



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:10 PM UTC

PDB ID : 6IV0 / pdb_00006iv0
Title : Crystal structure of a bacterial Bestrophin homolog from *Klebsiella pneumoniae* with a mutation I180A
Authors : Kittredge, A.; Chen, S.; Yang, T.
Deposited on : 2018-12-02
Resolution : 2.90 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

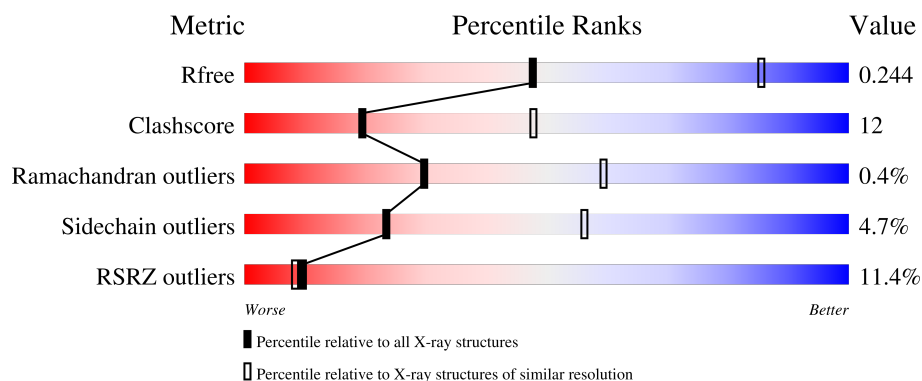
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	296	7% 68% 21% • 9%
1	B	296	11% 62% 26% • 9%
1	C	296	11% 72% 17% • 9%
1	D	296	12% 61% 26% • 9%
1	E	296	11% 69% 20% • 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10621 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 Bestrophin homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			2104	1363	353	379	9			
1	B	270	Total	C	N	O	S	0	0	0
			2139	1382	364	384	9			
1	C	269	Total	C	N	O	S	0	0	0
			2101	1353	362	377	9			
1	D	268	Total	C	N	O	S	0	0	0
			2111	1364	359	379	9			
1	E	270	Total	C	N	O	S	0	0	0
			2127	1374	364	380	9			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ASN	-	expression tag	UNP W1ELP7
A	0	ALA	-	expression tag	UNP W1ELP7
A	180	ALA	ILE	engineered mutation	UNP W1ELP7
B	-1	ASN	-	expression tag	UNP W1ELP7
B	0	ALA	-	expression tag	UNP W1ELP7
B	180	ALA	ILE	engineered mutation	UNP W1ELP7
C	-1	ASN	-	expression tag	UNP W1ELP7
C	0	ALA	-	expression tag	UNP W1ELP7
C	180	ALA	ILE	engineered mutation	UNP W1ELP7
D	-1	ASN	-	expression tag	UNP W1ELP7
D	0	ALA	-	expression tag	UNP W1ELP7
D	180	ALA	ILE	engineered mutation	UNP W1ELP7
E	-1	ASN	-	expression tag	UNP W1ELP7
E	0	ALA	-	expression tag	UNP W1ELP7
E	180	ALA	ILE	engineered mutation	UNP W1ELP7

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total 4	Zn 4	0	0
2	B	2	Total 2	Zn 2	0	0
2	C	3	Total 3	Zn 3	0	0
2	D	4	Total 4	Zn 4	0	0
2	E	2	Total 2	Zn 2	0	0

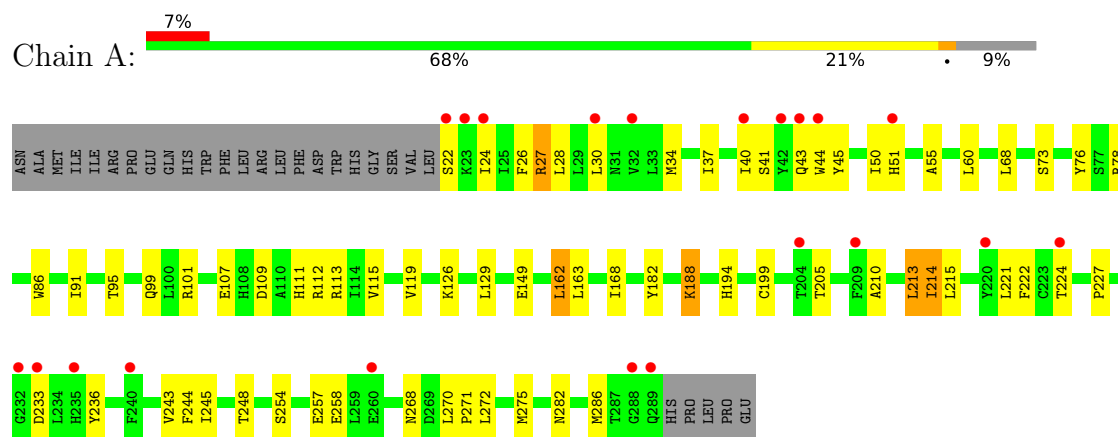
- Molecule 3 is water.

