



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:07 PM UTC

PDB ID : 5H01 / pdb_00005h01
Title : The crystal structure of D-2-halacid dehalogenase mutant
Authors : Xue, S.; Wang, Y.
Deposited on : 2016-10-02
Resolution : 2.19 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

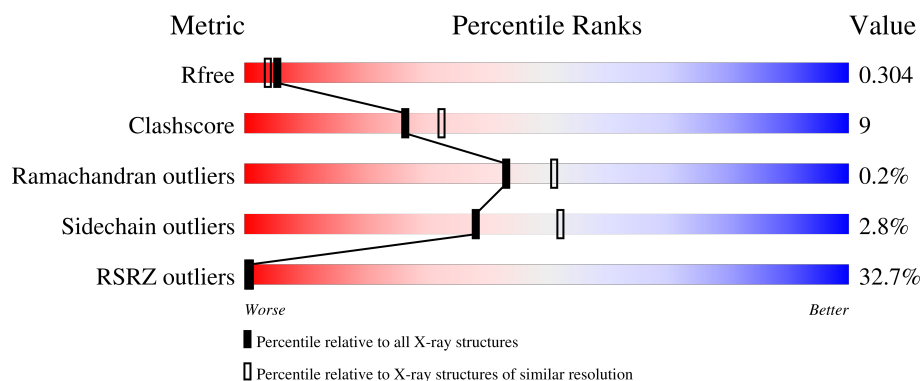
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	309	
1	B	309	
1	C	309	
1	D	309	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9743 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 (R)-2-haloacid dehalogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	0	0
			2327	1491	408	418	10			
1	B	292	Total	C	N	O	S	0	0	0
			2327	1491	408	418	10			
1	C	292	Total	C	N	O	S	0	0	0
			2327	1491	408	418	10			
1	D	292	Total	C	N	O	S	0	0	0
			2327	1491	408	418	10			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	288	ILE	LEU	engineered mutation	UNP Q52086
A	302	LEU	-	expression tag	UNP Q52086
A	303	GLU	-	expression tag	UNP Q52086
A	304	HIS	-	expression tag	UNP Q52086
A	305	HIS	-	expression tag	UNP Q52086
A	306	HIS	-	expression tag	UNP Q52086
A	307	HIS	-	expression tag	UNP Q52086
A	308	HIS	-	expression tag	UNP Q52086
A	309	HIS	-	expression tag	UNP Q52086
B	288	ILE	LEU	engineered mutation	UNP Q52086
B	302	LEU	-	expression tag	UNP Q52086
B	303	GLU	-	expression tag	UNP Q52086
B	304	HIS	-	expression tag	UNP Q52086
B	305	HIS	-	expression tag	UNP Q52086
B	306	HIS	-	expression tag	UNP Q52086
B	307	HIS	-	expression tag	UNP Q52086
B	308	HIS	-	expression tag	UNP Q52086
B	309	HIS	-	expression tag	UNP Q52086
C	288	ILE	LEU	engineered mutation	UNP Q52086
C	302	LEU	-	expression tag	UNP Q52086
C	303	GLU	-	expression tag	UNP Q52086

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Chain	Residue	Modelled	Actual	Comment	Reference
C	304	HIS	-	expression tag	UNP Q52086
C	305	HIS	-	expression tag	UNP Q52086
C	306	HIS	-	expression tag	UNP Q52086
C	307	HIS	-	expression tag	UNP Q52086
C	308	HIS	-	expression tag	UNP Q52086
C	309	HIS	-	expression tag	UNP Q52086
D	288	ILE	LEU	engineered mutation	UNP Q52086
D	302	LEU	-	expression tag	UNP Q52086
D	303	GLU	-	expression tag	UNP Q52086
D	304	HIS	-	expression tag	UNP Q52086
D	305	HIS	-	expression tag	UNP Q52086
D	306	HIS	-	expression tag	UNP Q52086
D	307	HIS	-	expression tag	UNP Q52086
D	308	HIS	-	expression tag	UNP Q52086
D	309	HIS	-	expression tag	UNP Q52086

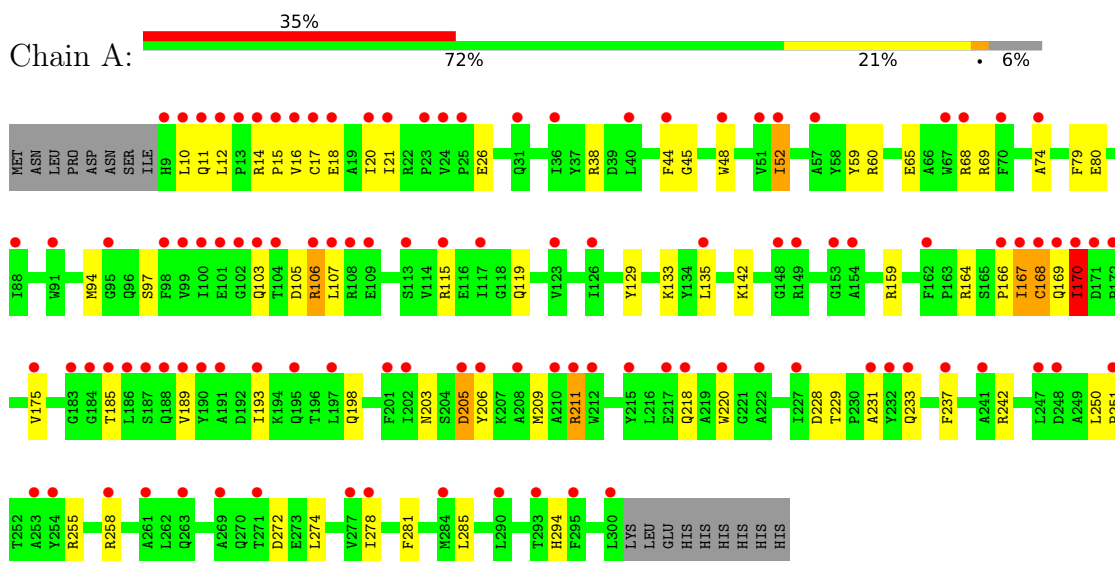
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	113	Total O 113 113	0	0
2	B	108	Total O 108 108	0	0
2	C	115	Total O 115 115	0	0
2	D	99	Total O 99 99	0	0

