASN:N[4_456]	2.09	0.11
1:A:-45:ASN:N	1:D:1184:GLU:OE1[3_545]	2.10	0.10
1:A:1183:PRO:CB	1:C:-48:GLY:O[4_446]	2.12	0.08
1:B:1184:GLU:OE1	1:D:-46:THR:OG1[4_456]	2.15	0.05
1:C:-21:ASN:O	1:D:1093:PRO:CG[4_456]	2.19	0.01

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	827/906 (91%)	796 (96%)	31 (4%)	0	100	100
1	B	667/906 (74%)	641 (96%)	26 (4%)	0	100	100
1	C	781/906 (86%)	753 (96%)	28 (4%)	0	100	100
1	D	827/906 (91%)	797 (96%)	30 (4%)	0	100	100
All	All	3102/3624 (86%)	2987 (96%)	115 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	721/777 (93%)	716 (99%)	5 (1%)	88	94
1	B	589/777 (76%)	586 (100%)	3 (0%)	92	96
1	C	686/777 (88%)	682 (99%)	4 (1%)	90	95
1	D	723/777 (93%)	719 (99%)	4 (1%)	90	95
All	All	2719/3108 (88%)	2703 (99%)	16 (1%)	90	95

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-57	PHE
1	A	67	LYS
1	A	147	ARG
1	A	268	TYR
1	A	1174	LEU
1	B	242	THR
1	B	268	TYR
1	B	1174	LEU
1	C	-57	PHE
1	C	268	TYR

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Mol	Chain	Res	Type
1	C	1174	LEU
1	C	1343	LEU
1	D	-57	PHE
1	D	268	TYR
1	D	1091	VAL
1	D	1174	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-29	ASN
1	D	-29	ASN
1	D	1287	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	833/906 (91%)	0.55	79 (9%) 10 15	211, 344, 728, 951	0
1	B	673/906 (74%)	0.47	65 (9%) 10 14	192, 330, 600, 858	0
1	C	789/906 (87%)	0.70	117 (14%) 3 9	226, 403, 694, 840	0
1	D	833/906 (91%)	0.93	172 (20%) 1 7	244, 456, 758, 955	0
All	All	3128/3624 (86%)	0.67	433 (13%) 4 10	192, 393, 718, 955	0

All (433) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1335	THR	15.7
1	A	1337	SER	14.9
1	B	1346	SER	14.8
1	A	1335	THR	14.6
1	B	1336	VAL	14.4
1	A	-112	ALA	14.1
1	A	1336	VAL	13.2
1	A	1346	SER	12.8
1	C	1233	LYS	12.7
1	C	1046	VAL	11.8
1	C	1117	TYR	10.8
1	D	280	GLY	10.8
1	C	1118	PRO	10.2
1	A	-110	GLY	10.1
1	B	1337	SER	9.9
1	C	1234	VAL	9.5
1	C	1337	SER	9.5
1	B	1237	LYS	9.3
1	A	1347	GLU	9.3
1	A	1345	SER	9.0
1	D	1048	VAL	9.0

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Mol	Chain	Res	Type	RSRZ
1	A	1338	GLY	8.8
1	C	1139	ASP	8.7
1	D	-116	GLU	8.7
1	C	1095	VAL	8.6
1	D	1079	THR	8.6
1	B	1238	ILE	8.4
1	D	-148	LEU	8.3
1	C	1235	VAL	8.3
1	D	1348	VAL	8.1
1	D	-112	ALA	8.0
1	A	1334	LEU	7.8
1	D	1096	GLY	7.8
1	D	-117	SER	7.8
1	A	-111	ILE	7.7
1	D	281	SER	7.7
1	C	1101	LEU	7.7
1	B	1265	THR	7.6
1	B	1345	SER	7.5
1	D	1084	LEU	7.3
1	D	1014	PHE	7.3
1	D	1070	GLN	7.3
1	C	1094	PRO	7.2
1	B	1334	LEU	7.1
1	D	1139	ASP	7.1
1	B	1250	LEU	7.1
1	C	1232	ASP	7.0
1	D	1142	LYS	6.9
1	C	1116	THR	6.7
1	B	1082	ARG	6.6
1	D	1233	LYS	6.6
1	A	-117	SER	6.6
1	D	-115	LEU	6.6
1	D	1334	LEU	6.6
1	A	-98	ALA	6.5
1	C	1142	LYS	6.4
1	D	1094	PRO	6.4
1	C	1096	GLY	6.4
1	D	1349	ALA	6.3
1	D	1013	ILE	6.3
1	B	1347	GLU	6.3
1	B	1264	GLU	6.3
1	C	1136	ALA	6.2