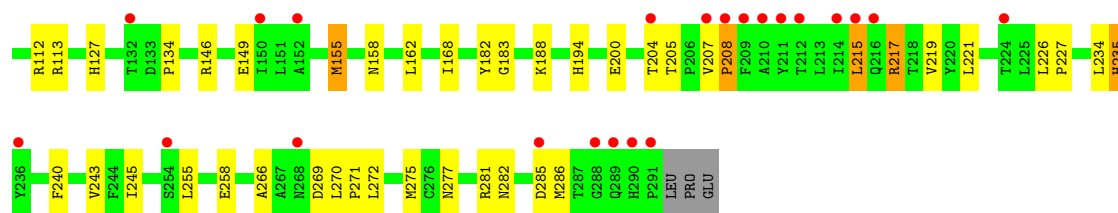
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	8	Total 8	O 8	0	0
3	B	4	Total 4	O 4	0	0
3	C	6	Total 6	O 6	0	0
3	D	3	Total 3	O 3	0	0
3	E	3	Total 3	O 3	0	0

3 Residue-property plots [i](#)

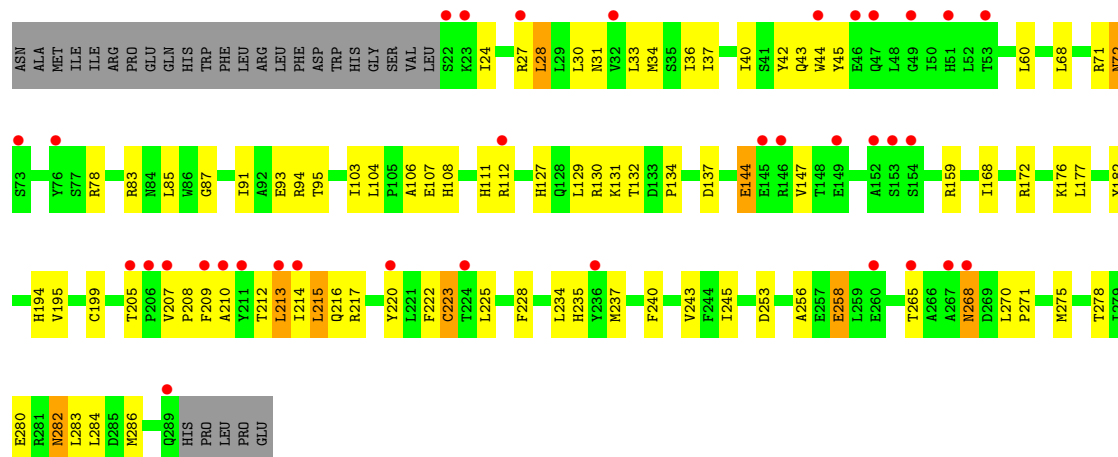
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

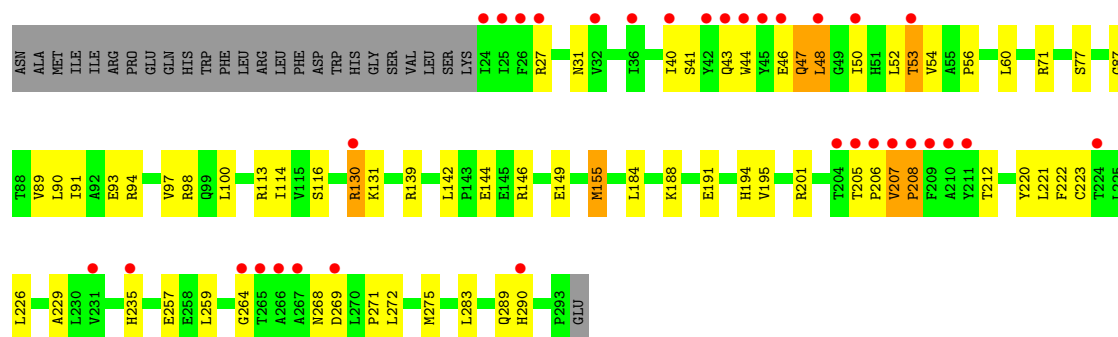




• Molecule 1: Bestrophin homolog



• Molecule 1: Bestrophin homolog



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.57Å 159.91Å 161.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.38 – 2.90 65.38 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (65.38-2.90) 99.8 (65.38-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.201 , 0.238 0.211 , 0.244	Depositor DCC
R_{free} test set	1996 reflections (3.04%)	wwPDB-VP
Wilson B-factor (Å ²)	79.1	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 35.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10621	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.66	0/2149	0.98	3/2929 (0.1%)
1	B	0.66	0/2187	0.98	3/2979 (0.1%)
1	C	0.63	0/2146	0.93	6/2925 (0.2%)
1	D	0.59	0/2156	0.99	3/2937 (0.1%)
1	E	0.68	0/2173	1.00	6/2961 (0.2%)
All	All	0.64	0/10811	0.98	21/14731 (0.1%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	206	PRO	N-CA-C	-8.90	94.14	112.47
1	D	217	ARG	N-CA-C	-8.32	101.90	110.97
1	A	214	ILE	CB-CA-C	-7.52	102.34	111.97
1	B	238	THR	CA-C-N	-7.32	110.69	119.84
1	B	238	THR	C-N-CA	-7.32	110.69	119.84
1	C	46	GLU	N-CA-C	-6.90	103.84	111.36
1	E	235	HIS	CB-CA-C	-6.51	109.05	116.54
1	C	207	VAL	CA-C-N	6.40	127.84	119.84
1	C	207	VAL	C-N-CA	6.40	127.84	119.84
1	B	210	ALA	N-CA-C	-6.25	99.45	109.39
1	E	264	GLY	N-CA-C	6.18	119.13	112.33
1	E	212	THR	N-CA-C	-5.84	106.12	113.18
1	D	223	CYS	N-CA-C	5.83	118.42	111.71
1	A	55	ALA	CA-C-N	-5.52	114.07	119.64
1	A	55	ALA	C-N-CA	-5.52	114.07	119.64
1	D	282	ASN	N-CA-C	5.16	117.57	111.33
1	C	235	HIS	CB-CA-C	-5.15	110.22	117.23
1	E	142	LEU	CA-C-N	5.07	124.98	119.76
1	E	142	LEU	C-N-CA	5.07	124.98	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	205	THR	CA-C-N	-5.00	114.43	119.83
1	C	205	THR	C-N-CA	-5.00	114.43	119.83

