



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:43 AM UTC

PDB ID : 1O60 / pdb_00001o60
Title : Crystal structure of KDO-8-phosphate synthase
Authors : Structural GenomiX
Deposited on : 2003-10-23
Resolution : 1.80 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

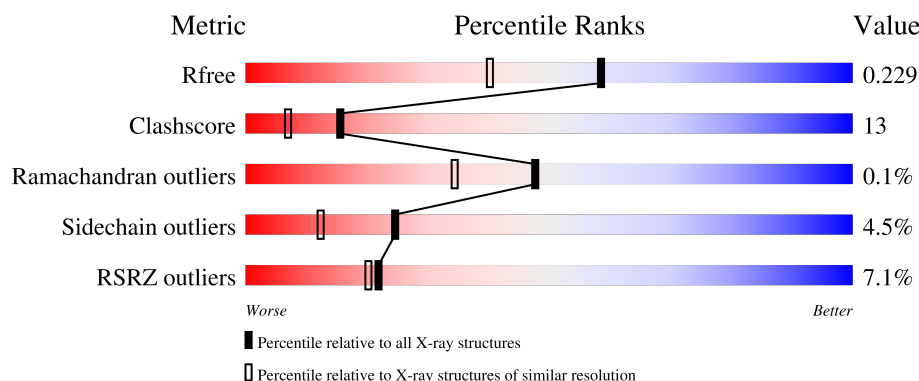
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	292	4% 73% 17% • 8%
1	B	292	8% 68% 21% • 8%
1	C	292	5% 65% 23% • 8%
1	D	292	8% 67% 23% • 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8811 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 2-dehydro-3-deoxyphosphooctonate aldolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	Se	0	3	0
			2067	1317	345	391	5	9			
1	B	269	Total	C	N	O	S	Se	0	0	0
			2059	1311	344	390	5	9			
1	C	269	Total	C	N	O	S	Se	0	2	0
			2066	1316	345	391	5	9			
1	D	269	Total	C	N	O	S	Se	0	1	0
			2051	1308	343	386	5	9			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP P45251
A	25	MSE	MET	modified residue	UNP P45251
A	33	MSE	MET	modified residue	UNP P45251
A	35	MSE	MET	modified residue	UNP P45251
A	74	MSE	MET	modified residue	UNP P45251
A	128	MSE	MET	modified residue	UNP P45251
A	148	MSE	MET	modified residue	UNP P45251
A	181	MSE	MET	modified residue	UNP P45251
A	187	MSE	MET	modified residue	UNP P45251
A	267	MSE	MET	modified residue	UNP P45251
A	285	GLY	-	cloning artifact	UNP P45251
A	286	SER	-	cloning artifact	UNP P45251
A	287	HIS	-	cloning artifact	UNP P45251
A	288	HIS	-	cloning artifact	UNP P45251
A	289	HIS	-	cloning artifact	UNP P45251
A	290	HIS	-	cloning artifact	UNP P45251
A	291	HIS	-	cloning artifact	UNP P45251
A	292	HIS	-	cloning artifact	UNP P45251
B	1	MSE	MET	modified residue	UNP P45251
B	25	MSE	MET	modified residue	UNP P45251
B	33	MSE	MET	modified residue	UNP P45251

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Chain	Residue	Modelled	Actual	Comment	Reference
B	35	MSE	MET	modified residue	UNP P45251
B	74	MSE	MET	modified residue	UNP P45251
B	128	MSE	MET	modified residue	UNP P45251
B	148	MSE	MET	modified residue	UNP P45251
B	181	MSE	MET	modified residue	UNP P45251
B	187	MSE	MET	modified residue	UNP P45251
B	267	MSE	MET	modified residue	UNP P45251
B	285	GLY	-	cloning artifact	UNP P45251
B	286	SER	-	cloning artifact	UNP P45251
B	287	HIS	-	cloning artifact	UNP P45251
B	288	HIS	-	cloning artifact	UNP P45251
B	289	HIS	-	cloning artifact	UNP P45251
B	290	HIS	-	cloning artifact	UNP P45251
B	291	HIS	-	cloning artifact	UNP P45251
B	292	HIS	-	cloning artifact	UNP P45251
C	1	MSE	MET	modified residue	UNP P45251
C	25	MSE	MET	modified residue	UNP P45251
C	33	MSE	MET	modified residue	UNP P45251
C	35	MSE	MET	modified residue	UNP P45251
C	74	MSE	MET	modified residue	UNP P45251
C	128	MSE	MET	modified residue	UNP P45251
C	148	MSE	MET	modified residue	UNP P45251
C	181	MSE	MET	modified residue	UNP P45251
C	187	MSE	MET	modified residue	UNP P45251
C	267	MSE	MET	modified residue	UNP P45251
C	285	GLY	-	cloning artifact	UNP P45251
C	286	SER	-	cloning artifact	UNP P45251
C	287	HIS	-	cloning artifact	UNP P45251
C	288	HIS	-	cloning artifact	UNP P45251
C	289	HIS	-	cloning artifact	UNP P45251
C	290	HIS	-	cloning artifact	UNP P45251
C	291	HIS	-	cloning artifact	UNP P45251
C	292	HIS	-	cloning artifact	UNP P45251
D	1	MSE	MET	modified residue	UNP P45251
D	25	MSE	MET	modified residue	UNP P45251
D	33	MSE	MET	modified residue	UNP P45251
D	35	MSE	MET	modified residue	UNP P45251
D	74	MSE	MET	modified residue	UNP P45251
D	128	MSE	MET	modified residue	UNP P45251
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Chain	Residue	Modelled	Actual	Comment	Reference
D	267	MSE	MET	modified residue	UNP P45251
D	285	GLY	-	cloning artifact	UNP P45251
D	286	SER	-	cloning artifact	UNP P45251
D	287	HIS	-	cloning artifact	UNP P45251
D	288	HIS	-	cloning artifact	UNP P45251
D	289	HIS	-	cloning artifact	UNP P45251
D	290	HIS	-	cloning artifact	UNP P45251
D	291	HIS	-	cloning artifact	UNP P45251
D	292	HIS	-	cloning artifact	UNP P45251