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Mol	Chain	Res	Type	RSRZ
1	D	1074	ASP	6.2
1	D	1097	ALA	6.0
1	D	1095	VAL	5.9
1	C	1100	VAL	5.8
1	C	-49	ALA	5.8
1	D	1143	SER	5.8
1	C	1137	PRO	5.8
1	C	1336	VAL	5.7
1	A	1236	LYS	5.7
1	D	-111	ILE	5.7
1	B	1338	GLY	5.6
1	B	1236	LYS	5.6
1	D	1015	LYS	5.5
1	D	1101	LEU	5.5
1	A	-116	GLU	5.5
1	D	1026	TYR	5.5
1	A	-114	ASP	5.4
1	D	1232	ASP	5.4
1	D	-97	GLU	5.4
1	A	1348	VAL	5.3
1	D	1313	ILE	5.3
1	D	1295	ALA	5.2
1	B	1182	PRO	5.2
1	D	1072	ASP	5.2
1	D	1069	GLY	5.1
1	D	-156	GLU	5.1
1	D	1118	PRO	5.1
1	D	1066	PHE	5.1
1	D	296	LYS	5.1
1	A	-95	LEU	5.1
1	A	-43	LEU	5.1
1	A	-97	GLU	5.1
1	D	1163	ASP	5.0
1	D	1141	GLY	5.0
1	D	1333	LYS	5.0
1	D	1127	LEU	4.9
1	D	1071	GLU	4.9
1	B	1359	PRO	4.9
1	A	-40	LEU	4.8
1	D	1027	LEU	4.8
1	D	-101	LYS	4.8
1	D	1332	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	1233	LYS	4.7
1	A	-108	ASN	4.7
1	D	1049	ASP	4.7
1	C	1070	GLN	4.7
1	C	1097	ALA	4.7
1	A	-78	LYS	4.7
1	B	1314	LYS	4.7
1	D	1098	MET	4.7
1	C	-34	ASP	4.7
1	A	1235	VAL	4.6
1	D	1231	THR	4.6
1	C	-48	GLY	4.6
1	C	1119	PHE	4.6
1	D	-147	ARG	4.6
1	D	1073	ILE	4.5
1	B	1142	LYS	4.5
1	D	-34	ASP	4.5
1	C	1014	PHE	4.5
1	D	118	THR	4.5
1	D	1028	GLY	4.5
1	C	1013	ILE	4.4
1	D	-100	ASP	4.4
1	C	1141	GLY	4.4
1	D	21	ARG	4.4
1	D	1316	GLY	4.4
1	D	1203	PRO	4.4
1	B	236	GLN	4.4
1	D	1202	LYS	4.4
1	D	-157	PHE	4.3
1	D	1080	PHE	4.3
1	C	1079	THR	4.3
1	D	-118	LYS	4.3
1	A	-109	ARG	4.3
1	A	1250	LEU	4.3
1	D	1099	SER	4.3
1	D	1238	ILE	4.2
1	B	1203	PRO	4.2
1	B	1235	VAL	4.2
1	A	-96	LYS	4.2
1	B	1232	ASP	4.1
1	C	-156	GLU	4.1
1	C	1027	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	1117	TYR	4.1
1	C	1048	VAL	4.1
1	D	-153	ARG	4.1
1	D	-32	ALA	4.1
1	D	1347	GLU	4.0
1	A	-34	ASP	4.0
1	C	1250	LEU	4.0
1	B	1196	GLN	4.0
1	D	1314	LYS	4.0
1	C	1045	VAL	4.0
1	A	1237	LYS	4.0
1	C	1115	ASN	4.0
1	C	-159	ASN	3.9
1	C	1128	PRO	3.9
1	D	-98	ALA	3.9
1	C	1138	GLN	3.9
1	C	1069	GLY	3.9
1	D	1144	CYS	3.9
1	B	1360	GLN	3.9
1	C	1143	SER	3.9
1	B	1183	PRO	3.9
1	D	1128	PRO	3.8
1	B	19	VAL	3.8
1	B	237	GLN	3.8
1	D	1234	VAL	3.8
1	A	-113	LYS	3.8
1	D	1336	VAL	3.8
1	B	1143	SER	3.8
1	C	1098	MET	3.8
1	C	1026	TYR	3.7
1	D	1346	SER	3.7
1	D	-33	GLU	3.7
1	B	234	ALA	3.7
1	D	1115	ASN	3.7
1	D	1324	ILE	3.7
1	D	265	TRP	3.7
1	D	-114	ASP	3.7
1	B	196	PRO	3.7
1	C	-35	TRP	3.7