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	2104	0	2122	58	0
1	B	2139	0	2160	70	0
1	C	2101	0	2110	42	0
1	D	2111	0	2138	61	0
1	E	2127	0	2162	57	0
2	A	4	0	0	0	0
2	B	2	0	0	0	0
2	C	3	0	0	0	0
2	D	4	0	0	0	0
2	E	2	0	0	0	0
3	A	8	0	0	0	0
3	B	4	0	0	0	0
3	C	6	0	0	0	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
All	All	10621	0	10692	247	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 12.

All (247) 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:68:LEU:HD23	1:C:215:LEU:CD1	1.77	1.13
1:D:212:THR:HG22	1:D:216:GLN:HE22	1.21	1.05
1:E:207:VAL:HG23	1:E:208:PRO:HD3	1.32	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:LEU:CD2	1:C:215:LEU:CD1	2.47	0.93
1:B:212:THR:HG22	1:B:216:GLN:NE2	1.84	0.91
1:A:236:TYR:HD2	1:E:48:LEU:O	1.55	0.90
1:E:201:ARG:O	1:E:205:THR:CB	2.21	0.89
1:E:130:ARG:HG2	1:E:130:ARG:HH21	1.38	0.89
1:A:76:TYR:HE1	1:E:207:VAL:HG21	1.40	0.86
1:B:236:TYR:O	1:B:237:MET:HG2	1.76	0.85
1:C:215:LEU:O	1:C:219:VAL:HG23	1.77	0.84
1:C:68:LEU:CD2	1:C:215:LEU:HD13	2.08	0.84
1:A:236:TYR:CD2	1:E:48:LEU:O	2.31	0.82
1:D:83:ARG:HG2	1:D:270:LEU:HD21	1.65	0.78
1:A:76:TYR:CE1	1:E:207:VAL:HG21	2.18	0.78
1:C:68:LEU:HD23	1:C:215:LEU:HD11	1.67	0.75
1:C:68:LEU:HD23	1:C:215:LEU:HD12	1.69	0.75
1:A:214:ILE:HD13	1:B:251:SER:HB3	1.69	0.74
1:B:271:PRO:HG2	1:B:275:MET:HE3	1.70	0.74
1:C:68:LEU:HD21	1:C:215:LEU:HD13	1.69	0.73
1:C:194:HIS:HA	1:E:91:ILE:HD13	1.71	0.72
1:A:51:HIS:ND1	1:B:235:HIS:HD2	1.86	0.71
1:E:130:ARG:HG2	1:E:130:ARG:NH2	2.01	0.70
1:A:22:SER:HB3	1:A:24:ILE:HG22	1.74	0.70
1:A:213:LEU:HD12	1:A:213:LEU:C	2.15	0.69
1:E:47:GLN:O	1:E:48:LEU:HB2	1.91	0.69
1:A:26:PHE:HD2	1:A:27:ARG:HD3	1.57	0.69
1:A:68:LEU:HD23	1:A:215:LEU:HD13	1.75	0.68
1:B:101:ARG:HD3	1:B:290:HIS:CG	2.28	0.68
1:B:41:SER:HA	1:B:44:TRP:HD1	1.58	0.68
1:B:212:THR:HG22	1:B:216:GLN:CD	2.19	0.67
1:C:91:ILE:HD13	1:D:194:HIS:HA	1.76	0.66
1:B:227:PRO:HA	1:B:230:LEU:HB2	1.78	0.65
1:A:271:PRO:HD2	1:A:275:MET:HE3	1.78	0.65
1:D:209:PHE:CE2	1:D:213:LEU:HD13	2.32	0.65
1:A:210:ALA:O	1:A:214:ILE:HG13	1.98	0.64
1:E:31:ASN:ND2	1:E:223:CYS:O	2.31	0.64
1:A:270:LEU:HD22	1:A:275:MET:HE1	1.80	0.64
1:A:51:HIS:ND1	1:B:235:HIS:CD2	2.66	0.63
1:A:109:ASP:HB3	1:A:113:ARG:HH12	1.63	0.62
1:D:270:LEU:HD22	1:D:275:MET:HE1	1.81	0.62
1:D:78:ARG:NH2	1:D:205:THR:O	2.26	0.62
1:D:43:GLN:HG3	1:D:44:TRP:CD1	2.34	0.62
1:D:78:ARG:HD2	1:D:207:VAL:HG23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:289:GLN:O	1:E:290:HIS:HD2	1.81	0.62
1:D:209:PHE:CZ	1:D:213:LEU:HD13	2.35	0.61
1:B:51:HIS:CE1	1:D:235:HIS:CE1	2.88	0.61
1:D:31:ASN:ND2	1:D:223:CYS:O	2.32	0.61
1:A:254:SER:HA	1:A:257:GLU:HG3	1.84	0.60
1:C:208:PRO:HG3	1:E:259:LEU:HD21	1.82	0.60
1:B:127:HIS:CD2	1:B:134:PRO:HA	2.37	0.59
1:E:90:LEU:HD23	1:E:94:ARG:NH2	2.18	0.59
1:D:258:GLU:OE1	1:D:268:ASN:ND2	2.36	0.58
1:A:149:GLU:HG2	1:B:291:PRO:HG3	1.85	0.58