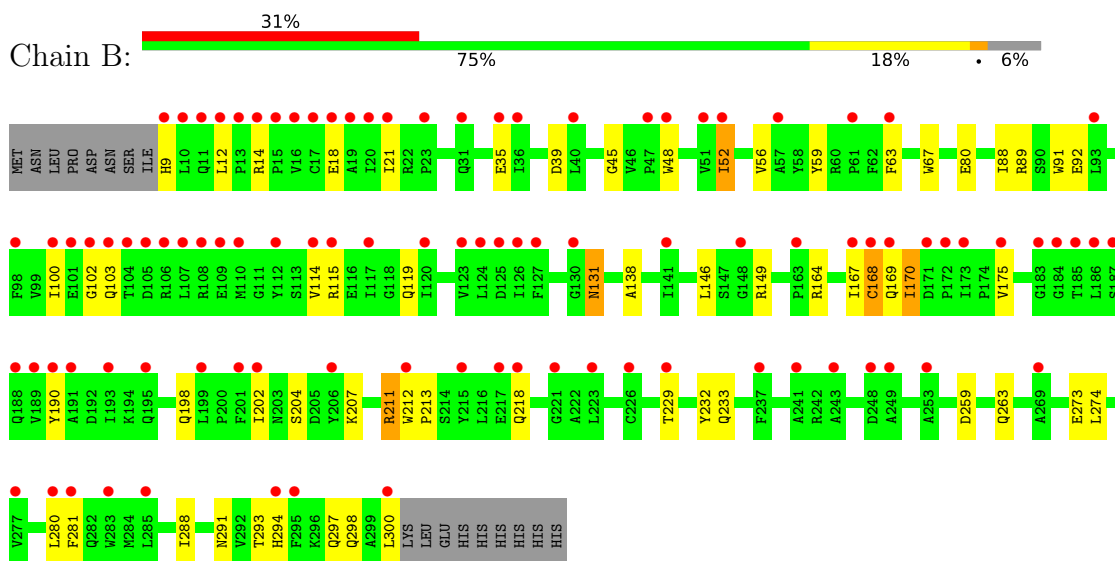
3 Residue-property plots

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: (R)-2-haloacid dehalogenase



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.71Å 97.18Å 93.75Å 90.00° 107.53° 90.00°	Depositor
Resolution (Å)	48.59 – 2.19 48.59 – 2.19	Depositor EDS
% Data completeness (in resolution range)	95.4 (48.59-2.19) 95.5 (48.59-2.19)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.253 , 0.312 0.250 , 0.304	Depositor DCC
R_{free} test set	3787 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.5	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9743	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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	0.55	0/2388	0.91	5/3244 (0.2%)
1	B	0.59	1/2388 (0.0%)	0.90	4/3244 (0.1%)
1	C	0.67	1/2388 (0.0%)	1.00	9/3244 (0.3%)
1	D	0.59	0/2388	0.95	9/3244 (0.3%)
All	All	0.60	2/9552 (0.0%)	0.94	27/12976 (0.2%)

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	B	0	1
1	C	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	284	MET	C-N	18.39	1.58	1.34
1	B	211	ARG	C-O	-5.04	1.17	1.24

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	284	MET	O-C-N	-14.87	106.56	122.03
1	C	284	MET	CA-C-N	10.55	135.79	120.38
1	C	284	MET	C-N-CA	10.55	135.79	120.38
1	A	229	THR	N-CA-C	-8.37	100.26	110.31
1	D	165	SER	CA-C-N	8.36	129.07	120.04
1	D	165	SER	C-N-CA	8.36	129.07	120.04
1	D	60	ARG	CA-C-N	-7.30	112.11	119.56
1	D	60	ARG	C-N-CA	-7.30	112.11	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	131	ASN	CA-C-N	-6.23	113.27	119.56
1	B	131	ASN	C-N-CA	-6.23	113.27	119.56
1	A	170	ILE	N-CA-C	-6.23	106.13	113.42
1	D	166	PRO	N-CA-C	6.17	122.60	114.27
1	C	60	ARG	CA-C-N	-6.15	112.67	119.19
1	C	60	ARG	C-N-CA	-6.15	112.67	119.19
1	A	60	ARG	CA-C-N	-5.96	113.55	119.56
1	A	60	ARG	C-N-CA	-5.96	113.55	119.56
1	D	277	VAL	N-CA-C	5.89	116.08	110.42
1	C	229	THR	N-CA-C	-5.85	102.52	110.36
1	A	211	ARG	N-CA-C	-5.71	105.20	111.82
1	B	12	LEU	CA-C-N	5.67	125.85	119.90
1	B	12	LEU	C-N-CA	5.67	125.85	119.90
1	C	165	SER	CA-C-N	5.64	126.89	119.84
1	C	165	SER	C-N-CA	5.64	126.89	119.84
1	C	11	GLN	N-CA-C	5.21	117.18	108.99
1	D	247	LEU	N-CA-C	5.19	116.94	111.28
1	D	250	LEU	CA-C-N	5.04	124.64	119.05
1	D	250	LEU	C-N-CA	5.04	124.64	119.05