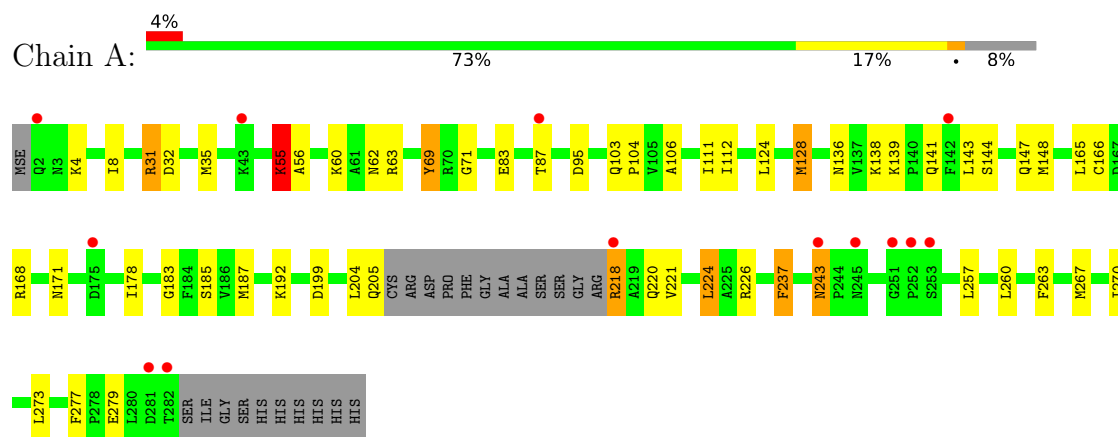
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	168	Total 168	O 168	0	0
2	B	137	Total 137	O 137	0	0
2	C	143	Total 143	O 143	0	0
2	D	120	Total 120	O 120	0	0

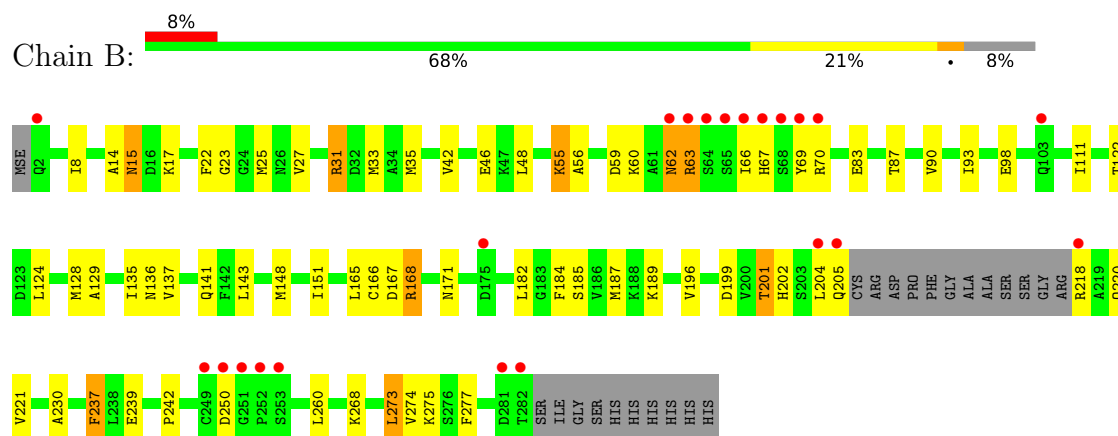
3 Residue-property plots [i](#)

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.

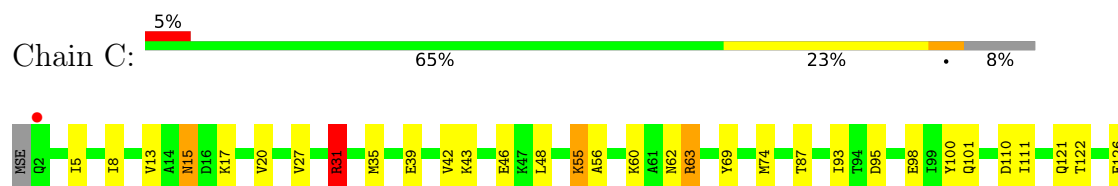
- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

