



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:52 AM UTC

PDB ID : 5GO3 / pdb_00005go3
Title : Crystal structure of a di-nucleotide cyclase Vibrio mutant
Authors : Ming, Z.H.; Wang, W.; Xie, Y.C.; Chen, Y.C.; Yan, L.M.; Lou, Z.Y.
Deposited on : 2016-07-26
Resolution : 2.20 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

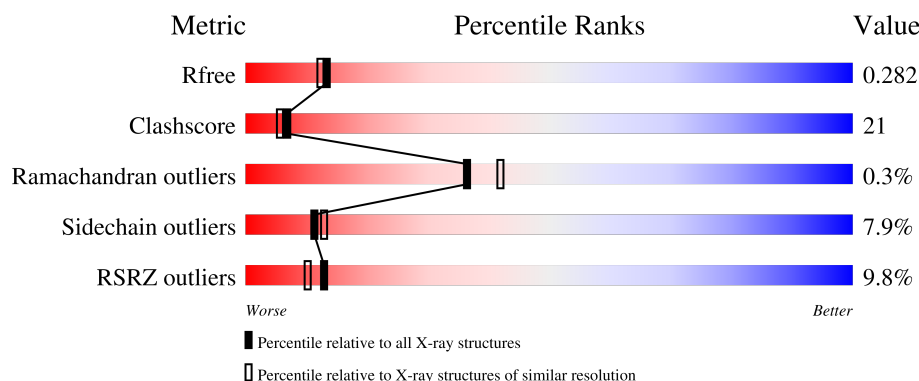
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	447	10% 49% 26% 5% 19%
1	B	447	6% 54% 22% 5% 19%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6104 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 Cyclic GMP-AMP synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2904	1837	503	548	16			
1	B	364	Total	C	N	O	S	0	0	0
			2922	1849	506	551	16			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q9KVG7
A	-3	PRO	-	expression tag	UNP Q9KVG7
A	-2	LEU	-	expression tag	UNP Q9KVG7
A	-1	GLY	-	expression tag	UNP Q9KVG7
A	0	SER	-	expression tag	UNP Q9KVG7
A	131	ASN	ASP	engineered mutation	UNP Q9KVG7
A	133	ASN	ASP	engineered mutation	UNP Q9KVG7
A	437	HIS	-	expression tag	UNP Q9KVG7
A	438	HIS	-	expression tag	UNP Q9KVG7
A	439	HIS	-	expression tag	UNP Q9KVG7
A	440	HIS	-	expression tag	UNP Q9KVG7
A	441	HIS	-	expression tag	UNP Q9KVG7
A	442	HIS	-	expression tag	UNP Q9KVG7
B	-4	GLY	-	expression tag	UNP Q9KVG7
B	-3	PRO	-	expression tag	UNP Q9KVG7
B	-2	LEU	-	expression tag	UNP Q9KVG7
B	-1	GLY	-	expression tag	UNP Q9KVG7
B	0	SER	-	expression tag	UNP Q9KVG7
B	131	ASN	ASP	engineered mutation	UNP Q9KVG7
B	133	ASN	ASP	engineered mutation	UNP Q9KVG7
B	437	HIS	-	expression tag	UNP Q9KVG7
B	438	HIS	-	expression tag	UNP Q9KVG7
B	439	HIS	-	expression tag	UNP Q9KVG7
B	440	HIS	-	expression tag	UNP Q9KVG7
B	441	HIS	-	expression tag	UNP Q9KVG7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	442	HIS	-	expression tag	UNP Q9KVG7

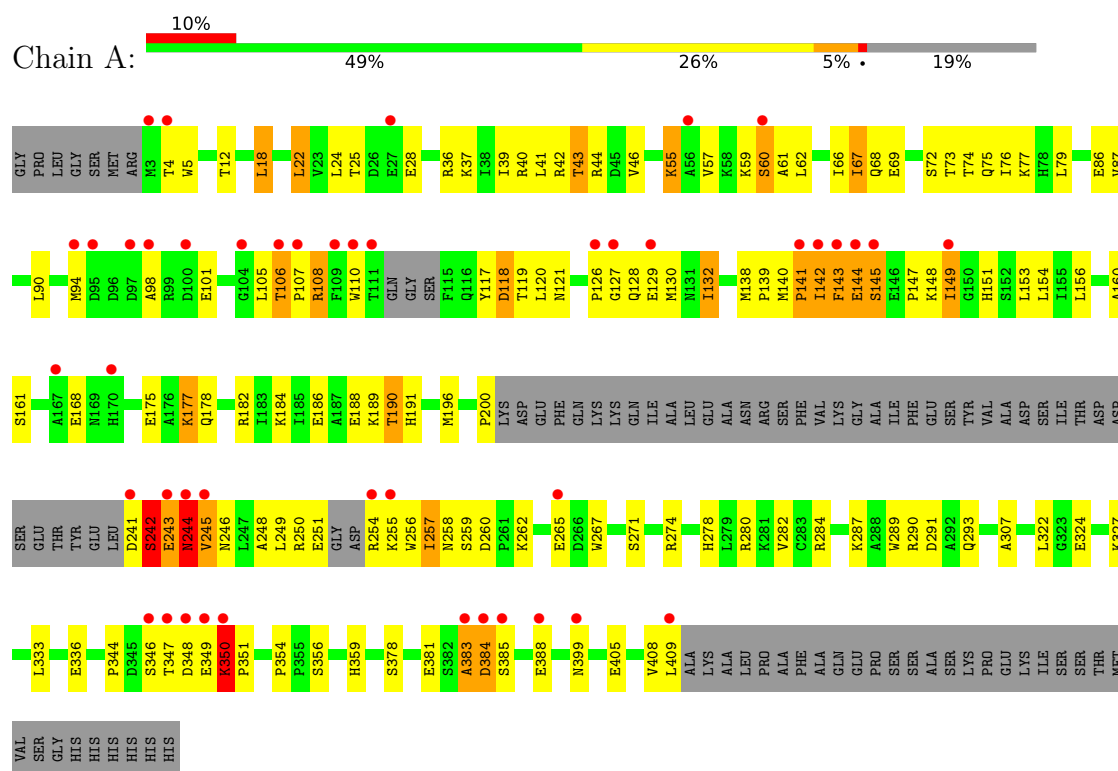
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	126	Total 126	O 126	0	0
2	B	152	Total 152	O 152	0	0