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	18	GLU	Peptide
1	C	284	MET	Mainchain

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	2327	0	2292	52	0
1	B	2327	0	2292	42	0
1	C	2327	0	2292	45	0
1	D	2327	0	2292	40	0
2	A	113	0	0	11	1
2	B	108	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	115	0	0	18	0
2	D	99	0	0	14	1
All	All	9743	0	9168	172	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 9.

All (172) 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:218:GLN:NE2	2:C:403:HOH:O	1.98	0.95
1:A:209:MET:HG3	2:A:428:HOH:O	1.66	0.92
1:B:14:ARG:NH1	1:B:198:GLN:O	2.02	0.92
1:C:211:ARG:NH2	2:C:404:HOH:O	2.03	0.90
1:C:228:ASP:OD1	2:C:401:HOH:O	1.90	0.89
1:A:258:ARG:NH2	1:A:272:ASP:OD1	2.08	0.87
1:A:198:GLN:NE2	2:A:401:HOH:O	2.04	0.84
1:D:148:GLY:O	2:D:402:HOH:O	1.94	0.83
1:D:96:GLN:NE2	2:D:404:HOH:O	2.11	0.82
1:D:110:MET:SD	2:D:406:HOH:O	2.37	0.82
1:C:65:GLU:OE1	1:C:68:ARG:NH1	2.14	0.79
1:B:273:GLU:OE1	2:B:401:HOH:O	2.01	0.78
1:D:258:ARG:NH2	1:D:272:ASP:OD1	2.17	0.78
1:B:211:ARG:HD3	1:B:211:ARG:C	2.11	0.76
1:D:26:GLU:HG3	2:D:454:HOH:O	1.87	0.74
1:A:106:ARG:HG2	1:A:107:LEU:N	2.05	0.72
1:B:103:GLN:OE1	1:B:218:GLN:NE2	2.22	0.72
1:A:103:GLN:HG2	1:A:106:ARG:HD3	1.72	0.72
1:C:260:ASP:OD1	2:C:405:HOH:O	2.09	0.70
1:A:242:ARG:O	2:A:402:HOH:O	2.11	0.69
1:D:149:ARG:NH2	2:D:413:HOH:O	2.27	0.67
1:A:12:LEU:HD23	1:A:237:PHE:HA	1.76	0.67
1:D:121:ARG:NH1	2:D:410:HOH:O	2.23	0.67
1:C:285:LEU:HA	1:C:288:ILE:HG22	1.76	0.66
1:A:20:ILE:O	2:A:403:HOH:O	2.15	0.65
1:D:64:ALA:O	1:D:68:ARG:HG2	1.97	0.65
1:C:115:ARG:NH2	2:C:412:HOH:O	2.29	0.64
1:B:89:ARG:NH1	1:B:92:GLU:OE1	2.28	0.64
1:D:192:ASP:O	1:D:196:THR:HG23	1.97	0.64
1:A:14:ARG:NH2	1:A:17:CYS:SG	2.68	0.64
1:B:300:LEU:O	2:B:402:HOH:O	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:GLU:HG3	2:C:437:HOH:O	1.96	0.64
1:D:116:GLU:OE2	2:D:405:HOH:O	2.15	0.63
1:B:100:ILE:HD13	1:B:297:GLN:HB3	1.80	0.62
1:A:26:GLU:OE1	2:A:404:HOH:O	2.16	0.62
1:C:52:ILE:HD11	1:C:278:ILE:HD12	1.81	0.62
1:C:298:GLN:OE1	2:C:403:HOH:O	2.16	0.61
1:A:52:ILE:HD11	1:A:278:ILE:HD12	1.83	0.61
1:C:211:ARG:NE	2:C:402:HOH:O	1.94	0.61
1:C:23:PRO:O	2:C:406:HOH:O	2.16	0.60
1:D:12:LEU:HD12	1:D:13:PRO:HD2	1.84	0.60
1:A:14:ARG:NH1	1:A:15:PRO:O	2.36	0.59
1:B:294:HIS:O	1:B:298:GLN:HG3	2.02	0.59
1:D:240:ASN:ND2	2:D:417:HOH:O	2.36	0.59
1:C:205:ASP:N	1:C:205:ASP:OD1	2.35	0.58
1:D:148:GLY:HA2	1:D:257:SER:HB3	1.84	0.58
1:A:168:CYS:SG	1:A:170:ILE:HG13	2.44	0.58
1:B:149:ARG:NH2	2:B:404:HOH:O	2.23	0.58
1:A:52:ILE:HD13	1:A:281:PHE:CB	2.34	0.57
1:C:105:ASP:OD1	1:C:108:ARG:NH1	2.26	0.57
1:C:31:GLN:H	1:C:31:GLN:CD	2.14	0.56