1:E:40:ILE:O	1:E:43:GLN:NE2	2.36	0.58
1:B:41:SER:HA	1:B:44:TRP:CD1	2.38	0.58
1:C:91:ILE:O	1:C:95:THR:HG23	2.03	0.58
1:C:155:MET:HG2	1:C:158:ASN:HB2	1.86	0.58
1:E:146:ARG:NH1	1:E:149:GLU:OE1	2.36	0.58
1:E:50:ILE:HG13	1:E:50:ILE:O	2.04	0.58
1:A:76:TYR:HE1	1:E:207:VAL:CG2	2.14	0.58
1:B:135:THR:HG23	1:B:151:LEU:HD11	1.86	0.57
1:C:245:ILE:HG12	1:D:60:LEU:HD13	1.87	0.57
1:D:278:THR:O	1:D:282:ASN:HB2	2.04	0.57
1:C:108:HIS:O	1:C:112:ARG:HG3	2.04	0.57
1:B:91:ILE:O	1:B:95:THR:HG23	2.05	0.57
1:E:87:GLY:O	1:E:91:ILE:HG13	2.05	0.56
1:C:277:ASN:O	1:C:281:ARG:HG3	2.04	0.56
1:E:43:GLN:HG3	1:E:44:TRP:CD2	2.41	0.56
1:D:27:ARG:HD3	1:D:220:TYR:CD1	2.40	0.56
1:A:168:ILE:HG22	1:A:182:TYR:CE1	2.40	0.56
1:D:91:ILE:O	1:D:95:THR:HG23	2.06	0.56
1:A:43:GLN:C	1:A:45:TYR:H	2.12	0.56
1:D:108:HIS:O	1:D:112:ARG:HG3	2.07	0.55
1:A:50:ILE:CG2	1:B:237:MET:HE2	2.36	0.55
1:A:282:ASN:HA	1:E:155:MET:HE3	1.88	0.54
1:B:194:HIS:HA	1:D:91:ILE:HD13	1.90	0.54
1:E:41:SER:C	1:E:43:GLN:H	2.15	0.54
1:E:207:VAL:CG2	1:E:208:PRO:HD3	2.21	0.54
1:E:90:LEU:HD23	1:E:94:ARG:HH21	1.72	0.54
1:E:90:LEU:HB3	1:E:94:ARG:HH21	1.72	0.54
1:C:50:ILE:C	1:C:51:HIS:HD2	2.16	0.54
1:C:168:ILE:HG22	1:C:182:TYR:CE2	2.43	0.54
1:A:258:GLU:OE1	1:A:268:ASN:ND2	2.41	0.53
1:B:127:HIS:HD1	1:B:132:THR:HG1	1.54	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:TYR:HA	1:D:45:TYR:CD1	2.43	0.53
1:A:26:PHE:CD2	1:A:27:ARG:HD3	2.41	0.53
1:D:127:HIS:NE2	1:D:137:ASP:OD2	2.28	0.53
1:B:71:ARG:NH1	1:B:253:ASP:OD1	2.38	0.53
1:B:139:ARG:HG3	1:B:147:VAL:HG11	1.91	0.53
1:A:107:GLU:O	1:A:111:HIS:CD2	2.62	0.52
1:D:87:GLY:O	1:D:91:ILE:HG13	2.09	0.52
1:B:211:TYR:CD1	1:B:211:TYR:C	2.86	0.52
1:D:168:ILE:HG22	1:D:182:TYR:CD2	2.44	0.52
1:E:53:THR:HG22	1:E:54:VAL:H	1.75	0.52
1:B:256:ALA:O	1:B:260:GLU:HG3	2.11	0.51
1:A:30:LEU:O	1:A:34:MET:HG2	2.11	0.51
1:A:205:THR:HG21	1:B:83:ARG:HG2	1.91	0.51
1:D:68:LEU:HD23	1:D:215:LEU:HD13	1.92	0.51
1:E:97:VAL:HG21	1:E:283:LEU:HD22	1.93	0.51
1:D:72:ASN:OD1	1:D:256:ALA:HB2	2.11	0.50
1:D:127:HIS:CD2	1:D:134:PRO:HA	2.47	0.50
1:B:35:SER:HB3	1:B:239:PRO:HA	1.93	0.50
1:B:39:ILE:HD13	1:B:236:TYR:HD1	1.75	0.50
1:B:212:THR:HA	1:B:216:GLN:HG2	1.94	0.50
1:B:150:ILE:HD13	1:B:160:ILE:HG12	1.92	0.50
1:B:240:PHE:O	1:B:243:VAL:HG12	2.11	0.50
1:A:91:ILE:HD13	1:E:194:HIS:HA	1.94	0.49
1:B:205:THR:OG1	1:D:83:ARG:NH2	2.45	0.49
1:C:226:LEU:N	1:C:227:PRO:HD2	2.27	0.49
1:E:27:ARG:NH1	1:E:220:TYR:CZ	2.80	0.49
1:A:78:ARG:NH1	1:A:205:THR:O	2.45	0.49
1:D:265:THR:O	1:D:265:THR:OG1	2.28	0.49
1:E:191:GLU:O	1:E:195:VAL:HG23	2.13	0.49
1:E:60:LEU:HD23	1:E:222:PHE:HD1	1.77	0.48
1:A:60:LEU:HD23	1:A:222:PHE:HD1	1.78	0.48
1:B:204:THR:O	1:B:206:PRO:HD3	2.12	0.48
1:C:255:LEU:HD13	1:D:210:ALA:HB3	1.95	0.48
1:C:285:ASP:O	1:D:159:ARG:NH2	2.46	0.48
1:B:52:LEU:HD23	1:D:234:LEU:HD22	1.95	0.48
1:E:52:LEU:HB3	1:E:229:ALA:HA	1.95	0.48