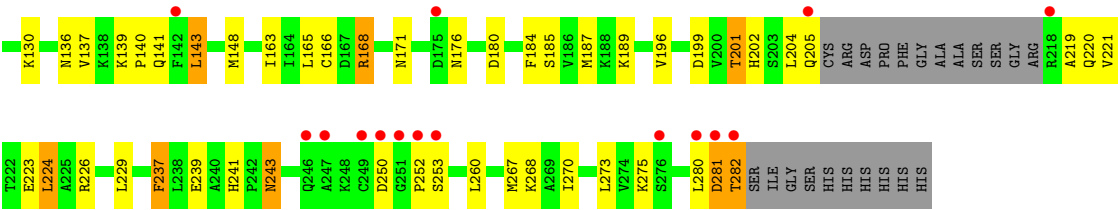


- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

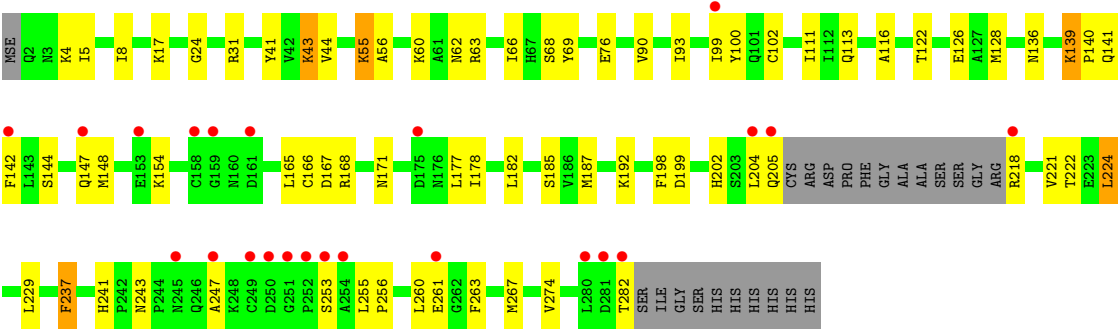


- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase





● Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.97Å 92.89Å 82.30Å 90.00° 116.82° 90.00°	Depositor
Resolution (Å)	39.22 – 1.80 39.22 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (39.22-1.80) 97.5 (39.22-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.23 (at 1.81Å)	Xtriage
Refinement program	REFMAC 4.0	Depositor
R, R_{free}	0.207 , 0.242 0.197 , 0.229	Depositor DCC
R_{free} test set	9540 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8811	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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	0.75	1/2103 (0.0%)	1.35	13/2822 (0.5%)
1	B	0.72	0/2084	1.30	9/2798 (0.3%)
1	C	0.74	0/2099	1.35	16/2818 (0.6%)
1	D	0.70	0/2080	1.30	4/2793 (0.1%)
All	All	0.73	1/8366 (0.0%)	1.33	42/11231 (0.4%)

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	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	128	MSE	SE-CE	-6.39	1.76	1.95

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	226	ARG	CD-NE-CZ	11.60	140.64	124.40
1	A	226	ARG	NE-CZ-NH2	10.94	129.04	119.20
1	C	226	ARG	NE-CZ-NH2	9.00	127.30	119.20
1	A	226	ARG	NE-CZ-NH1	-8.77	112.73	121.50
1	C	237	PHE	CA-CB-CG	8.38	122.18	113.80
1	B	22	PHE	CA-C-N	-8.27	116.03	121.65
1	B	22	PHE	C-N-CA	-8.27	116.03	121.65
1	C	226	ARG	NE-CZ-NH1	-7.57	113.93	121.50
1	B	237	PHE	CA-CB-CG	7.25	121.05	113.80
1	A	277	PHE	CA-CB-CG	7.20	121.00	113.80
1	A	95	ASP	CA-CB-CG	7.06	119.66	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	31	ARG	CA-CB-CG	6.84	127.79	114.10
1	A	243	ASN	CA-C-N	6.84	126.35	119.24
1	A	243	ASN	C-N-CA	6.84	126.35	119.24
1	B	202	HIS	CA-CB-CG	-6.69	107.11	113.80
1	B	260	LEU	N-CA-C	6.26	117.77	111.07
1	D	55	LYS	CB-CG-CD	6.18	125.52	111.30
1	D	237	PHE	CA-CB-CG	6.04	119.84	113.80
1	B	122	THR	N-CA-C	5.86	117.34	111.07
1	A	226	ARG	CD-NE-CZ	5.85	132.59	124.40
1	C	122	THR	N-CA-C	5.72	117.97	111.11
1	C	260	LEU	N-CA-C	5.69	117.16	111.07
1	C	55	LYS	CB-CG-CD	5.67	124.34	111.30
1	C	163	ILE	N-CA-C	5.67	116.05	108.11
1	B	90	VAL	CB-CA-C	-5.61	103.88	111.63
1	A	55	LYS	CB-CG-CD	5.54	124.04	111.30
1	C	15	ASN	OD1-CG-ND2	5.50	128.10	122.60
1	C	31	ARG	CB-CG-CD	5.50	123.95	111.30
1	C	95	ASP	CA-CB-CG	5.49	118.09	112.60
1	A	260	LEU	N-CA-C	5.47	117.68	111.11
1	A	71	GLY	CA-C-N	5.44	125.05	119.56
1	A	71	GLY	C-N-CA	5.44	125.05	119.56
1	D	274	VAL	N-CA-C	5.33	116.06	110.62
1	B	15	ASN	CA-CB-CG	-5.27	107.33	112.60
1	C	253	SER	N-CA-C	5.27	119.22	112.26
1	A	69	TYR	CA-C-O	-5.23	115.43	121.19
1	A	237	PHE	CA-CB-CG	5.08	118.88	113.80
1	C	243	ASN	CA-C-N	5.07	126.18	119.84
1	C	243	ASN	C-N-CA	5.07	126.18	119.84
1	D	90	VAL	CB-CA-C	-5.04	105.81	111.45
1	B	23	GLY	O-C-N	5.03	127.51	123.49
1	C	110	ASP	CA-CB-CG	-5.00	107.60	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	252	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	2067	0	2091	45	0
1	B	2059	0	2089	51	0
1	C	2066	0	2093	73	0
1	D	2051	0	2080	68	0
2	A	168	0	0	3	0
2	B	137	0	0	1	0
2	C	143	0	0	2	0
2	D	120	0	0	1	0
All	All	8811	0	8353	223	0