1:B:204:SER:HA	1:B:207:LYS:HE2	1.87	0.56
1:A:45:GLY:HA2	1:A:168:CYS:SG	2.46	0.55
1:B:259:ASP:O	1:B:263:GLN:HG2	2.07	0.55
1:A:170:ILE:HD12	1:A:170:ILE:N	2.22	0.54
1:B:45:GLY:HA2	1:B:168:CYS:SG	2.47	0.54
1:A:103:GLN:HA	2:A:456:HOH:O	2.07	0.54
1:A:228:ASP:HA	1:A:233:GLN:HG3	1.90	0.54
1:D:48:TRP:HH2	1:D:131:ASN:OD1	1.90	0.53
1:A:142:LYS:NZ	2:A:423:HOH:O	2.42	0.53
1:B:232:TYR:OH	2:B:403:HOH:O	2.19	0.53
1:A:135:LEU:HA	1:A:285:LEU:HD13	1.91	0.53
1:D:196:THR:OG1	1:D:220:TRP:HH2	1.92	0.53
1:D:204:SER:HA	1:D:207:LYS:HE2	1.91	0.52
1:D:43:THR:HG23	1:D:75:LYS:HG2	1.92	0.52
1:D:196:THR:HG21	1:D:224:LYS:HE3	1.91	0.52
1:B:211:ARG:HD3	1:B:211:ARG:O	2.09	0.52
1:A:106:ARG:CZ	1:A:218:GLN:OE1	2.58	0.52
1:A:52:ILE:HD13	1:A:281:PHE:HB3	1.90	0.51
1:B:56:VAL:HG12	1:B:63:PHE:HB2	1.91	0.51
1:C:80:GLU:OE1	1:C:164:ARG:HD2	2.10	0.51
1:C:247:LEU:HD12	1:C:250:LEU:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:ARG:HD2	1:B:212:TRP:CD2	2.46	0.51
1:A:167:ILE:HD12	1:D:129:TYR:CD1	2.45	0.51
1:B:21:ILE:HD11	1:B:280:LEU:HD23	1.93	0.50
1:B:39:ASP:OD2	1:B:67:TRP:NE1	2.35	0.50
1:C:38:ARG:HD2	2:C:425:HOH:O	2.12	0.50
1:B:21:ILE:HD13	1:B:281:PHE:CE2	2.46	0.50
1:D:184:GLY:N	2:D:414:HOH:O	2.30	0.49
1:A:193:ILE:HG12	1:A:220:TRP:CE2	2.47	0.49
1:D:150:THR:OG1	2:D:403:HOH:O	2.00	0.49
1:A:65:GLU:OE2	1:A:68:ARG:NH2	2.40	0.49
1:C:137:PHE:CZ	1:C:141:ILE:HD11	2.47	0.49
1:D:52:ILE:HD11	1:D:278:ILE:HD12	1.93	0.49
1:C:204:SER:HA	1:C:207:LYS:HE2	1.94	0.49
1:D:218:GLN:OE1	2:D:406:HOH:O	2.20	0.49
1:B:52:ILE:HD12	1:B:138:ALA:HB2	1.95	0.48
1:A:69:ARG:HD3	1:A:255:ARG:O	2.14	0.48
1:A:209:MET:N	2:A:428:HOH:O	2.46	0.48
1:D:148:GLY:HA2	1:D:257:SER:CB	2.43	0.48
1:A:48:TRP:CD1	1:A:48:TRP:N	2.81	0.48
1:A:105:ASP:HB2	2:A:456:HOH:O	2.14	0.48
1:B:80:GLU:HB2	1:B:164:ARG:HB2	1.95	0.48
1:A:59:TYR:CD2	1:A:274:LEU:HD13	2.49	0.47
1:B:168:CYS:SG	1:B:170:ILE:HG23	2.54	0.47
1:A:175:VAL:HG21	1:B:175:VAL:HG21	1.95	0.47
1:B:9:HIS:ND1	1:B:9:HIS:O	2.48	0.47
1:D:292:VAL:HA	1:D:295:PHE:CD2	2.49	0.47
1:C:38:ARG:NH1	2:C:425:HOH:O	2.48	0.47
1:D:48:TRP:CD1	1:D:48:TRP:N	2.82	0.47
2:C:412:HOH:O	1:D:29:ALA:N	2.48	0.46
1:A:103:GLN:HB3	1:A:106:ARG:NH1	2.30	0.46
1:A:94:MET:HE2	1:A:294:HIS:HB2	1.98	0.46
1:D:142:LYS:HE2	1:D:146:LEU:HD11	1.98	0.46
1:A:97:SER:HB3	1:A:231:ALA:HB1	1.97	0.46
1:B:211:ARG:C	1:B:213:PRO:HD3	2.41	0.46
1:C:141:ILE:HA	2:C:432:HOH:O	2.16	0.46
1:A:11:GLN:N	2:A:411:HOH:O	2.29	0.45
1:D:80:GLU:HB2	1:D:164:ARG:HB2	1.99	0.45
1:D:238:ASP:O	1:D:242:ARG:HG2	2.16	0.45
1:A:129:TYR:HB2	1:D:166:PRO:HG2	1.98	0.45
1:B:164:ARG:NH2	2:B:421:HOH:O	2.50	0.45