1:A:194:HIS:HA	1:B:91:ILE:HD13	1.96	0.48
1:D:212:THR:HG22	1:D:216:GLN:NE2	2.07	0.48
1:E:130:ARG:NH2	1:E:269:ASP:OD2	2.46	0.48
1:C:109:ASP:HB3	1:C:113:ARG:HH12	1.79	0.48
1:D:60:LEU:HD23	1:D:222:PHE:HD1	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:43:GLN:HG3	1:E:44:TRP:CE2	2.48	0.48
1:A:101:ARG:HD2	1:A:286:MET:O	2.13	0.48
1:C:183:GLY:HA2	1:E:184:LEU:HD11	1.96	0.48
1:C:271:PRO:HG2	1:C:275:MET:HE3	1.96	0.48
1:B:85:LEU:HD22	1:B:195:VAL:HA	1.96	0.47
1:B:155:MET:HG3	1:B:158:ASN:HB3	1.96	0.47
1:D:144:GLU:HA	1:D:147:VAL:HB	1.96	0.47
1:D:93:GLU:HB3	1:D:283:LEU:HD11	1.97	0.47
1:C:50:ILE:C	1:C:51:HIS:CD2	2.93	0.47
1:B:224:THR:O	1:B:227:PRO:HD2	2.15	0.47
1:C:146:ARG:NH1	1:C:149:GLU:OE1	2.47	0.47
1:D:30:LEU:O	1:D:34:MET:HG2	2.15	0.47
1:E:41:SER:O	1:E:43:GLN:N	2.42	0.47
1:C:266:ALA:O	1:C:269:ASP:HB2	2.15	0.46
1:B:137:ASP:OD1	1:B:140:ARG:NH2	2.46	0.46
1:B:24:ILE:HG22	1:B:28:LEU:HG	1.98	0.46
1:C:50:ILE:O	1:C:50:ILE:HG13	2.16	0.46
1:D:129:LEU:HD21	1:D:199:CYS:HB3	1.96	0.46
1:C:76:TYR:HE1	1:D:208:PRO:HD2	1.81	0.46
1:E:100:LEU:HD11	1:E:114:ILE:HD13	1.97	0.46
1:A:245:ILE:HG12	1:E:60:LEU:HD13	1.97	0.46
1:A:115:VAL:O	1:A:119:VAL:HG23	2.15	0.46
1:A:224:THR:O	1:A:227:PRO:HD2	2.15	0.46
1:B:51:HIS:CD2	1:B:51:HIS:N	2.83	0.46
1:B:234:LEU:O	1:B:235:HIS:HB2	2.16	0.46
1:C:217:ARG:O	1:C:221:LEU:N	2.44	0.46
1:D:280:GLU:O	1:D:284:LEU:HG	2.16	0.46
1:B:60:LEU:HD13	1:D:245:ILE:HG12	1.98	0.46
1:E:48:LEU:HD13	1:E:48:LEU:N	2.31	0.46
1:D:33:LEU:O	1:D:37:ILE:HG13	2.16	0.46
1:E:27:ARG:NH1	1:E:220:TYR:OH	2.49	0.46
1:A:28:LEU:HD22	1:A:243:VAL:HG13	1.97	0.45
1:B:44:TRP:O	1:B:48:LEU:HD12	2.16	0.45
1:A:95:THR:HG21	1:A:188:LYS:HE2	1.98	0.45
1:A:109:ASP:OD1	1:A:112:ARG:NH2	2.50	0.45
1:D:172:ARG:HA	1:D:177:LEU:HB2	1.98	0.45
1:D:282:ASN:O	1:D:286:MET:HG3	2.16	0.45
1:B:139:ARG:CG	1:B:147:VAL:HG11	2.46	0.45
1:D:85:LEU:HD22	1:D:195:VAL:HA	1.98	0.45
1:A:213:LEU:O	1:A:214:ILE:C	2.59	0.45
1:B:211:TYR:CD1	1:B:211:TYR:O	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ILE:O	1:A:41:SER:HB3	2.17	0.45
1:C:270:LEU:O	1:C:272:LEU:N	2.51	0.44
1:B:22:SER:C	1:B:24:ILE:H	2.26	0.44
1:B:101:ARG:HH21	1:B:290:HIS:CD2	2.34	0.44
1:D:33:LEU:HA	1:D:36:ILE:HG12	1.99	0.44
1:B:231:VAL:HA	1:B:238:THR:OG1	2.17	0.44
1:B:155:MET:HE3	1:D:94:ARG:NH2	2.33	0.44
1:B:209:PHE:C	1:B:211:TYR:N	2.75	0.44
1:D:106:ALA:O	1:D:108:HIS:N	2.50	0.44
1:B:51:HIS:ND1	1:D:235:HIS:CE1	2.86	0.44
1:A:244:PHE:CE1	1:E:221:LEU:HD23	2.52	0.44
1:A:50:ILE:HG13	1:A:50:ILE:O	2.18	0.43
1:A:86:TRP:CE2	1:A:272:LEU:HD22	2.53	0.43
1:B:28:LEU:HD23	1:B:28:LEU:HA	1.88	0.43
1:E:289:GLN:C	1:E:290:HIS:HD2	2.26	0.43
1:A:244:PHE:CZ	1:E:221:LEU:HB3	2.53	0.43
1:C:71:ARG:HD2	1:C:71:ARG:C	2.43	0.43
1:C:168:ILE:HG22	1:C:182:TYR:CD2	2.53	0.43
1:E:222:PHE:O	1:E:226:LEU:HB2	2.18	0.43
1:C:127:HIS:CD2	1:C:134:PRO:HA	2.53	0.43
1:D:107:GLU:OE2	1:D:176:LYS:HD2	2.18	0.43