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 13.

All (223) 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:C:220[B]:GLN:NE2	1:C:223[B]:GLU:CD	2.03	1.17
1:C:220[B]:GLN:NE2	1:C:223[B]:GLU:OE1	1.82	1.09
1:B:137:VAL:HG11	1:B:151:ILE:HD12	1.45	0.98
1:A:165:LEU:HB3	1:A:187:MSE:HE1	1.51	0.92
1:C:148:MSE:HE2	1:C:165:LEU:HD22	1.52	0.91
1:D:44:VAL:HG22	1:D:261:GLU:HG3	1.52	0.91
1:C:148:MSE:HG3	1:C:187:MSE:HE3	1.54	0.90
1:B:141:GLN:HG3	1:B:171:ASN:HD21	1.38	0.88
1:A:148:MSE:HG3	1:A:187:MSE:HE3	1.54	0.88
1:D:148:MSE:HG3	1:D:187:MSE:HE3	1.56	0.87
1:B:201:THR:HG21	1:B:239:GLU:H	1.42	0.84
1:D:141:GLN:HG3	1:D:171:ASN:HD21	1.42	0.84
1:C:137:VAL:HG11	1:C:148:MSE:HE1	1.59	0.83
1:C:220[B]:GLN:NE2	1:C:223[B]:GLU:OE2	2.08	0.83
1:C:201:THR:HG21	1:C:239:GLU:H	1.44	0.81
1:C:220[B]:GLN:OE1	1:D:185[B]:SER:OG	1.99	0.81
1:A:165:LEU:HB3	1:A:187:MSE:CE	2.11	0.80
1:C:165:LEU:HB3	1:C:187:MSE:HE1	1.63	0.79
1:B:35:MSE:HE1	1:B:87:THR:HG21	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:HIS:HD2	1:C:243:ASN:H	1.27	0.78
1:A:55:LYS:HD2	1:A:56:ALA:N	1.99	0.78
1:D:55:LYS:HD2	1:D:56:ALA:N	1.99	0.77
1:D:165:LEU:HB3	1:D:187:MSE:HE1	1.68	0.76
1:B:141:GLN:HG3	1:B:171:ASN:ND2	2.02	0.74
1:C:148:MSE:CG	1:C:187:MSE:HE3	2.19	0.73
1:D:165:LEU:HD13	1:D:187:MSE:HE2	1.70	0.73
1:C:220[B]:GLN:HE22	1:C:223[B]:GLU:CD	1.84	0.73
1:D:141:GLN:HG3	1:D:171:ASN:ND2	2.04	0.72
1:D:241:HIS:HD2	1:D:243:ASN:H	1.37	0.72
1:C:74:MSE:CE	1:C:101:GLN:HG2	2.19	0.72
1:C:140:PRO:HG2	1:C:143:LEU:HD23	1.71	0.72
1:B:204:LEU:CD1	1:B:221:VAL:HG22	2.20	0.71
1:D:165:LEU:HB3	1:D:187:MSE:CE	2.21	0.71
1:A:141:GLN:OE1	1:A:171:ASN:ND2	2.22	0.71
1:A:185:SER:HB2	2:A:363:HOH:O	1.91	0.70
1:C:220[B]:GLN:HE21	1:C:223[B]:GLU:CD	2.00	0.69
1:D:148:MSE:HE3	1:D:165:LEU:HD22	1.73	0.68
1:B:204:LEU:HD13	1:B:221:VAL:HG22	1.76	0.68
1:C:74:MSE:HE1	1:C:100:TYR:CE1	2.28	0.68
1:D:148:MSE:CG	1:D:187:MSE:HE3	2.23	0.68
1:B:148:MSE:O	1:B:151:ILE:HG12	1.94	0.67
1:B:25:MSE:HE1	1:B:33:MSE:HG2	1.76	0.67
1:A:148:MSE:CG	1:A:187:MSE:HE3	2.24	0.67
1:B:148:MSE:HE3	1:B:165:LEU:HD22	1.76	0.66
1:A:165:LEU:HD13	1:A:187:MSE:HE2	1.78	0.66
1:C:165:LEU:HB3	1:C:187:MSE:CE	2.24	0.66
1:A:139:LYS:HB2	1:A:148:MSE:HE2	1.77	0.66
1:D:144:SER:OG	1:D:147:GLN:HG2	1.95	0.65
1:A:204:LEU:CD1	1:A:221:VAL:HG22	2.27	0.65
1:D:204:LEU:HD12	1:D:253:SER:HB2	1.77	0.65
1:B:8:ILE:HD13	1:B:111:ILE:HD11	1.78	0.65
1:B:148:MSE:SE	1:B:151:ILE:HD11	2.46	0.65