1:C:274:LEU:O	1:C:278:ILE:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:PHE:O	1:A:133:LYS:NZ	2.43	0.45
1:C:21:ILE:HD11	1:C:280:LEU:HD23	1.98	0.45
1:C:103:GLN:HG3	2:C:403:HOH:O	2.16	0.45
1:A:185:THR:O	1:A:189:VAL:HG23	2.16	0.45
1:A:38:ARG:NH1	1:A:170:ILE:HG22	2.32	0.45
1:C:11:GLN:HG2	2:C:450:HOH:O	2.17	0.45
1:C:71:ALA:O	1:C:75:LYS:HG3	2.16	0.45
1:C:94:MET:SD	1:C:290:LEU:HD22	2.57	0.45
1:C:165:SER:HA	1:C:166:PRO:HD3	1.82	0.44
1:D:97:SER:HB3	1:D:231:ALA:HB1	1.99	0.44
1:B:229:THR:O	1:B:233:GLN:HG3	2.17	0.44
1:C:9:HIS:ND1	2:C:407:HOH:O	2.19	0.44
1:D:11:GLN:NE2	2:D:409:HOH:O	2.26	0.44
1:D:71:ALA:O	1:D:75:LYS:HG3	2.18	0.44
1:C:11:GLN:OE1	1:C:233:GLN:NE2	2.50	0.44
1:A:80:GLU:OE1	1:A:164:ARG:HD2	2.18	0.44
1:A:115:ARG:NE	2:A:431:HOH:O	2.50	0.44
1:A:205:ASP:OD1	1:A:205:ASP:N	2.51	0.44
1:A:250:LEU:HA	1:A:251:PRO:HD3	1.80	0.44
1:C:48:TRP:CD1	1:C:48:TRP:N	2.86	0.44
1:B:91:TRP:CZ3	1:B:297:GLN:HG2	2.52	0.44
1:B:293:THR:O	1:B:297:GLN:HG3	2.18	0.44
1:A:211:ARG:NE	1:B:175:VAL:HG13	2.33	0.44
1:C:292:VAL:HA	1:C:295:PHE:CD2	2.52	0.44
1:A:115:ARG:O	1:A:119:GLN:HG3	2.18	0.43
1:A:159:ARG:HE	1:A:159:ARG:HB2	1.69	0.43
1:C:80:GLU:HB2	1:C:164:ARG:HB2	2.00	0.43
1:C:89:ARG:O	1:C:93:LEU:HB2	2.18	0.43
1:A:203:ASN:HB2	1:A:206:TYR:CD2	2.53	0.43
1:A:211:ARG:HE	1:B:175:VAL:HG13	1.84	0.43
1:C:107:LEU:HD23	1:C:107:LEU:HA	1.77	0.43
1:A:74:ALA:HA	1:A:79:PHE:CD2	2.54	0.43
1:C:270:GLN:OE1	2:C:408:HOH:O	2.21	0.43
1:B:146:LEU:HD23	1:B:146:LEU:HA	1.89	0.43
1:C:103:GLN:OE1	1:C:106:ARG:NH1	2.52	0.43
1:A:14:ARG:HE	1:A:198:GLN:HB3	1.84	0.43
1:B:88:ILE:HG13	1:C:77:HIS:CE1	2.54	0.43
1:D:203:ASN:HD22	1:D:206:TYR:HE2	1.67	0.42
1:B:169:GLN:H	1:C:167:ILE:HD11	1.83	0.42
1:C:211:ARG:NH1	2:C:410:HOH:O	2.27	0.42
1:B:190:TYR:O	1:B:202:ILE:HD11	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:MET:SD	1:D:290:LEU:HD22	2.60	0.42
1:B:288:ILE:HA	1:B:291:ASN:HB2	2.01	0.42
1:C:48:TRP:HH2	1:C:131:ASN:OD1	2.03	0.42
1:D:250:LEU:HA	1:D:251:PRO:HD3	1.84	0.42
1:B:149:ARG:HE	1:B:149:ARG:HB3	1.56	0.41
1:A:16:VAL:HG22	1:A:18:GLU:HG3	2.02	0.41
1:D:229:THR:O	1:D:233:GLN:HG3	2.20	0.41
1:A:106:ARG:NH2	1:A:218:GLN:HE22	2.19	0.41
1:B:115:ARG:O	1:B:119:GLN:HG3	2.21	0.41
1:C:59:TYR:OH	1:C:273:GLU:OE1	2.38	0.41
1:B:103:GLN:HB3	1:B:218:GLN:NE2	2.36	0.40
1:D:255:ARG:HH21	1:D:260:ASP:CG	2.28	0.40
1:B:48:TRP:HH2	1:B:131:ASN:OD1	2.04	0.40
1:B:59:TYR:CD1	1:B:274:LEU:HD13	2.56	0.40
1:C:185:THR:HG21	2:D:414:HOH:O	2.21	0.40
1:B:211:ARG:C	1:B:211:ARG:CD	2.86	0.40
1:C:11:GLN:CD	1:C:233:GLN:HE21	2.29	0.40
1:D:108:ARG:HB2	2:D:444:HOH:O	2.21	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)
2:A:414:HOH:O	2:D:487:HOH:O[2_757]	2.17	0.03