1:C:98:ARG:HH11	1:C:98:ARG:HG2	1.82	0.43
1:B:24:ILE:O	1:B:28:LEU:N	2.47	0.43
1:B:52:LEU:HD11	1:D:237:MET:HE2	2.01	0.43
1:D:34:MET:HE3	1:D:228:PHE:HE2	1.84	0.43
1:D:215:LEU:HD23	1:D:215:LEU:HA	1.62	0.43
1:E:268:ASN:O	1:E:271:PRO:HD2	2.19	0.43
1:B:39:ILE:HD13	1:B:236:TYR:CD1	2.53	0.42
1:E:139:ARG:HG2	1:E:144:GLU:OE1	2.19	0.42
1:A:271:PRO:O	1:A:275:MET:HG3	2.19	0.42
1:B:209:PHE:C	1:B:211:TYR:H	2.27	0.42
1:B:216:GLN:CG	1:B:217:ARG:N	2.82	0.42
1:D:103:ILE:O	1:D:104:LEU:HD23	2.19	0.42
1:E:272:LEU:HD12	1:E:272:LEU:HA	1.81	0.42
1:D:108:HIS:HA	1:D:111:HIS:ND1	2.34	0.42
1:E:53:THR:HB	1:E:56:PRO:HD3	2.02	0.42
1:D:71:ARG:NH2	1:D:253:ASP:OD1	2.35	0.42
1:D:130:ARG:O	1:D:132:THR:HG23	2.18	0.42
1:D:213:LEU:O	1:D:214:ILE:C	2.63	0.42
1:E:289:GLN:C	1:E:290:HIS:CD2	2.97	0.42
1:A:188:LYS:N	1:A:188:LYS:HD3	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:LEU:O	1:C:235:HIS:HB2	2.19	0.42
1:E:188:LYS:HD3	1:E:188:LYS:HA	1.64	0.42
1:A:60:LEU:HD13	1:B:245:ILE:HG12	2.02	0.42
1:C:51:HIS:CD2	1:C:51:HIS:N	2.88	0.42
1:C:240:PHE:O	1:C:243:VAL:HG12	2.20	0.42
1:A:43:GLN:C	1:A:45:TYR:N	2.77	0.42
1:B:161:LEU:HD23	1:B:161:LEU:HA	1.86	0.42
1:E:100:LEU:HA	1:E:100:LEU:HD23	1.82	0.42
1:A:26:PHE:HB3	1:A:27:ARG:NH1	2.35	0.42
1:A:221:LEU:HG	1:B:244:PHE:CE2	2.55	0.42
1:C:83:ARG:NE	1:D:205:THR:OG1	2.34	0.42
1:A:50:ILE:HB	1:B:237:MET:CE	2.50	0.41
1:A:163:LEU:HD23	1:A:163:LEU:HA	1.76	0.41
1:E:47:GLN:HG3	1:E:48:LEU:HD13	2.01	0.41
1:A:215:LEU:HA	1:A:215:LEU:HD23	1.80	0.41
1:B:28:LEU:O	1:B:32:VAL:HG23	2.20	0.41
1:E:113:ARG:O	1:E:116:SER:HB2	2.20	0.41
1:A:162:LEU:HD12	1:B:98:ARG:HG3	2.02	0.41
1:B:83:ARG:HA	1:B:83:ARG:HD2	1.89	0.41
1:C:162:LEU:HD12	1:E:98:ARG:HG3	2.02	0.41
1:C:200:GLU:O	1:C:204:THR:HG23	2.20	0.41
1:B:173:GLU:C	1:B:175:GLY:H	2.29	0.41
1:A:99:GLN:HE22	1:A:188:LYS:NZ	2.19	0.41
1:B:129:LEU:HD22	1:B:263:PHE:CD2	2.56	0.41
1:B:213:LEU:HD12	1:B:213:LEU:HA	1.80	0.41
1:B:260:GLU:C	1:B:262:PRO:HD3	2.46	0.41
1:D:42:TYR:O	1:D:45:TYR:HB2	2.21	0.41
1:A:233:ASP:HB3	1:E:53:THR:OG1	2.20	0.40
1:B:138:LEU:HB3	1:B:147:VAL:HG13	2.03	0.40
1:D:28:LEU:HD23	1:D:28:LEU:HA	1.88	0.40
1:D:271:PRO:HD2	1:D:275:MET:HE3	2.03	0.40
1:A:244:PHE:CD1	1:E:221:LEU:HD23	2.56	0.40
1:B:115:VAL:O	1:B:119:VAL:HG23	2.22	0.40
1:B:146:ARG:HD3	1:B:146:ARG:HA	1.79	0.40
1:D:240:PHE:O	1:D:243:VAL:HG12	2.21	0.40
1:C:188:LYS:HD3	1:C:188:LYS:HA	1.72	0.40
1:C:282:ASN:O	1:C:286:MET:HG3	2.20	0.40
1:E:89:VAL:O	1:E:93:GLU:HG3	2.20	0.40
1:A:129:LEU:HD21	1:A:199:CYS:HB3	2.04	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	266/296 (90%)	254 (96%)	10 (4%)	2 (1%)	16	44
1	B	268/296 (90%)	241 (90%)	27 (10%)	0	100	100
1	C	267/296 (90%)	249 (93%)	17 (6%)	1 (0%)	30	59
1	D	266/296 (90%)	252 (95%)	13 (5%)	1 (0%)	30	59
1	E	268/296 (90%)	255 (95%)	12 (4%)	1 (0%)	30	59
All	All	1335/1480 (90%)	1251 (94%)	79 (6%)	5 (0%)	30	59