1:C:224:LEU:HG	1:D:182:LEU:HD21	1.79	0.65
1:D:218:ARG:O	1:D:221:VAL:HG23	1.96	0.64
1:B:184:PHE:HD1	1:B:196:VAL:HG11	1.63	0.64
1:C:184:PHE:HD1	1:C:196:VAL:HG11	1.61	0.64
1:A:8:ILE:HD13	1:A:111:ILE:HD11	1.80	0.63
1:C:141:GLN:OE1	1:C:171:ASN:ND2	2.32	0.62
1:D:199:ASP:OD2	1:D:202:HIS:HD2	1.82	0.62
1:A:220[B]:GLN:NE2	1:B:185:SER:OG	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:LEU:HD13	1:C:187:MSE:HE2	1.80	0.62
1:C:280:LEU:HD23	1:D:222:THR:HG21	1.82	0.62
1:C:280:LEU:O	1:C:281:ASP:C	2.43	0.62
1:C:74:MSE:HE2	1:C:101:GLN:HG2	1.82	0.61
1:C:5:ILE:HD13	1:C:17:LYS:NZ	2.15	0.61
1:A:35:MSE:HE1	1:A:87:THR:HG21	1.83	0.61
1:A:63:ARG:HD3	1:A:69:TYR:O	2.01	0.61
1:C:241:HIS:CD2	1:C:243:ASN:H	2.15	0.60
1:D:148:MSE:HE2	1:D:187:MSE:HE1	1.83	0.60
1:C:55:LYS:HD2	1:C:56:ALA:N	2.15	0.60
1:C:63:ARG:HD3	1:C:69:TYR:O	2.02	0.60
1:D:8:ILE:HD13	1:D:111:ILE:HD11	1.84	0.60
1:C:31:ARG:HD3	1:C:31:ARG:C	2.26	0.59
1:B:137:VAL:HG11	1:B:151:ILE:CD1	2.27	0.59
1:B:148:MSE:SE	1:B:151:ILE:CD1	3.00	0.59
1:B:199:ASP:HA	1:B:237:PHE:HB3	1.83	0.59
1:C:280:LEU:HD23	1:D:222:THR:CG2	2.32	0.59
1:C:241:HIS:HD2	1:C:243:ASN:N	1.99	0.59
1:D:136:ASN:HD21	1:D:166:CYS:HB2	1.68	0.58
1:C:137:VAL:CG1	1:C:148:MSE:HE1	2.32	0.58
1:C:180:ASP:CG	1:D:178:ILE:HD12	2.29	0.57
1:A:141:GLN:HG3	1:A:171:ASN:OD1	2.03	0.57
1:D:60:LYS:HE2	1:D:60:LYS:HA	1.87	0.57
1:D:204:LEU:CD1	1:D:221:VAL:HG22	2.34	0.57
1:A:218:ARG:O	1:A:221:VAL:HG23	2.05	0.57
1:D:218:ARG:N	1:D:253:SER:HA	2.19	0.57
1:C:204:LEU:CD1	1:C:221:VAL:HG22	2.35	0.57
1:C:126:GLU:HG2	1:C:130:LYS:HE3	1.87	0.57
1:A:183:GLY:HA3	2:A:316:HOH:O	2.04	0.56
1:A:270:ILE:HD13	1:B:273:LEU:HD13	1.86	0.56
1:D:205:GLN:HB2	2:D:350:HOH:O	2.04	0.56
1:B:33:MSE:HE2	1:B:242:PRO:HG2	1.87	0.55
1:C:199:ASP:OD2	1:C:202:HIS:HD2	1.89	0.55
1:A:139:LYS:HE2	2:A:319:HOH:O	2.07	0.54
1:A:55:LYS:HD2	1:A:55:LYS:C	2.32	0.54
1:B:31:ARG:HD2	1:B:83:GLU:OE1	2.07	0.54
1:A:204:LEU:HD13	1:A:221:VAL:HG22	1.89	0.54
1:B:136:ASN:HD21	1:B:166:CYS:HB2	1.72	0.54
1:B:184:PHE:HD1	1:B:196:VAL:CG1	2.21	0.54
1:B:59:ASP:OD1	1:B:70:ARG:HD3	2.08	0.53
1:D:148:MSE:HG3	1:D:187:MSE:CE	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:ILE:HD13	1:C:17:LYS:HZ2	1.72	0.53
1:C:168:ARG:HG2	1:C:168:ARG:HH11	1.74	0.53
1:C:199:ASP:HA	1:C:237:PHE:HB3	1.91	0.53
1:A:199:ASP:HA	1:A:237:PHE:HB3	1.91	0.52
1:C:8:ILE:HD13	1:C:111:ILE:HD11	1.91	0.52
1:C:136:ASN:HD21	1:C:166:CYS:HB2	1.74	0.52