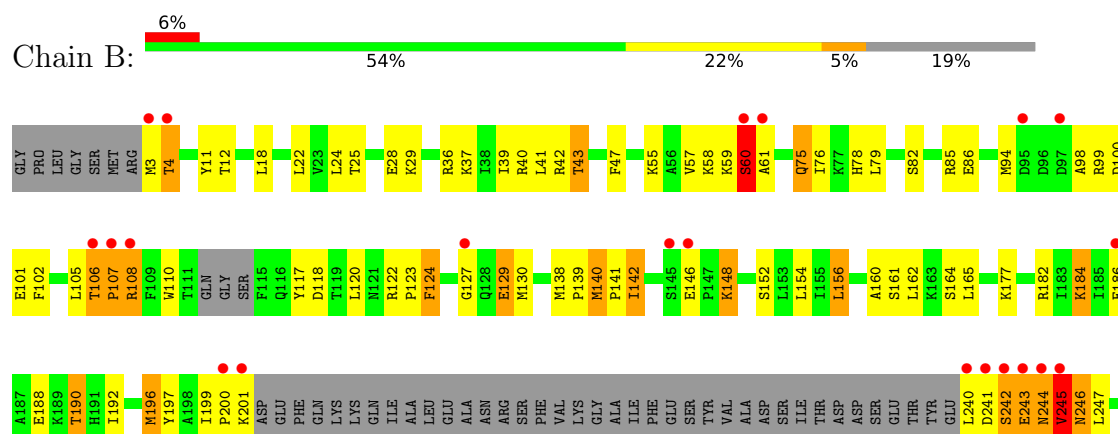
3 Residue-property plots

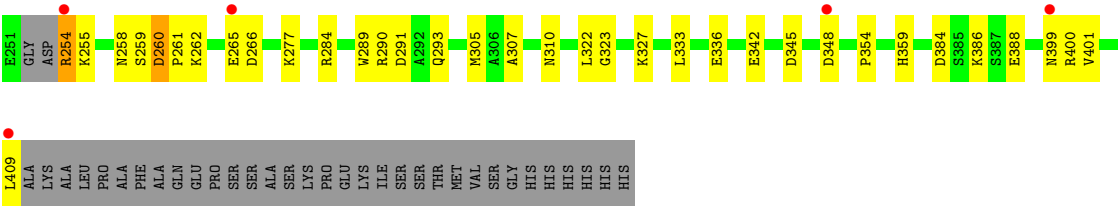
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Cyclic GMP-AMP synthase



• Molecule 1: Cyclic GMP-AMP synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.75Å 46.27Å 121.79Å 90.00° 99.82° 90.00°	Depositor
Resolution (Å)	43.17 – 2.20 43.17 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (43.17-2.20) 94.9 (43.17-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.24 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.7.1 _743	Depositor
R, R_{free}	0.228 , 0.292 0.228 , 0.282	Depositor DCC
R_{free} test set	2118 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	26.8	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6104	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.58 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.6676e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.58	1/2961 (0.0%)	1.22	30/3991 (0.8%)
1	B	0.57	1/2979 (0.0%)	1.45	32/4014 (0.8%)
All	All	0.57	2/5940 (0.0%)	1.34	62/8005 (0.8%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	107	PRO	N-CD	13.43	1.66	1.47
1	B	106	THR	C-N	6.63	1.39	1.33