1	D	-110	GLY	3.7
1	C	196	PRO	3.7
1	C	1093	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	-36	ARG	3.6
1	A	-93	ASN	3.6
1	C	1322	MET	3.6
1	D	237	GLN	3.6
1	B	1361	PRO	3.6
1	C	280	GLY	3.6
1	C	1163	ASP	3.6
1	C	1236	LYS	3.6
1	D	295	ALA	3.6
1	B	21	ARG	3.5
1	B	235	ALA	3.5
1	A	1238	ILE	3.5
1	D	-119	ALA	3.5
1	C	31	LEU	3.5
1	D	1267	GLU	3.5
1	D	1047	LEU	3.4
1	A	1070	GLN	3.4
1	D	1162	GLU	3.4
1	A	1082	ARG	3.4
1	D	1335	THR	3.4
1	A	1233	LYS	3.4
1	C	-47	PHE	3.4
1	A	237	GLN	3.4
1	D	1068	TYR	3.4
1	C	17	THR	3.4
1	C	1114	ASP	3.4
1	B	1066	PHE	3.3
1	B	1230	ASN	3.3
1	A	1265	THR	3.3
1	D	-120	ALA	3.3
1	B	1069	GLY	3.3
1	D	1165	ILE	3.3
1	A	-94	PHE	3.3
1	D	1100	VAL	3.3
1	D	1093	PRO	3.3
1	A	-39	GLN	3.3
1	A	-35	TRP	3.3
1	D	1034	ASP	3.3
1	C	1047	LEU	3.3
1	A	1344	THR	3.2
1	D	1082	ARG	3.2
1	B	1141	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	1144	CYS	3.2
1	D	2	CYS	3.2
1	D	1201	ASP	3.2
1	C	1335	THR	3.2
1	A	1251	TYR	3.2
1	C	1295	ALA	3.2
1	A	1142	LYS	3.2
1	C	1346	SER	3.2
1	D	1337	SER	3.2
1	C	1339	PHE	3.2
1	D	-146	LEU	3.2
1	B	1079	THR	3.2
1	A	265	TRP	3.2
1	A	1257	VAL	3.1
1	A	1048	VAL	3.1
1	D	1131	VAL	3.1
1	D	1294	ILE	3.1
1	C	1102	THR	3.1
1	B	1239	LYS	3.1
1	B	1313	ILE	3.0
1	D	-51	GLY	3.0
1	C	1015	LYS	3.0
1	D	-121	ASN	3.0
1	C	-97	GLU	3.0
1	D	1050	PRO	3.0
1	A	196	PRO	3.0
1	D	1081	ARG	3.0
1	A	1234	VAL	3.0
1	C	1135	PRO	3.0
1	B	1251	TYR	3.0
1	A	1197	PHE	3.0
1	D	1106	GLU	3.0
1	D	-52	THR	3.0
1	D	1315	GLU	3.0
1	D	1039	VAL	2.9
1	C	1348	VAL	2.9
1	C	1071	GLU	2.9
1	A	-148	LEU	2.9
1	C	-103	ILE	2.9
1	A	-99	GLU	2.9
1	A	1141	GLY	2.9
1	D	1293	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	22	SER	2.9
1	B	1256	TYR	2.9
1	C	-37	LYS	2.9
1	B	1231	THR	2.9
1	C	1237	LYS	2.8
1	C	1238	ILE	2.9
1	C	1092	TYR	2.8
1	C	1334	LEU	2.8
1	A	1256	TYR	2.8
1	D	1200	SER	2.8
1	D	1317	ILE	2.8
1	B	1197	PHE	2.8
1	D	-35	TRP	2.8
1	D	-113	LYS	2.8
1	D	1230	ASN	2.8
1	D	-31	ALA	2.8
1	D	1046	VAL	2.8
1	C	197	GLU	2.8
1	B	1202	LYS	2.8
1	C	14	SER	2.8
1	B	233	ALA	2.8
1	B	20	VAL	2.8
1	B	1322	MET	2.8
1	D	1025	ILE	2.8
1	D	282	CYS	2.8
1	C	1072	ASP	2.7
1	D	-102	THR	2.7
1	A	1109	LEU	2.7
1	D	-107	THR	2.7
1	D	1265	THR	2.7
1	C	1324	ILE	2.7
1	D	-140	THR	2.7
1	D	28	GLN	2.7
1	B	1257	VAL	2.7
1	D	1282	VAL	2.7
1	D	326	ASN	2.7
1	A	-103	ILE	2.7
1	C	1200	SER	2.6
1	C	1265	THR	2.6
1	D	1318	ASP	2.6