1:D:5:ILE:HD13	1:D:17:LYS:NZ	2.25	0.52
1:D:204:LEU:HD13	1:D:221:VAL:HG22	1.92	0.52
1:A:148:MSE:HG3	1:A:187:MSE:CE	2.32	0.52
1:B:63:ARG:HE	1:B:63:ARG:HA	1.74	0.52
1:B:201:THR:HG21	1:B:239:GLU:N	2.20	0.52
1:B:141:GLN:NE2	1:B:171:ASN:OD1	2.28	0.51
1:B:218:ARG:O	1:B:221:VAL:HG23	2.10	0.51
1:D:204:LEU:O	1:D:205:GLN:C	2.54	0.51
1:B:55:LYS:HB2	1:B:93:ILE:CG2	2.40	0.51
1:C:148:MSE:HG3	1:C:187:MSE:CE	2.36	0.51
1:B:66:ILE:HG22	1:D:122:THR:HG22	1.91	0.51
1:C:74:MSE:HE1	1:C:101:GLN:HG2	1.90	0.51
1:A:165:LEU:HD13	1:A:187:MSE:CE	2.39	0.51
1:A:112:ILE:HG22	1:A:128:MSE:HE3	1.91	0.51
1:C:35:MSE:HE1	1:C:87:THR:HG21	1.92	0.50
1:C:184:PHE:HD1	1:C:196:VAL:CG1	2.25	0.50
1:C:27:VAL:HG22	1:C:60:LYS:HE3	1.94	0.50
1:D:177:LEU:O	1:D:178:ILE:HD13	2.11	0.50
1:D:241:HIS:CD2	1:D:243:ASN:H	2.24	0.50
1:A:31:ARG:NH2	1:A:83:GLU:OE2	2.45	0.50
1:C:201:THR:HG21	1:C:239:GLU:N	2.20	0.50
1:C:185:SER:O	1:C:189:LYS:HG3	2.12	0.50
1:A:138:LYS:NZ	1:A:168:ARG:HH11	2.11	0.49
1:A:106:ALA:HB2	1:A:112:ILE:HD11	1.93	0.49
1:B:14:ALA:HB3	1:B:17:LYS:HG3	1.95	0.49
1:D:63:ARG:HD2	1:D:69:TYR:O	2.13	0.49
1:D:199:ASP:HA	1:D:237:PHE:HB3	1.93	0.49
1:D:241:HIS:CE1	1:D:247:ALA:HA	2.47	0.49
1:D:43:LYS:NZ	1:D:43:LYS:HB2	2.28	0.48
1:B:42:VAL:O	1:B:46:GLU:HG2	2.14	0.48
1:C:220[B]:GLN:CD	1:C:223[B]:GLU:OE1	2.55	0.48
1:C:204:LEU:O	1:C:205:GLN:C	2.56	0.48
1:B:124:LEU:O	1:B:128:MSE:HG3	2.12	0.48
1:B:8:ILE:CD1	1:B:111:ILE:HD11	2.43	0.48
1:C:148:MSE:CB	1:C:187:MSE:HE3	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:ARG:HD3	1:B:69:TYR:O	2.14	0.47
1:D:99:ILE:HG13	1:D:100:TYR:N	2.28	0.47
1:D:241:HIS:HD2	1:D:243:ASN:N	2.10	0.47
1:C:55:LYS:HB2	1:C:93:ILE:HG23	1.95	0.47
1:C:141:GLN:HG3	1:C:171:ASN:OD1	2.15	0.47
1:B:55:LYS:HB2	1:B:93:ILE:HG23	1.97	0.46
1:A:31:ARG:HG3	1:A:32:ASP:N	2.29	0.46
1:D:165:LEU:CD1	1:D:187:MSE:HE2	2.43	0.46
1:D:55:LYS:HB2	1:D:93:ILE:CG2	2.45	0.46
1:D:148:MSE:CB	1:D:187:MSE:HE3	2.45	0.46
1:C:42:VAL:O	1:C:46:GLU:HB2	2.16	0.46
1:A:136:ASN:HD21	1:A:166:CYS:HB2	1.80	0.46
1:C:224:LEU:HG	1:D:182:LEU:CD2	2.45	0.46
1:B:129:ALA:HA	1:B:135:ILE:HD11	1.97	0.46
1:C:8:ILE:CD1	1:C:111:ILE:HD11	2.45	0.46
1:A:144:SER:H	1:A:147[B]:GLN:HE21	1.63	0.46
1:A:144:SER:OG	1:A:147[B]:GLN:HG3	2.17	0.45
1:B:63:ARG:HA	1:B:63:ARG:NE	2.31	0.45
1:B:167:ASP:HB2	1:B:187:MSE:HE1	1.98	0.45
1:C:219:ALA:HA	1:D:282:THR:HG23	1.98	0.45
1:D:199:ASP:OD2	1:D:202:HIS:CD2	2.66	0.45
1:C:48:LEU:O	1:C:268:LYS:HE3	2.16	0.45