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	107	PRO	CB-CA-C	-35.18	79.39	111.40
1	A	141	PRO	N-CA-C	30.72	152.26	113.86
1	B	245	VAL	N-CA-C	28.79	137.53	111.91
1	B	245	VAL	N-CA-CB	-22.09	86.55	112.39
1	B	245	VAL	CB-CA-C	-16.56	93.14	112.19
1	A	60	SER	N-CA-C	-15.66	85.60	109.24
1	B	244	ASN	N-CA-C	-15.34	93.87	112.89
1	B	61	ALA	N-CA-CB	-14.30	86.56	109.87
1	B	4	THR	N-CA-C	-14.12	85.50	108.52
1	B	108	ARG	N-CA-CB	-14.05	88.64	110.56
1	B	3	MET	N-CA-CB	-13.32	87.85	110.50
1	B	3	MET	N-CA-C	-12.04	77.28	111.00
1	A	145	SER	N-CA-C	-11.59	100.15	114.75
1	A	244	ASN	N-CA-C	-11.16	99.11	113.17
1	B	243	GLU	CB-CA-C	-10.96	93.37	111.02
1	A	142	ILE	CB-CA-C	-10.95	93.33	111.29
1	B	60	SER	CB-CA-C	-10.59	86.06	109.56
1	B	244	ASN	CB-CA-C	10.03	130.96	109.99
1	B	400	ARG	N-CA-C	10.00	132.11	110.80
1	B	246	ASN	N-CA-C	-9.87	94.15	109.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	346	SER	CB-CA-C	-9.84	92.29	110.01
1	A	142	ILE	N-CA-C	-9.32	89.96	109.34
1	B	243	GLU	N-CA-C	9.28	123.92	112.59
1	B	242	SER	CB-CA-C	9.14	125.22	110.88
1	A	144	GLU	CB-CA-C	9.11	128.30	112.00
1	B	3	MET	CB-CA-C	-9.06	92.88	110.10
1	A	61	ALA	N-CA-CB	-9.05	93.72	110.56
1	B	242	SER	N-CA-C	-8.90	101.54	111.07
1	A	145	SER	N-CA-CB	-8.74	98.39	111.15
1	A	106	THR	CB-CA-C	8.56	122.24	109.22
1	A	128	GLN	N-CA-C	-8.56	96.33	109.95
1	A	141	PRO	CB-CA-C	-8.48	99.30	111.68
1	A	60	SER	CB-CA-C	-8.29	91.83	110.07
1	A	243	GLU	CB-CA-C	-8.18	96.44	110.09
1	B	246	ASN	CB-CA-C	8.14	123.64	110.29
1	A	107	PRO	CA-N-CD	-7.82	101.05	112.00
1	B	401	VAL	CB-CA-C	-7.61	102.18	111.08
1	B	247	LEU	N-CA-C	-7.43	97.58	109.76
1	B	241	ASP	N-CA-C	7.12	120.87	111.75
1	A	384	ASP	N-CA-C	7.01	120.94	112.38
1	A	383	ALA	CB-CA-C	-6.99	99.00	109.90
1	A	59	LYS	CB-CA-C	-6.75	96.62	110.38
1	A	143	PHE	N-CA-C	6.47	118.04	107.23
1	B	124	PHE	CB-CA-C	-6.45	98.58	109.03
1	A	383	ALA	N-CA-C	6.43	119.69	110.10
1	A	143	PHE	N-CA-CB	-6.38	100.39	110.79
1	A	242	SER	N-CA-C	-6.35	105.18	113.12
1	A	246	ASN	N-CA-C	6.24	119.67	107.57
1	B	399	ASN	N-CA-C	6.10	123.79	110.80
1	B	124	PHE	N-CA-C	6.08	121.36	113.88
1	B	246	ASN	N-CA-CB	5.76	119.25	109.87
1	A	68	GLN	N-CA-C	5.70	117.50	111.28
1	B	400	ARG	N-CA-CB	-5.70	100.86	110.49
1	A	350	LYS	CA-C-N	-5.65	113.96	119.78
1	A	350	LYS	C-N-CA	-5.65	113.96	119.78
1	A	107	PRO	N-CA-C	-5.41	101.03	111.69
1	B	60	SER	N-CA-C	-5.38	100.89	109.23
1	B	243	GLU	N-CA-CB	-5.25	102.52	110.92
1	A	140	MET	CA-C-N	-5.24	114.27	119.56
1	A	140	MET	C-N-CA	-5.24	114.27	119.56
1	B	260	ASP	CA-C-N	5.06	124.85	119.28
1	B	260	ASP	C-N-CA	5.06	124.85	119.28

There are no chirality outliers.

There are no planarity outliers.

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	2904	0	2899	138	0
1	B	2922	0	2926	111	1
2	A	126	0	0	6	0
2	B	152	0	0	7	0
All	All	6104	0	5825	248	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 21.