1	C	1028	GLY	2.6
1	D	299	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	1025	ILE	2.6
1	A	-36	ARG	2.6
1	C	142	PRO	2.6
1	C	1201	ASP	2.6
1	D	-103	ILE	2.6
1	A	-80	ASN	2.6
1	A	1232	ASP	2.6
1	C	-157	PHE	2.6
1	D	121	GLY	2.5
1	B	1181	ALA	2.5
1	D	1235	VAL	2.5
1	D	1140	VAL	2.5
1	A	1333	LYS	2.5
1	D	1197	PHE	2.5
1	B	1084	LEU	2.5
1	C	1197	PHE	2.5
1	D	1164	LYS	2.5
1	D	1114	ASP	2.5
1	B	36	GLN	2.5
1	C	1267	GLU	2.5
1	D	1092	TYR	2.5
1	D	240	SER	2.5
1	A	-115	LEU	2.4
1	C	-85	ARG	2.4
1	A	1084	LEU	2.4
1	A	-146	LEU	2.4
1	C	1177	LYS	2.4
1	B	1118	PRO	2.4
1	C	1338	GLY	2.4
1	C	-153	ARG	2.4
1	A	-118	LYS	2.4
1	C	1323	GLY	2.4
1	A	-79	ALA	2.4
1	B	1344	THR	2.4
1	D	1125	ASP	2.4
1	D	-126	LYS	2.4
1	A	1094	PRO	2.4
1	A	195	LYS	2.4
1	B	1068	TYR	2.4
1	D	1102	THR	2.4
1	C	1120	LEU	2.3
1	B	197	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	-99	GLU	2.3
1	C	282	CYS	2.3
1	D	-159	ASN	2.3
1	D	1312	ILE	2.3
1	C	20	VAL	2.3
1	B	1240	VAL	2.3
1	C	-50	VAL	2.3
1	C	1144	CYS	2.3
1	B	1109	LEU	2.3
1	C	21	ARG	2.3
1	C	1231	THR	2.3
1	D	266	VAL	2.2
1	A	1079	THR	2.2
1	D	1292	ARG	2.2
1	C	-152	ILE	2.2
1	D	1133	LEU	2.2
1	B	265	TRP	2.2
1	C	237	GLN	2.2
1	D	-84	GLY	2.2
1	B	1092	TYR	2.2
1	C	16	ALA	2.2
1	A	1106	GLU	2.2
1	A	1231	THR	2.2
1	C	1313	ILE	2.2
1	D	1322	MET	2.2
1	D	32	ALA	2.2
1	D	-106	ASN	2.2
1	C	1162	GLU	2.2
1	C	1182	PRO	2.2
1	D	1239	LYS	2.2
1	C	1084	LEU	2.1
1	A	1143	SER	2.1
1	D	122	GLU	2.1
1	D	279	GLN	2.1
1	C	121	GLY	2.1
1	D	-125	SER	2.1
1	D	1132	MET	2.1
1	C	281	SER	2.1
1	D	-122	LEU	2.1
1	D	1268	LYS	2.1
1	D	1225	VAL	2.1
1	D	1250	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	1082	ARG	2.1
1	A	1183	PRO	2.1
1	C	2	CYS	2.1
1	C	1099	SER	2.1
1	D	1111	LYS	2.1
1	D	1156	ASP	2.1
1	D	1195	TRP	2.1
1	A	-42	ARG	2.1
1	C	242	THR	2.1
1	A	236	GLN	2.1
1	C	-51	GLY	2.1
1	C	1140	VAL	2.1
1	D	-1	ALA	2.1
1	A	-59	MET	2.1
1	A	1101	LEU	2.1
1	A	1249	VAL	2.1
1	C	1133	LEU	2.1
1	D	1045	VAL	2.1
1	D	1104	LEU	2.1
1	A	-38	GLN	2.1
1	C	1321	VAL	2.1
1	D	1283	PRO	2.1
1	C	15	ASN	2.1
1	D	1350	THR	2.0
1	D	143	MET	2.0
1	B	1200	SER	2.0
1	D	1075	VAL	2.0
1	C	1202	LYS	2.0
1	D	-123	SER	2.0
1	C	1024	THR	2.0
1	A	-32	ALA	2.0
1	C	1039	VAL	2.0
1	B	1094	PRO	2.0
1	A	1283	PRO	2.0

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

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.