1:B:66:ILE:HG13	1:B:67:HIS:CD2	2.52	0.45
1:D:41:TYR:CD1	1:D:260:LEU:HD21	2.52	0.45
1:A:224:LEU:HG	1:B:182:LEU:HD21	1.99	0.45
1:B:55:LYS:HD2	1:B:56:ALA:N	2.32	0.45
1:C:199:ASP:OD2	1:C:202:HIS:CD2	2.70	0.45
1:B:218:ARG:HG3	1:B:220:GLN:H	1.82	0.45
1:D:4:LYS:HE3	1:D:192:LYS:O	2.16	0.45
1:D:165:LEU:HB3	1:D:187:MSE:HE2	1.99	0.45
1:B:273:LEU:HD22	1:B:277:PHE:CZ	2.53	0.44
1:C:202:HIS:HE1	2:C:435:HOH:O	2.00	0.44
1:A:62:ASN:OD1	1:C:121:GLN:NE2	2.50	0.44
1:C:165:LEU:CD1	1:C:187:MSE:HE2	2.48	0.44
1:D:63:ARG:HD3	1:D:68:SER:HB3	1.98	0.44
1:D:165:LEU:HD13	1:D:187:MSE:CE	2.43	0.44
1:A:165:LEU:CD1	1:A:187:MSE:HE2	2.46	0.44
1:C:165:LEU:HD13	1:C:187:MSE:CE	2.46	0.44
1:D:122:THR:HG23	1:D:154:LYS:CE	2.48	0.44
1:A:204:LEU:O	1:A:205:GLN:C	2.61	0.43
1:B:171:ASN:ND2	1:D:142:PHE:HB2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:LEU:HD11	1:A:221:VAL:HG22	2.01	0.43
1:D:5:ILE:HD13	1:D:17:LYS:HZ1	1.83	0.43
1:A:8:ILE:CD1	1:A:111:ILE:HD11	2.48	0.43
1:A:263:PHE:O	1:A:267:MSE:HG2	2.18	0.43
1:C:55:LYS:HD2	1:C:55:LYS:C	2.44	0.43
1:C:60:LYS:HE2	2:C:340:HOH:O	2.19	0.43
1:B:62:ASN:C	1:B:62:ASN:HD22	2.27	0.42
1:B:63:ARG:HE	1:B:63:ARG:CA	2.32	0.42
1:C:15:ASN:O	1:C:275:LYS:HE2	2.20	0.42
1:D:198:PHE:HZ	1:D:224:LEU:HD13	1.84	0.42
1:A:4:LYS:HE3	1:A:192:LYS:O	2.19	0.42
1:A:124:LEU:O	1:A:128:MSE:HG3	2.19	0.42
2:B:373:HOH:O	1:D:66:ILE:HG23	2.18	0.42
1:B:230:ALA:HA	1:B:274:VAL:HG21	2.02	0.42
1:D:141:GLN:NE2	1:D:171:ASN:OD1	2.53	0.42
1:D:116:ALA:HB1	1:D:140:PRO:HA	2.02	0.42
1:B:15:ASN:O	1:B:275:LYS:HE2	2.20	0.42
1:B:168:ARG:HD3	1:B:168:ARG:C	2.44	0.42
1:D:204:LEU:CD1	1:D:253:SER:HB2	2.46	0.42
1:C:39:GLU:HG2	1:C:43:LYS:NZ	2.35	0.41
1:A:103:GLN:N	1:A:104:PRO:HD2	2.35	0.41
1:D:113:GLN:HE22	1:D:237:PHE:HE2	1.66	0.41
1:D:139:LYS:NZ	1:D:167:ASP:OD1	2.53	0.41
1:D:255:LEU:HA	1:D:256:PRO:HD3	1.94	0.41
1:D:24:GLY:HA3	1:D:55:LYS:O	2.20	0.41
1:A:178:ILE:HD13	1:A:178:ILE:HG21	1.91	0.41
1:C:176:ASN:HA	1:C:205:GLN:HG3	2.03	0.41
1:D:55:LYS:HB2	1:D:93:ILE:HG23	2.02	0.41
1:C:229:LEU:CD1	1:C:267:MSE:HB3	2.51	0.40
1:C:280:LEU:O	1:C:282:THR:N	2.54	0.40
1:D:31:ARG:HD3	1:D:31:ARG:C	2.45	0.40
1:D:229:LEU:CD1	1:D:267:MSE:HB3	2.51	0.40
1:B:48:LEU:O	1:B:268:LYS:HE3	2.21	0.40
1:B:25:MSE:HE2	1:B:27:VAL:O	2.21	0.40
1:C:13:VAL:HG22	1:C:20:VAL:HG21	2.02	0.40
1:A:60:LYS:HA	1:A:60:LYS:HE2	2.02	0.40
1:C:280:LEU:CD2	1:D:263:PHE:HA	2.50	0.40
1:D:102:CYS:SG	1:D:128:MSE:HG2	2.61	0.40