All (248) 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:385:SER:HB3	1:A:388:GLU:OE1	1.22	1.29
1:A:245:VAL:HG12	1:A:259:SER:N	1.53	1.21
1:B:290:ARG:NH1	1:B:291:ASP:OD1	1.73	1.20
1:A:385:SER:CB	1:A:388:GLU:OE1	2.02	1.08
1:B:24:LEU:HD11	1:B:130:MET:HE1	1.38	1.06
1:A:245:VAL:HB	1:A:258:ASN:OD1	1.58	1.03
1:B:142:ILE:H	1:B:142:ILE:HD12	1.26	0.99
1:A:245:VAL:O	1:A:258:ASN:HA	1.61	0.99
1:A:350:LYS:NZ	1:A:350:LYS:HA	1.80	0.97
1:A:245:VAL:HG11	1:A:258:ASN:ND2	1.78	0.96
1:A:24:LEU:HD11	1:A:130:MET:HE1	1.48	0.96
1:A:200:PRO:HD3	1:A:243:GLU:O	1.66	0.95
1:B:101:GLU:HG3	1:B:148:LYS:HE2	1.49	0.94
1:A:245:VAL:HG12	1:A:258:ASN:C	1.92	0.93
1:A:350:LYS:HD3	1:A:351:PRO:HD2	1.52	0.92
1:A:245:VAL:O	1:A:259:SER:N	2.03	0.91
1:B:94:MET:HE1	1:B:102:PHE:HB2	1.53	0.91
1:A:241:ASP:O	1:A:245:VAL:CG2	2.19	0.89
1:B:105:LEU:HD21	1:B:138:MET:CE	2.01	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:LEU:HD21	1:B:138:MET:HE3	1.55	0.89
1:B:199:ILE:HG22	1:B:244:ASN:O	1.73	0.87
1:B:108:ARG:HH21	1:B:108:ARG:HG3	1.38	0.87
1:B:120:LEU:HD21	1:B:130:MET:HE2	1.55	0.87
1:B:200:PRO:HD3	1:B:243:GLU:O	1.74	0.87
1:B:245:VAL:CG1	1:B:258:ASN:HA	2.05	0.86
1:A:74:THR:O	1:A:77:LYS:HE3	1.76	0.86
1:B:79:LEU:HD11	1:B:160:ALA:HB2	1.56	0.86
1:B:254:ARG:HG2	1:B:254:ARG:HH11	1.42	0.85
1:A:117:TYR:O	1:A:118:ASP:HB2	1.75	0.85
1:B:24:LEU:HD11	1:B:130:MET:CE	2.07	0.84
1:B:242:SER:O	1:B:258:ASN:OD1	1.98	0.81
1:B:245:VAL:HG11	1:B:258:ASN:OD1	1.80	0.81
1:A:245:VAL:HG13	1:A:260:ASP:N	1.96	0.80
1:B:28:GLU:OE2	1:B:122:ARG:NH1	2.16	0.79
1:B:245:VAL:HG23	1:B:260:ASP:HB2	1.64	0.79
1:B:307:ALA:HB1	1:B:336:GLU:HG2	1.66	0.78
1:A:350:LYS:HA	1:A:350:LYS:CE	2.07	0.77
1:A:350:LYS:HD3	1:A:351:PRO:CD	2.14	0.77
1:B:245:VAL:HG22	1:B:259:SER:N	1.98	0.77
1:A:79:LEU:HD11	1:A:160:ALA:HB2	1.66	0.76
1:B:58:LYS:NZ	1:B:100:ASP:OD1	2.16	0.76
1:A:118:ASP:O	1:A:284:ARG:NH1	2.18	0.76
1:B:245:VAL:HG11	1:B:258:ASN:HA	1.69	0.75
1:B:36:ARG:HD2	2:B:547:HOH:O	1.86	0.75
1:B:36:ARG:HD3	1:B:40:ARG:CZ	2.16	0.75
1:A:245:VAL:HB	1:A:258:ASN:CG	2.12	0.74
1:A:290:ARG:NH1	1:A:291:ASP:OD1	2.21	0.73
1:B:142:ILE:H	1:B:142:ILE:CD1	2.01	0.73
1:B:245:VAL:HG13	1:B:258:ASN:HA	1.69	0.73
1:B:245:VAL:HG13	1:B:245:VAL:O	1.82	0.73
1:A:120:LEU:HD22	1:A:132:ILE:HD11	1.71	0.72
1:A:200:PRO:HG3	1:A:243:GLU:HB2	1.71	0.72
1:A:399:ASN:ND2	2:A:501:HOH:O	2.17	0.72
1:A:105:LEU:HD21	1:A:138:MET:HE2	1.72	0.71
1:A:347:THR:O	1:A:348:ASP:OD1	2.07	0.71
1:A:245:VAL:O	1:A:258:ASN:CA	2.38	0.71
1:B:24:LEU:CD1	1:B:130:MET:HE1	2.19	0.70
1:B:245:VAL:HG22	1:B:259:SER:C	2.15	0.70
1:A:42:ARG:NH1	2:A:503:HOH:O	2.25	0.69
1:B:94:MET:HE2	1:B:98:ALA:C	2.17	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:LEU:HB2	1:B:244:ASN:HD22	1.55	0.69