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	290/309 (94%)	281 (97%)	8 (3%)	1 (0%)	36 42
1	B	290/309 (94%)	281 (97%)	8 (3%)	1 (0%)	36 42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	290/309 (94%)	282 (97%)	8 (3%)	0	100	100
1	D	290/309 (94%)	286 (99%)	4 (1%)	0	100	100
All	All	1160/1236 (94%)	1130 (97%)	28 (2%)	2 (0%)	43	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	PRO
1	B	102	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	240/257 (93%)	231 (96%)	9 (4%)	29	40
1	B	240/257 (93%)	234 (98%)	6 (2%)	42	56
1	C	240/257 (93%)	236 (98%)	4 (2%)	53	69
1	D	240/257 (93%)	232 (97%)	8 (3%)	33	45
All	All	960/1028 (93%)	933 (97%)	27 (3%)	38	52

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	21	ILE
1	A	52	ILE
1	A	106	ARG
1	A	167	ILE
1	A	168	CYS
1	A	169	GLN
1	A	170	ILE
1	A	205	ASP
1	B	35	GLU

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Mol	Chain	Res	Type
1	B	52	ILE
1	B	114	VAL
1	B	167	ILE
1	B	168	CYS
1	B	170	ILE
1	C	52	ILE
1	C	167	ILE
1	C	205	ASP
1	C	224	LYS
1	D	21	ILE
1	D	35	GLU
1	D	52	ILE
1	D	53	THR
1	D	68	ARG
1	D	93	LEU
1	D	169	GLN
1	D	211	ARG

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	31	GLN
1	B	218	GLN
1	C	77	HIS
1	C	198	GLN
1	C	218	GLN
1	C	233	GLN
1	D	31	GLN
1	D	240	ASN

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 [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	292/309 (94%)	1.86	108 (36%) 1 0	20, 30, 48, 68	0
1	B	292/309 (94%)	1.78	97 (33%) 1 0	22, 30, 47, 70	0
1	C	292/309 (94%)	1.70	83 (28%) 1 1	21, 30, 46, 64	0
1	D	292/309 (94%)	1.72	94 (32%) 1 0	20, 30, 47, 66	0
All	All	1168/1236 (94%)	1.77	382 (32%) 1 0	20, 30, 47, 70	0