There are no symmetry-related clashes.

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	268/292 (92%)	262 (98%)	6 (2%)	0	100	100
1	B	265/292 (91%)	257 (97%)	8 (3%)	0	100	100
1	C	267/292 (91%)	260 (97%)	6 (2%)	1 (0%)	30	19
1	D	266/292 (91%)	257 (97%)	9 (3%)	0	100	100
All	All	1066/1168 (91%)	1036 (97%)	29 (3%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	281	ASP

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	229/236 (97%)	221 (96%)	8 (4%)	32	19
1	B	228/236 (97%)	215 (94%)	13 (6%)	18	8
1	C	229/236 (97%)	216 (94%)	13 (6%)	18	8
1	D	226/236 (96%)	219 (97%)	7 (3%)	35	23
All	All	912/944 (97%)	871 (96%)	41 (4%)	24	12

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ARG
1	A	55	LYS
1	A	143	LEU
1	A	218	ARG
1	A	224	LEU
1	A	243	ASN
1	A	257	LEU
1	A	273	LEU
1	B	31	ARG
1	B	55	LYS
1	B	60	LYS
1	B	62	ASN
1	B	63	ARG
1	B	98	GLU
1	B	143	LEU
1	B	168	ARG
1	B	189	LYS
1	B	201	THR
1	B	205	GLN
1	B	250	ASP
1	B	273	LEU
1	C	31	ARG
1	C	62	ASN
1	C	63	ARG
1	C	98	GLU
1	C	139	LYS
1	C	143	LEU
1	C	168	ARG
1	C	201	THR
1	C	224	LEU
1	C	250	ASP
1	C	270	ILE
1	C	273	LEU
1	C	282	THR
1	D	43	LYS
1	D	62	ASN
1	D	76	GLU
1	D	126	GLU
1	D	139	LYS
1	D	168	ARG
1	D	224	LEU

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

Mol	Chain	Res	Type
1	A	62	ASN
1	A	113	GLN
1	A	136	ASN
1	B	62	ASN
1	B	67	HIS
1	B	97	HIS
1	B	103	GLN
1	B	113	GLN
1	B	136	ASN
1	B	141	GLN
1	B	171	ASN
1	C	62	ASN
1	C	113	GLN
1	C	121	GLN
1	C	136	ASN
1	C	202	HIS
1	C	205	GLN
1	C	241	HIS
1	D	36	GLN
1	D	62	ASN
1	D	103	GLN
1	D	113	GLN
1	D	136	ASN
1	D	141	GLN
1	D	171	ASN
1	D	202	HIS
1	D	220	GLN
1	D	241	HIS

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 ⓘ

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	260/292 (89%)	0.10	13 (5%) 34 33	11, 19, 34, 44	3 (1%)
1	B	260/292 (89%)	0.37	22 (8%) 16 14	11, 20, 46, 63	0
1	C	260/292 (89%)	0.41	16 (6%) 26 25	14, 21, 43, 66	2 (0%)
1	D	260/292 (89%)	0.62	23 (8%) 15 13	14, 25, 45, 64	1 (0%)
All	All	1040/1168 (89%)	0.38	74 (7%) 22 20	11, 21, 43, 66	6 (0%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	282	THR	5.6
1	C	252	PRO	5.4
1	C	250	ASP	5.1
1	B	66	ILE	4.7
1	B	249	CYS	4.5
1	B	282	THR	4.3
1	C	281	ASP	4.2
1	D	250	ASP	4.2
1	D	253	SER	4.2
1	B	67	HIS	4.2
1	D	252	PRO	4.2
1	C	175	ASP	4.1
1	C	280	LEU	4.1
1	C	251	GLY	4.0
1	D	249	CYS	4.0
1	C	205	GLN	3.8
1	B	250	ASP	3.7
1	B	252	PRO	3.7
1	B	64	SER	3.6
1	C	247	ALA	3.5
1	C	282	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	175	ASP	3.3
1	B	62	ASN	3.0
1	A	282	THR	3.0
1	D	161	ASP	3.0
1	A	245	ASN	3.0
1	C	142	PHE	3.0
1	D	205	GLN	2.9
1	D	218	ARG	2.9
1	B	69	TYR	2.8
1	B	70	ARG	2.8
1	A	281	ASP	2.8
1	D	281	ASP	2.8
1	B	65	SER	2.8
1	B	68	SER	2.7
1	B	204	LEU	2.6
1	B	2	GLN	2.6
1	B	251	GLY	2.6
1	C	249	CYS	2.5
1	C	2	GLN	2.5
1	A	218	ARG	2.5
1	B	103	GLN	2.5
1	A	243	ASN	2.5
1	D	280	LEU	2.4
1	C	246	GLN	2.4
1	C	253	SER	2.4
1	D	159	GLY	2.3
1	B	205	GLN	2.3
1	A	87	THR	2.3
1	A	142	PHE	2.3
1	D	142	PHE	2.3
1	B	253	SER	2.3
1	B	63	ARG	2.3
1	D	99	ILE	2.2
1	D	245	ASN	2.2
1	D	254	ALA	2.2
1	A	2	GLN	2.2
1	C	276	SER	2.2
1	D	175	ASP	2.2
1	D	204	LEU	2.2
1	D	153	GLU	2.1
1	A	253	SER	2.1
1	D	261	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	147	GLN	2.1
1	A	175	ASP	2.1
1	D	251	GLY	2.1
1	A	43	LYS	2.1
1	D	247	ALA	2.1
1	B	281	ASP	2.1
1	B	218	ARG	2.1
1	C	218	ARG	2.1
1	D	158	CYS	2.1
1	A	252	PRO	2.0
1	A	251	GLY	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.