1:A:43:THR:HG22	1:A:161:SER:HB3	1.73	0.69
1:A:354:PRO:O	1:A:359:HIS:HE1	1.76	0.68
1:B:142:ILE:HD12	1:B:142:ILE:N	2.06	0.68
1:B:254:ARG:HG2	1:B:254:ARG:NH1	2.05	0.68
1:A:245:VAL:CG1	1:A:258:ASN:ND2	2.55	0.68
1:A:249:LEU:HD11	1:A:257:ILE:HG13	1.76	0.68
1:A:245:VAL:HG12	1:A:259:SER:CA	2.23	0.68
1:A:105:LEU:HD11	1:A:138:MET:HE3	1.74	0.68
1:B:201:LYS:HD2	2:B:589:HOH:O	1.93	0.67
1:A:43:THR:HG22	1:A:161:SER:CB	2.25	0.67
1:A:105:LEU:HD22	1:A:149:ILE:HD12	1.75	0.67
1:A:129:GLU:OE1	1:A:191:HIS:CD2	2.49	0.66
1:A:141:PRO:C	1:A:142:ILE:HG13	2.20	0.66
1:A:350:LYS:HA	1:A:350:LYS:HZ3	1.61	0.65
1:A:57:VAL:O	1:A:60:SER:O	2.15	0.65
1:A:241:ASP:O	1:A:245:VAL:HG21	1.96	0.65
1:B:307:ALA:CB	1:B:336:GLU:HG2	2.27	0.65
1:A:5:TRP:NE1	1:A:383:ALA:O	2.25	0.64
1:A:101:GLU:HG3	1:A:148:LYS:CE	2.28	0.64
1:B:245:VAL:HG21	1:B:258:ASN:OD1	1.98	0.64
1:A:36:ARG:HD3	1:A:40:ARG:CZ	2.28	0.62
1:B:55:LYS:HD3	1:B:55:LYS:C	2.24	0.62
1:A:94:MET:HE1	1:A:98:ALA:O	1.99	0.62
1:B:240:LEU:HB2	1:B:244:ASN:ND2	2.14	0.62
1:A:69:GLU:O	1:A:72:SER:OG	2.18	0.62
1:B:409:LEU:C	2:B:569:HOH:O	2.42	0.62
1:B:82:SER:O	1:B:86:GLU:HG3	2.00	0.61
1:B:79:LEU:HD11	1:B:160:ALA:CB	2.29	0.60
1:B:261:PRO:O	1:B:265:GLU:HG3	2.01	0.60
1:B:108:ARG:HG3	1:B:108:ARG:NH2	2.11	0.60
1:B:108:ARG:NH2	1:B:139:PRO:HG2	2.16	0.60
1:A:307:ALA:HB1	1:A:336:GLU:HG2	1.84	0.59
1:A:25:THR:OG1	1:A:28:GLU:HG3	2.02	0.59
1:B:28:GLU:CD	1:B:122:ARG:HH12	2.09	0.59
1:B:39:ILE:O	1:B:43:THR:HG23	2.02	0.59
1:B:188:GLU:O	1:B:190:THR:HG23	2.03	0.59
1:A:200:PRO:HD2	1:A:244:ASN:HA	1.85	0.58
1:B:354:PRO:O	1:B:359:HIS:HE1	1.86	0.58
1:A:79:LEU:HD11	1:A:160:ALA:CB	2.33	0.58
1:A:24:LEU:CD1	1:A:130:MET:HE1	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:THR:OG1	1:A:348:ASP:N	2.36	0.57
1:B:160:ALA:O	1:B:164:SER:HB3	2.05	0.57
1:B:76:ILE:HG23	1:B:79:LEU:HD13	1.86	0.57
1:A:101:GLU:OE1	1:A:141:PRO:HG3	2.05	0.56
1:B:101:GLU:HG3	1:B:148:LYS:CE	2.30	0.56
1:A:129:GLU:HG2	1:A:189:LYS:HA	1.86	0.56
1:B:75:GLN:HG2	1:B:164:SER:HB2	1.88	0.56
1:A:24:LEU:HD11	1:A:130:MET:CE	2.31	0.55
1:A:241:ASP:O	1:A:245:VAL:HG22	2.05	0.55
1:A:245:VAL:CG1	1:A:259:SER:N	2.48	0.55
1:B:310:ASN:ND2	1:B:336:GLU:OE2	2.28	0.55
1:B:47:PHE:CE2	1:B:138:MET:HE1	2.41	0.55
1:B:57:VAL:O	1:B:60:SER:O	2.25	0.55
1:A:108:ARG:HG3	1:A:139:PRO:HG3	1.89	0.55
1:A:24:LEU:HD21	1:A:130:MET:HE1	1.89	0.54
1:A:307:ALA:CB	1:A:336:GLU:HG2	2.36	0.54
1:B:106:THR:CG2	1:B:108:ARG:CZ	2.85	0.54
1:B:39:ILE:HD11	1:B:192:ILE:HD12	1.89	0.54
1:B:177:LYS:HE3	1:B:182:ARG:NH1	2.23	0.54
1:A:241:ASP:OD1	1:A:260:ASP:OD2	2.26	0.54
1:A:245:VAL:CG1	1:A:258:ASN:CG	2.81	0.53
1:A:241:ASP:N	1:A:244:ASN:ND2	2.56	0.53
1:B:25:THR:HG23	1:B:28:GLU:OE1	2.08	0.53