All (382) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	167	ILE	7.3
1	D	10	LEU	6.6
1	A	16	VAL	6.5
1	D	16	VAL	6.4
1	A	167	ILE	6.2
1	B	16	VAL	6.0
1	B	168	CYS	6.0
1	D	167	ILE	6.0
1	A	168	CYS	5.9
1	D	168	CYS	5.9
1	B	18	GLU	5.8
1	C	168	CYS	5.7
1	C	155	ALA	5.5
1	A	9	HIS	5.5
1	A	300	LEU	5.5
1	B	48	TRP	5.3
1	C	16	VAL	5.3
1	C	300	LEU	5.3
1	B	20	ILE	5.3
1	B	167	ILE	5.2
1	A	12	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	21	ILE	5.0
1	C	100	ILE	4.9
1	C	9	HIS	4.9
1	D	17	CYS	4.8
1	C	169	GLN	4.8
1	C	285	LEU	4.7
1	A	48	TRP	4.7
1	B	10	LEU	4.7
1	B	9	HIS	4.6
1	B	101	GLU	4.5
1	A	17	CYS	4.4
1	C	18	GLU	4.4
1	B	184	GLY	4.3
1	D	9	HIS	4.3
1	B	17	CYS	4.3
1	D	97	SER	4.3
1	A	188	GLN	4.3
1	A	20	ILE	4.3
1	A	99	VAL	4.2
1	B	102	GLY	4.2
1	A	13	PRO	4.2
1	B	300	LEU	4.2
1	D	300	LEU	4.2
1	A	166	PRO	4.2
1	D	48	TRP	4.1
1	A	218	GLN	4.1
1	C	99	VAL	4.1
1	B	185	THR	4.1
1	C	19	ALA	4.1
1	D	184	GLY	4.0
1	D	155	ALA	4.0
1	C	170	ILE	4.0
1	B	12	LEU	3.9
1	D	104	THR	3.9
1	C	20	ILE	3.9
1	C	287	GLY	3.9
1	B	188	GLN	3.9
1	B	241	ALA	3.7
1	C	10	LEU	3.7
1	A	170	ILE	3.7
1	D	74	ALA	3.7
1	A	108	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	12	LEU	3.7
1	B	19	ALA	3.7
1	B	280	LEU	3.6
1	A	21	ILE	3.6
1	C	48	TRP	3.6
1	A	102	GLY	3.6
1	A	184	GLY	3.6
1	A	23	PRO	3.6
1	B	212	TRP	3.5
1	B	15	PRO	3.5
1	A	106	ARG	3.5
1	A	201	PHE	3.5
1	C	265	GLY	3.5
1	D	169	GLN	3.5
1	A	100	ILE	3.4
1	D	202	ILE	3.4
1	A	186	LEU	3.4
1	B	202	ILE	3.4
1	B	169	GLN	3.4
1	D	15	PRO	3.4
1	D	19	ALA	3.4
1	B	109	GLU	3.3
1	A	51	VAL	3.3
1	A	189	VAL	3.3
1	D	261	ALA	3.3
1	C	17	CYS	3.3
1	A	15	PRO	3.3
1	A	18	GLU	3.3
1	B	13	PRO	3.3
1	A	210	ALA	3.3
1	D	20	ILE	3.3
1	D	183	GLY	3.2
1	B	191	ALA	3.2
1	A	10	LEU	3.2
1	D	186	LEU	3.2
1	A	169	GLN	3.2
1	C	96	GLN	3.2
1	A	67	TRP	3.2
1	A	57	ALA	3.2
1	C	12	LEU	3.2
1	B	189	VAL	3.1
1	C	202	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	170	ILE	3.1
1	A	14	ARG	3.1
1	D	18	GLU	3.1
1	B	199	LEU	3.1
1	C	145	LEU	3.1
1	D	197	LEU	3.1
1	D	185	THR	3.1
1	C	228	ASP	3.1
1	C	191	ALA	3.1
1	D	190	TYR	3.1
1	B	126	ILE	3.1
1	B	183	GLY	3.0
1	A	115	ARG	3.0
1	D	219	ALA	3.0
1	D	96	GLN	3.0
1	D	187	SER	3.0
1	A	148	GLY	3.0
1	B	108	ARG	3.0
1	C	258	ARG	3.0
1	D	228	ASP	3.0
1	A	269	ALA	3.0
1	D	51	VAL	3.0
1	A	11	GLN	3.0
1	B	11	GLN	3.0
1	A	101	GLU	3.0
1	B	173	ILE	3.0
1	A	103	GLN	2.9
1	B	14	ARG	2.9
1	A	191	ALA	2.9
1	C	104	THR	2.9
1	B	47	PRO	2.9
1	B	190	TYR	2.9
1	C	201	PHE	2.9
1	C	254	TYR	2.9
1	D	191	ALA	2.9
1	D	265	GLY	2.9
1	B	193	ILE	2.9
1	B	218	GLN	2.9
1	C	109	GLU	2.9
1	C	129	TYR	2.9
1	A	241	ALA	2.9
1	C	183	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	195	GLN	2.8
1	C	233	GLN	2.8
1	D	135	LEU	2.8
1	A	24	VAL	2.8
1	A	104	THR	2.8
1	A	185	THR	2.8
1	D	35	GLU	2.8
1	C	15	PRO	2.8
1	A	205	ASP	2.8
1	B	112	TYR	2.8
1	C	71	ALA	2.8
1	D	249	ALA	2.8
1	D	269	ALA	2.8
1	C	185	THR	2.8
1	A	172	PRO	2.8
1	A	278	ILE	2.8
1	B	201	PHE	2.8
1	A	206	TYR	2.8
1	A	295	PHE	2.7
1	B	127	PHE	2.7
1	C	74	ALA	2.7
1	A	290	LEU	2.7
1	C	46	VAL	2.7
1	A	202	ILE	2.7
1	D	227	ILE	2.7
1	D	257	SER	2.7
1	A	248	ASP	2.7
1	C	184	GLY	2.7
1	C	154	ALA	2.7
1	C	186	LEU	2.7
1	D	196	THR	2.7
1	A	232	TYR	2.7
1	B	100	ILE	2.7
1	D	100	ILE	2.7
1	D	220	TRP	2.7
1	D	63	PHE	2.7
1	D	254	TYR	2.7
1	B	51	VAL	2.7
1	C	97	SER	2.7
1	C	189	VAL	2.7
1	C	239	ILE	2.7
1	D	189	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	107	LEU	2.6