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	208	PRO
1	A	44	TRP
1	A	40	ILE
1	D	40	ILE
1	E	208	PRO

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	225/258 (87%)	218 (97%)	7 (3%)	35	69
1	B	231/258 (90%)	215 (93%)	16 (7%)	14	41
1	C	223/258 (86%)	215 (96%)	8 (4%)	31	65
1	D	227/258 (88%)	217 (96%)	10 (4%)	25	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	230/258 (89%)	218 (95%)	12 (5%)	21	52
All	All	1136/1290 (88%)	1083 (95%)	53 (5%)	23	56

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ARG
1	A	73	SER
1	A	126	LYS
1	A	162	LEU
1	A	188	LYS
1	A	213	LEU
1	A	248	THR
1	B	30	LEU
1	B	39	ILE
1	B	46	GLU
1	B	51	HIS
1	B	80	VAL
1	B	95	THR
1	B	126	LYS
1	B	131	LYS
1	B	157	THR
1	B	188	LYS
1	B	211	TYR
1	B	213	LEU
1	B	217	ARG
1	B	218	THR
1	B	282	ASN
1	B	290	HIS
1	C	40	ILE
1	C	50	ILE
1	C	51	HIS
1	C	58	SER
1	C	155	MET
1	C	215	LEU
1	C	217	ARG
1	C	258	GLU
1	D	24	ILE
1	D	28	LEU
1	D	72	ASN
1	D	131	LYS
1	D	144	GLU

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Mol	Chain	Res	Type
1	D	213	LEU
1	D	215	LEU
1	D	225	LEU
1	D	258	GLU
1	D	268	ASN
1	E	46	GLU
1	E	47	GLN
1	E	48	LEU
1	E	53	THR
1	E	71	ARG
1	E	77	SER
1	E	130	ARG
1	E	131	LYS
1	E	155	MET
1	E	207	VAL
1	E	257	GLU
1	E	275	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	B	99	GLN
1	B	216	GLN
1	B	235	HIS
1	B	268	ASN
1	C	235	HIS
1	C	268	ASN
1	C	289	GLN
1	D	51	HIS
1	D	128	GLN
1	D	216	GLN
1	D	282	ASN
1	E	31	ASN
1	E	43	GLN
1	E	47	GLN
1	E	235	HIS
1	E	290	HIS

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](#)