1:A:120:LEU:HD21	1:A:130:MET:HE2	1.90	0.53
1:B:106:THR:HG23	1:B:108:ARG:NE	2.24	0.53
1:B:199:ILE:HB	1:B:200:PRO:HD2	1.91	0.53
1:A:177:LYS:HE3	1:A:182:ARG:NH1	2.24	0.53
1:B:108:ARG:HH21	1:B:108:ARG:CG	2.14	0.53
1:A:327:LYS:NZ	1:A:381:GLU:OE1	2.41	0.52
1:A:350:LYS:HA	1:A:350:LYS:HZ2	1.72	0.52
1:A:141:PRO:O	1:A:142:ILE:HG13	2.09	0.52
1:B:55:LYS:HD3	1:B:55:LYS:O	2.09	0.52
1:B:262:LYS:HG2	1:B:266:ASP:OD2	2.09	0.52
1:B:124:PHE:O	1:B:124:PHE:CD1	2.63	0.51
1:B:245:VAL:HG22	1:B:259:SER:H	1.72	0.51
1:B:108:ARG:NH2	1:B:108:ARG:CG	2.73	0.51
1:A:151:HIS:HB3	1:A:255:LYS:HE2	1.92	0.51
1:B:106:THR:CG2	1:B:108:ARG:NE	2.73	0.51
1:A:55:LYS:HD3	1:A:55:LYS:C	2.36	0.51
1:A:188:GLU:O	1:A:190:THR:HG23	2.10	0.51
1:A:271:SER:HA	1:A:274:ARG:NH1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ARG:HH21	1:A:168:GLU:CD	2.18	0.50
1:A:245:VAL:CB	1:A:258:ASN:CG	2.82	0.50
1:A:143:PHE:HZ	1:A:256:TRP:CE2	2.29	0.50
1:A:245:VAL:CG1	1:A:259:SER:CA	2.90	0.50
1:A:245:VAL:CB	1:A:258:ASN:OD1	2.47	0.50
1:A:90:LEU:HD13	1:A:153:LEU:HB2	1.94	0.49
1:A:66:ILE:O	1:A:67:ILE:C	2.55	0.49
1:A:76:ILE:HD13	1:A:87:VAL:HG11	1.95	0.49
1:A:106:THR:HG21	1:A:108:ARG:NH2	2.27	0.49
1:A:248:ALA:HB2	1:A:256:TRP:CZ3	2.48	0.49
1:A:69:GLU:O	1:A:73:THR:HG23	2.13	0.48
1:A:200:PRO:CD	1:A:243:GLU:O	2.51	0.48
1:A:245:VAL:HG11	1:A:258:ASN:HD21	1.67	0.48
1:A:12:THR:HG22	1:A:322:LEU:HD12	1.94	0.48
1:A:37:LYS:O	1:A:41:LEU:HG	2.13	0.48
1:A:94:MET:CE	1:A:98:ALA:C	2.86	0.48
1:A:129:GLU:OE1	1:A:191:HIS:NE2	2.46	0.48
1:B:110:TRP:CH2	1:B:262:LYS:HE2	2.47	0.48
1:A:129:GLU:OE2	1:A:186:GLU:HA	2.13	0.48
1:A:242:SER:C	1:A:245:VAL:HG23	2.38	0.48
1:B:29:LYS:HE2	2:B:649:HOH:O	2.12	0.48
1:A:250:ARG:O	1:A:251:GLU:O	2.32	0.48
1:B:117:TYR:O	1:B:118:ASP:HB2	2.13	0.48
1:A:175:GLU:OE2	1:A:184:LYS:HE3	2.14	0.48
1:A:405:GLU:O	1:B:277:LYS:HE2	2.14	0.47
1:A:39:ILE:O	1:A:43:THR:HG23	2.14	0.47
1:A:260:ASP:OD1	1:A:262:LYS:HB3	2.15	0.47
1:B:196:MET:O	1:B:196:MET:HG3	2.15	0.47
1:B:118:ASP:O	1:B:284:ARG:NH1	2.47	0.47
1:A:118:ASP:HB2	1:A:280:ARG:NE	2.30	0.47
1:B:105:LEU:HD11	1:B:138:MET:HE3	1.98	0.46
1:B:94:MET:HE1	1:B:102:PHE:CB	2.36	0.46
1:A:245:VAL:O	1:A:258:ASN:C	2.57	0.46
1:A:249:LEU:CD1	1:A:257:ILE:HG13	2.42	0.46
1:B:348:ASP:HB3	2:B:599:HOH:O	2.16	0.46
1:A:117:TYR:O	1:A:118:ASP:CB	2.53	0.46
1:B:289:TRP:O	1:B:293:GLN:HG2	2.16	0.46
1:A:22:LEU:HG	1:A:121:ASN:OD1	2.15	0.46
1:A:57:VAL:C	1:A:60:SER:O	2.59	0.46
1:B:117:TYR:HD2	1:B:305:MET:HE1	1.81	0.46
1:A:76:ILE:HG23	1:A:79:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:VAL:HG13	1:A:259:SER:C	2.41	0.46
1:B:43:THR:HA	1:B:161:SER:OG	2.15	0.46
1:B:37:LYS:O	1:B:41:LEU:HG	2.16	0.45
1:B:42:ARG:HB3	1:B:165:LEU:HD11	1.97	0.45