1	B	206	TYR	2.6
1	C	288	ILE	2.6
1	B	40	LEU	2.6
1	C	106	ARG	2.6
1	C	114	VAL	2.6
1	B	31	GLN	2.6
1	B	253	ALA	2.6
1	B	93	LEU	2.6
1	B	105	ASP	2.6
1	C	21	ILE	2.6
1	C	175	VAL	2.6
1	A	293	THR	2.6
1	C	182	ALA	2.6
1	D	182	ALA	2.6
1	A	197	LEU	2.6
1	A	212	TRP	2.6
1	D	247	LEU	2.6
1	C	98	PHE	2.5
1	D	46	VAL	2.5
1	C	249	ALA	2.5
1	C	261	ALA	2.5
1	D	231	ALA	2.5
1	A	107	LEU	2.5
1	B	223	LEU	2.5
1	A	237	PHE	2.5
1	A	227	ILE	2.5
1	B	175	VAL	2.5
1	C	206	TYR	2.5
1	C	211	ARG	2.5
1	D	108	ARG	2.5
1	C	146	LEU	2.5
1	B	130	GLY	2.5
1	B	277	VAL	2.5
1	B	226	CYS	2.5
1	D	215	TYR	2.5
1	B	285	LEU	2.5
1	A	277	VAL	2.4
1	C	52	ILE	2.5
1	C	141	ILE	2.5
1	D	114	VAL	2.4
1	D	141	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	125	ASP	2.4
1	B	195	GLN	2.4
1	D	206	TYR	2.4
1	A	231	ALA	2.4
1	C	108	ARG	2.4
1	D	38	ARG	2.4
1	A	193	ILE	2.4
1	D	31	GLN	2.4
1	B	114	VAL	2.4
1	B	123	VAL	2.4
1	B	57	ALA	2.4
1	A	135	LEU	2.4
1	B	217	GLU	2.4
1	D	295	PHE	2.4
1	C	193	ILE	2.4
1	D	52	ILE	2.4
1	A	25	PRO	2.4
1	B	61	PRO	2.4
1	D	285	LEU	2.4
1	A	183	GLY	2.4
1	C	31	GLN	2.4
1	A	44	PHE	2.4
1	D	70	PHE	2.4
1	A	211	ARG	2.4
1	D	99	VAL	2.4
1	A	113	SER	2.4
1	B	172	PRO	2.4
1	A	208	ALA	2.3
1	A	31	GLN	2.3
1	C	135	LEU	2.3
1	C	188	GLN	2.3
1	A	95	GLY	2.3
1	D	68	ARG	2.3
1	B	141	ILE	2.3
1	A	253	ALA	2.3
1	C	231	ALA	2.3
1	D	154	ALA	2.3
1	D	208	ALA	2.3
1	D	243	ALA	2.3
1	B	148	GLY	2.3
1	B	186	LEU	2.3
1	A	284	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	162	PHE	2.3
1	C	51	VAL	2.3
1	B	103	GLN	2.3
1	A	261	ALA	2.3
1	B	269	ALA	2.3
1	A	171	ASP	2.3
1	A	190	TYR	2.3
1	B	124	LEU	2.3
1	B	221	GLY	2.3
1	D	58	TYR	2.3
1	C	242	ARG	2.3
1	D	146	LEU	2.3
1	B	237	PHE	2.3
1	B	52	ILE	2.3
1	A	68	ARG	2.3
1	A	222	ALA	2.3
1	D	64	ALA	2.3
1	A	40	LEU	2.3
1	C	247	LEU	2.3
1	A	215	TYR	2.3
1	D	129	TYR	2.3
1	D	162	PHE	2.2
1	A	117	ILE	2.2
1	A	123	VAL	2.2
1	D	271	THR	2.2
1	A	149	ARG	2.2
1	D	222	ALA	2.2
1	D	287	GLY	2.2
1	D	299	ALA	2.2
1	D	145	LEU	2.2
1	B	35	GLU	2.2
1	C	190	TYR	2.2
1	D	109	GLU	2.2
1	D	112	TYR	2.2
1	A	220	TRP	2.2
1	A	70	PHE	2.2
1	A	258	ARG	2.2
1	B	63	PHE	2.2
1	A	154	ALA	2.2
1	C	217	GLU	2.2
1	C	243	ALA	2.2
1	A	233	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	294	HIS	2.2
1	B	106	ARG	2.2
1	A	98	PHE	2.2
1	B	104	THR	2.2
1	B	120	ILE	2.2
1	B	281	PHE	2.2
1	C	225	PRO	2.2
1	C	271	THR	2.2
1	B	248	ASP	2.2
1	A	175	VAL	2.2
1	A	109	GLU	2.2
1	A	217	GLU	2.2
1	C	159	ARG	2.2
1	D	14	ARG	2.2
1	D	106	ARG	2.2
1	B	215	TYR	2.2
1	B	171	ASP	2.2
1	A	88	ILE	2.1
1	B	117	ILE	2.1
1	C	227	ILE	2.1
1	D	281	PHE	2.1
1	D	175	VAL	2.1
1	A	247	LEU	2.1
1	C	40	LEU	2.1
1	B	110	MET	2.1
1	A	251	PRO	2.1
1	D	43	THR	2.1
1	D	200	PRO	2.1
1	B	36	ILE	2.1
1	A	153	GLY	2.1
1	B	243	ALA	2.1
1	A	187	SER	2.1
1	C	93	LEU	2.1
1	C	35	GLU	2.1
1	B	229	THR	2.1
1	A	126	ILE	2.1
1	B	115	ARG	2.1
1	D	258	ARG	2.1
1	C	64	ALA	2.1
1	B	187	SER	2.1
1	A	263	GLN	2.1
1	C	276	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	254	TYR	2.1
1	B	163	PRO	2.1
1	A	52	ILE	2.1
1	B	295	PHE	2.1
1	A	91	TRP	2.1
1	B	283	TRP	2.1
1	A	74	ALA	2.1
1	B	249	ALA	2.1
1	D	101	GLU	2.0
1	A	271	THR	2.0
1	A	36	ILE	2.0
1	C	275	ILE	2.0
1	D	21	ILE	2.0
1	D	239	ILE	2.0
1	B	98	PHE	2.0
1	C	292	VAL	2.0
1	D	214	SER	2.0
1	D	140	ALA	2.0
1	C	107	LEU	2.0
1	D	195	GLN	2.0
1	D	233	GLN	2.0
1	B	23	PRO	2.0
1	D	166	PRO	2.0
1	C	221	GLY	2.0
1	D	102	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.