Of 15 ligands modelled in this entry, 15 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	268/296 (90%)	0.22	21 (7%) 19 16	46, 69, 119, 141	0
1	B	270/296 (91%)	0.60	32 (11%) 9 7	49, 77, 115, 133	0
1	C	269/296 (90%)	0.59	32 (11%) 9 7	51, 75, 128, 149	0
1	D	268/296 (90%)	0.58	35 (13%) 7 6	52, 86, 120, 130	0
1	E	270/296 (91%)	0.48	33 (12%) 8 7	46, 70, 120, 146	0
All	All	1345/1480 (90%)	0.49	153 (11%) 10 8	46, 76, 121, 149	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	204	THR	9.0
1	C	210	ALA	8.3
1	B	287	THR	6.7
1	B	213	LEU	6.3
1	E	45	TYR	5.8
1	B	214	ILE	5.8
1	B	215	LEU	5.7
1	D	154	SER	5.7
1	D	211	TYR	5.0
1	E	42	TYR	4.9
1	D	153	SER	4.9
1	E	209	PHE	4.7
1	B	210	ALA	4.7
1	E	266	ALA	4.6
1	C	291	PRO	4.6
1	C	289	GLN	4.6
1	C	207	VAL	4.3
1	E	26	PHE	4.2
1	E	211	TYR	4.0
1	B	205	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	236	TYR	3.8
1	B	204	THR	3.8
1	C	208	PRO	3.8
1	E	130	ARG	3.8
1	B	211	TYR	3.7
1	E	265	THR	3.7
1	C	268	ASN	3.7
1	E	48	LEU	3.6
1	B	155	MET	3.6
1	D	46	GLU	3.5
1	C	27	ARG	3.5
1	E	44	TRP	3.5
1	C	209	PHE	3.5
1	C	47	GLN	3.4
1	C	214	ILE	3.4
1	C	150	ILE	3.4
1	B	216	GLN	3.4
1	A	42	TYR	3.3
1	C	211	TYR	3.3
1	D	268	ASN	3.3
1	A	233	ASP	3.3
1	E	24	ILE	3.3
1	D	152	ALA	3.3
1	C	51	HIS	3.2
1	D	146	ARG	3.2
1	D	265	THR	3.2
1	C	285	ASP	3.2
1	D	209	PHE	3.2
1	B	24	ILE	3.2
1	B	207	VAL	3.1
1	D	47	GLN	3.1
1	D	289	GLN	3.1
1	D	206	PRO	3.1
1	D	149	GLU	3.1
1	D	23	LYS	3.1
1	E	210	ALA	3.0
1	C	288	GLY	3.0
1	C	46	GLU	3.0
1	B	32	VAL	3.0
1	E	231	VAL	3.0
1	E	50	ILE	2.9
1	E	205	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	40	ILE	2.9
1	E	267	ALA	2.9
1	D	260	GLU	2.8
1	D	112	ARG	2.8
1	B	237	MET	2.8
1	E	206	PRO	2.8
1	A	51	HIS	2.8
1	A	204	THR	2.8
1	C	254	SER	2.8
1	C	204	THR	2.8
1	B	241	VAL	2.7
1	D	32	VAL	2.7
1	A	23	LYS	2.7
1	E	207	VAL	2.7
1	C	212	THR	2.7
1	B	46	GLU	2.7
1	A	40	ILE	2.7
1	B	289	GLN	2.7
1	D	213	LEU	2.7
1	C	290	HIS	2.7
1	D	205	THR	2.7
1	E	269	ASP	2.7
1	A	289	GLN	2.7
1	E	43	GLN	2.7
1	A	30	LEU	2.7
1	B	33	LEU	2.7
1	E	25	ILE	2.6
1	D	27	ARG	2.6
1	B	206	PRO	2.6
1	A	235	HIS	2.6
1	E	46	GLU	2.6
1	A	288	GLY	2.6
1	C	132	THR	2.6
1	C	109	ASP	2.5
1	A	32	VAL	2.5
1	D	53	THR	2.5
1	B	190	ASP	2.5
1	E	208	PRO	2.5
1	B	247	TYR	2.5
1	D	145	GLU	2.5
1	B	71	ARG	2.5
1	C	152	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	224	THR	2.5
1	D	207	VAL	2.4
1	B	291	PRO	2.4
1	D	22	SER	2.4
1	C	45	TYR	2.4
1	B	37	ILE	2.4
1	A	260	GLU	2.4
1	C	24	ILE	2.3
1	E	32	VAL	2.3
1	B	288	GLY	2.3
1	A	220	TYR	2.3
1	B	47	GLN	2.3
1	C	103	ILE	2.3
1	D	51	HIS	2.3
1	E	36	ILE	2.3
1	D	210	ALA	2.2
1	E	235	HIS	2.2
1	A	24	ILE	2.2
1	E	264	GLY	2.2
1	B	48	LEU	2.2
1	E	290	HIS	2.2
1	A	240	PHE	2.2
1	B	239	PRO	2.1
1	A	224	THR	2.1
1	E	53	THR	2.1
1	A	44	TRP	2.1
1	A	209	PHE	2.1
1	D	73	SER	2.1
1	D	214	ILE	2.1
1	E	224	THR	2.1
1	A	22	SER	2.1
1	A	43	GLN	2.1
1	C	216	GLN	2.1
1	A	232	GLY	2.1
1	B	212	THR	2.1
1	B	285	ASP	2.1
1	E	27	ARG	2.1
1	D	267	ALA	2.1
1	D	220	TYR	2.1
1	C	224	THR	2.1
1	D	76	TYR	2.1
1	C	215	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	106	ALA	2.0
1	B	236	TYR	2.0
1	D	236	TYR	2.0
1	B	43	GLN	2.0
1	D	49	GLY	2.0
1	C	40	ILE	2.0
1	D	44	TRP	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ZN	D	303	1/1	0.70	0.20	117,117,117,117	0
2	ZN	B	301	1/1	0.89	0.15	133,133,133,133	0
2	ZN	D	304	1/1	0.92	0.09	128,128,128,128	0
2	ZN	A	304	1/1	0.93	0.07	80,80,80,80	0
2	ZN	E	302	1/1	0.96	0.10	71,71,71,71	0
2	ZN	D	302	1/1	0.97	0.07	87,87,87,87	0
2	ZN	A	302	1/1	0.98	0.10	76,76,76,76	0
2	ZN	C	303	1/1	0.99	0.07	75,75,75,75	0
2	ZN	A	301	1/1	0.99	0.06	74,74,74,74	0
2	ZN	A	303	1/1	0.99	0.07	81,81,81,81	0
2	ZN	B	302	1/1	0.99	0.08	73,73,73,73	0
2	ZN	E	301	1/1	0.99	0.08	63,63,63,63	0
2	ZN	C	302	1/1	0.99	0.04	76,76,76,76	0
2	ZN	D	301	1/1	1.00	0.05	76,76,76,76	0
2	ZN	C	301	1/1	1.00	0.08	69,69,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.