1:A:22:LEU:HG	1:A:121:ASN:CG	2.42	0.45
1:A:178:GLN:HG3	1:A:250:ARG:O	2.15	0.45
1:B:11:TYR:CE2	1:B:323:GLY:HA2	2.52	0.45
1:A:245:VAL:HG13	1:A:260:ASP:H	1.79	0.45
1:B:36:ARG:HD3	1:B:40:ARG:NH2	2.31	0.45
1:B:260:ASP:HA	1:B:261:PRO:HD2	1.81	0.45
1:B:24:LEU:HD21	1:B:130:MET:CE	2.47	0.44
1:A:245:VAL:HG22	1:A:260:ASP:HB2	1.99	0.44
1:A:324:GLU:HG2	2:A:606:HOH:O	2.18	0.44
1:A:105:LEU:HD12	1:A:139:PRO:HD2	2.00	0.44
1:A:129:GLU:HG2	1:A:189:LYS:CA	2.48	0.44
1:B:327:LYS:HB2	1:B:327:LYS:HE3	1.85	0.44
1:B:245:VAL:HG22	1:B:259:SER:CA	2.47	0.44
1:A:79:LEU:HD12	1:A:79:LEU:N	2.32	0.44
1:A:324:GLU:OE1	1:A:327:LYS:NZ	2.44	0.44
1:B:123:PRO:HG3	1:B:130:MET:HG3	1.98	0.44
1:A:94:MET:HE2	1:A:98:ALA:C	2.43	0.44
1:B:76:ILE:C	1:B:78:HIS:N	2.75	0.44
1:B:129:GLU:N	1:B:129:GLU:CD	2.75	0.43
1:A:44:ARG:O	2:A:502:HOH:O	2.21	0.43
1:A:408:VAL:HG12	1:A:409:LEU:N	2.33	0.43
1:B:79:LEU:N	1:B:79:LEU:HD12	2.33	0.43
1:B:129:GLU:CD	1:B:129:GLU:H	2.25	0.43
1:A:144:GLU:OE2	1:A:144:GLU:HA	2.18	0.43
1:B:197:TYR:HA	1:B:246:ASN:O	2.18	0.43
1:A:289:TRP:O	1:A:293:GLN:HG2	2.19	0.43
1:A:356:SER:HA	1:A:359:HIS:CD2	2.52	0.43
1:B:141:PRO:HG2	1:B:148:LYS:HG3	2.01	0.43
1:B:24:LEU:HD21	1:B:130:MET:HE3	2.01	0.42
1:B:106:THR:O	1:B:108:ARG:HG2	2.19	0.42
1:B:245:VAL:CG1	1:B:258:ASN:OD1	2.60	0.42
1:A:143:PHE:CZ	1:A:147:PRO:HG3	2.54	0.42
1:B:120:LEU:HD21	1:B:130:MET:CE	2.36	0.42
1:A:106:THR:CG2	1:A:108:ARG:NH2	2.82	0.42
1:A:256:TRP:O	1:A:257:ILE:HG12	2.20	0.42
1:A:242:SER:O	1:A:258:ASN:OD1	2.38	0.42
1:B:106:THR:CG2	1:B:108:ARG:NH1	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:LEU:HD23	1:B:322:LEU:HA	1.83	0.42
1:A:110:TRP:NE1	1:A:265:GLU:OE1	2.53	0.42
1:B:12:THR:HG22	1:B:322:LEU:HD12	2.02	0.42
1:A:119:THR:HA	1:A:284:ARG:NH1	2.35	0.42
1:A:126:PRO:HA	1:A:127:GLY:HA2	1.70	0.41
1:B:140:MET:O	1:B:200:PRO:O	2.37	0.41
1:B:152:SER:O	1:B:156:LEU:HD22	2.20	0.41
1:A:24:LEU:HD21	1:A:130:MET:CE	2.49	0.41
1:A:267:TRP:CD1	1:A:344:PRO:HB3	2.55	0.41
1:B:345:ASP:OD1	1:B:345:ASP:C	2.63	0.41
1:B:342:GLU:HG2	2:B:647:HOH:O	2.20	0.41
1:A:76:ILE:HA	1:A:79:LEU:HD13	2.03	0.41
1:B:384:ASP:HB2	1:B:388:GLU:OE1	2.20	0.41
1:A:118:ASP:HB2	1:A:280:ARG:HE	1.84	0.41
1:A:175:GLU:OE1	1:A:177:LYS:HE2	2.20	0.41
1:A:12:THR:CG2	1:A:322:LEU:HD12	2.51	0.41
1:A:278:HIS:O	1:A:282:VAL:HG22	2.21	0.41
1:B:184:LYS:HE2	2:B:559:HOH:O	2.20	0.41
1:B:188:GLU:O	1:B:190:THR:CG2	2.68	0.41
1:A:254:ARG:HG2	2:A:613:HOH:O	2.19	0.41
1:A:287:LYS:HB3	2:A:579:HOH:O	2.19	0.40
1:B:58:LYS:HB2	1:B:99:ARG:HD2	2.02	0.40
1:A:57:VAL:HA	1:A:62:LEU:HG	2.04	0.40
1:A:18:LEU:HA	1:A:18:LEU:HD23	1.81	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:B:85:ARG:NH2	1:B:127:GLY:O[2_444]	1.90	0.30

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	354/447 (79%)	340 (96%)	12 (3%)	2 (1%)	21	23
1	B	356/447 (80%)	345 (97%)	11 (3%)	0	100	100
All	All	710/894 (79%)	685 (96%)	23 (3%)	2 (0%)	36	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	ASP
1	A	67	ILE

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	320/391 (82%)	294 (92%)	26 (8%)	11	12
1	B	323/391 (83%)	298 (92%)	25 (8%)	12	13
All	All	643/782 (82%)	592 (92%)	51 (8%)	11	13

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	18	LEU
1	A	22	LEU
1	A	43	THR
1	A	46	VAL
1	A	55	LYS
1	A	75	GLN
1	A	86	GLU
1	A	108	ARG
1	A	132	ILE
1	A	145	SER
1	A	149	ILE

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Mol	Chain	Res	Type
1	A	154	LEU
1	A	156	LEU
1	A	177	LYS
1	A	190	THR
1	A	196	MET
1	A	242	SER
1	A	244	ASN
1	A	245	VAL
1	A	257	ILE
1	A	333	LEU
1	A	349	GLU
1	A	350	LYS
1	A	378	SER
1	A	384	ASP
1	B	4	THR
1	B	18	LEU
1	B	22	LEU
1	B	43	THR
1	B	59	LYS
1	B	60	SER
1	B	75	GLN
1	B	107	PRO
1	B	129	GLU
1	B	140	MET
1	B	142	ILE
1	B	146	GLU
1	B	148	LYS
1	B	154	LEU
1	B	156	LEU
1	B	162	LEU
1	B	184	LYS
1	B	186	GLU
1	B	190	THR
1	B	196	MET
1	B	245	VAL
1	B	254	ARG
1	B	255	LYS
1	B	333	LEU
1	B	386	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	244	ASN
1	A	246	ASN
1	A	359	HIS
1	B	178	GLN
1	B	244	ASN
1	B	359	HIS
1	B	399	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 oligosaccharides 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	362/447 (80%)	0.58	45 (12%) 8 6	15, 31, 56, 68	0
1	B	364/447 (81%)	0.31	26 (7%) 22 19	14, 27, 47, 63	0
All	All	726/894 (81%)	0.44	71 (9%) 13 10	14, 29, 53, 68	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	244	ASN	8.7
1	A	245	VAL	8.1
1	B	245	VAL	7.0
1	A	244	ASN	6.9
1	A	142	ILE	6.7
1	A	106	THR	6.3
1	B	127	GLY	6.2
1	A	349	GLU	5.2
1	A	141	PRO	5.1
1	B	243	GLU	5.0
1	B	240	LEU	5.0
1	B	3	MET	4.9
1	A	143	PHE	4.9
1	B	95	ASP	4.7
1	A	243	GLU	4.4
1	A	129	GLU	4.4
1	A	348	ASP	4.3
1	B	241	ASP	4.2
1	A	145	SER	4.1
1	B	348	ASP	4.1
1	A	127	GLY	4.0
1	A	350	LYS	4.0
1	A	60	SER	3.7
1	B	107	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	61	ALA	3.5
1	A	347	THR	3.5
1	B	409	LEU	3.5
1	A	126	PRO	3.4
1	A	3	MET	3.2
1	A	409	LEU	3.1
1	A	144	GLU	3.1
1	A	109	PHE	3.1
1	A	95	ASP	3.1
1	A	254	ARG	3.1
1	A	4	THR	3.0
1	B	146	GLU	3.0
1	A	384	ASP	2.9
1	A	385	SER	2.9
1	A	265	GLU	2.8
1	A	110	TRP	2.8
1	A	383	ALA	2.8
1	B	4	THR	2.8
1	B	97	ASP	2.8
1	B	145	SER	2.7
1	B	201	LYS	2.7
1	A	97	ASP	2.6
1	B	186	GLU	2.6
1	A	170	HIS	2.6
1	B	399	ASN	2.6
1	A	241	ASP	2.6
1	A	56	ALA	2.5
1	B	242	SER	2.4
1	A	94	MET	2.4
1	B	200	PRO	2.4
1	B	254	ARG	2.4
1	A	98	ALA	2.4
1	B	106	THR	2.4
1	A	149	ILE	2.4
1	A	107	PRO	2.3
1	B	60	SER	2.3
1	A	111	THR	2.3
1	A	100	ASP	2.3
1	A	167	ALA	2.2
1	B	265	GLU	2.2
1	A	346	SER	2.2
1	A	388	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	399	ASN	2.1
1	B	108	ARG	2.1
1	A	27	GLU	2.1
1	A	104	GLY	2.0
1	A	255	LYS	2.0

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.