



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:13 PM UTC

PDB ID : 6IVW / pdb_00006ivw
Title : Crystal structure of a bacterial Bestrophin homolog from *Klebsiella pneumoniae* with a mutation D269A
Authors : Kittredge, A.; Chen, S.; Yang, T.
Deposited on : 2018-12-04
Resolution : 3.72 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

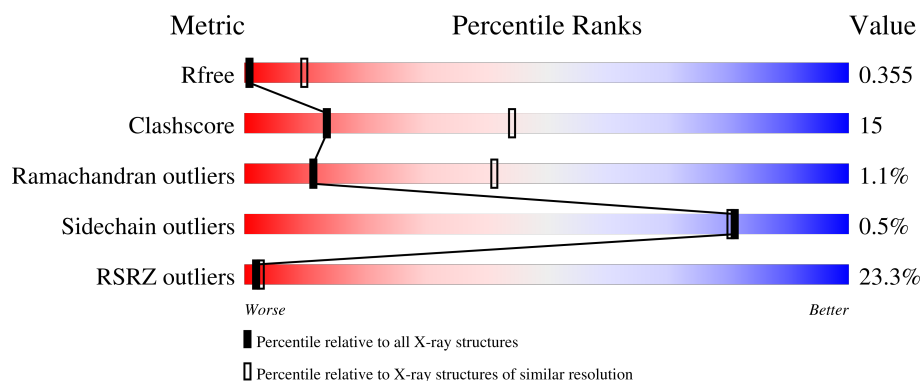
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.72 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	1182 (3.84-3.60)
Clashscore	190562	1222 (3.84-3.60)
Ramachandran outliers	187476	1178 (3.84-3.60)
Sidechain outliers	187428	1174 (3.84-3.60)
RSRZ outliers	180081	1181 (3.84-3.60)

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	21% 60% 30% 9%
1	B	296	25% 61% 28% 10%
1	C	296	15% 61% 28% 10%
1	D	296	17% 61% 29% 9%
1	E	296	27% 57% 33% 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10562 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.

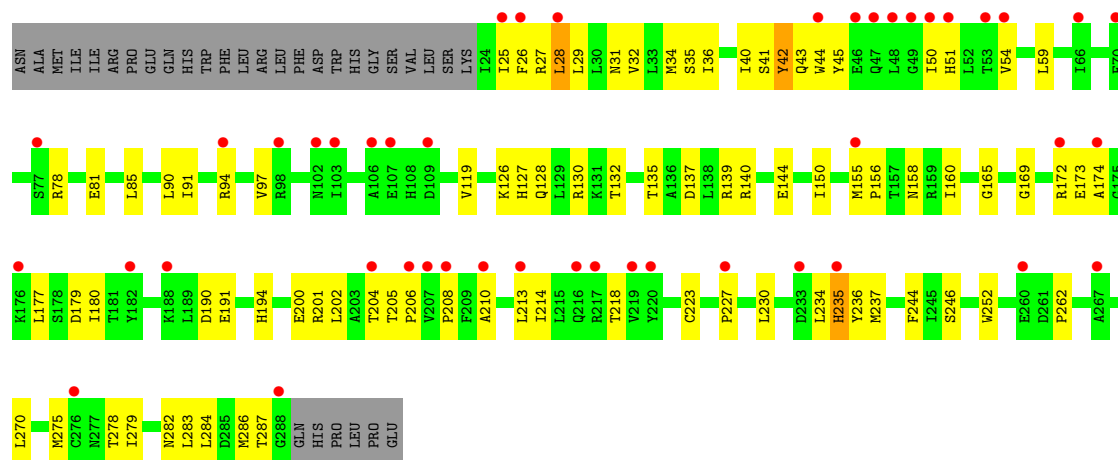
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			2117	1372	359	377	9			
1	B	266	Total	C	N	O	S	0	0	0
			2100	1364	353	375	8			
1	C	265	Total	C	N	O	S	0	0	0
			2076	1342	355	370	9			
1	D	268	Total	C	N	O	S	0	0	0
			2111	1366	359	377	9			
1	E	270	Total	C	N	O	S	0	0	0
			2149	1395	364	381	9			

There are 15 discrepancies between the modelled and reference sequences:

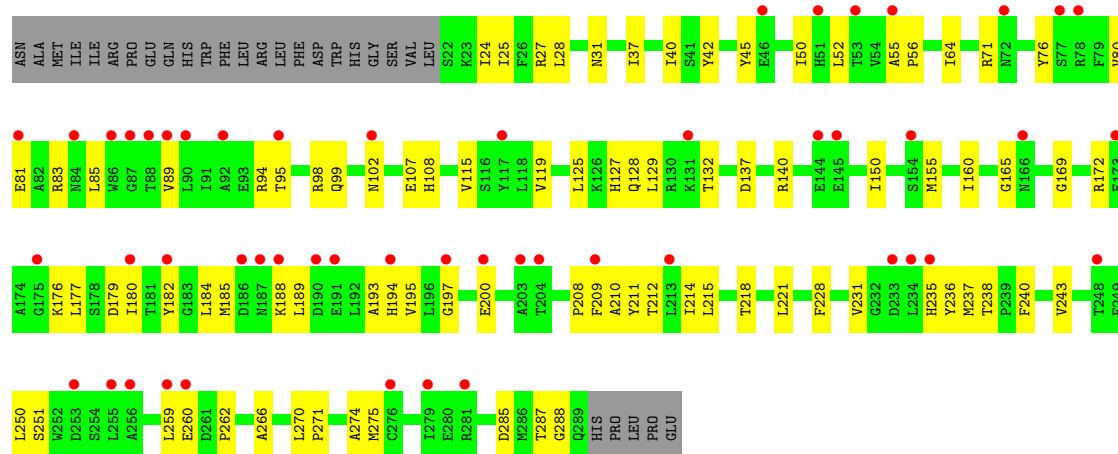
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ASN	-	expression tag	UNP W1ELP7
A	0	ALA	-	expression tag	UNP W1ELP7
A	269	ALA	ASP	engineered mutation	UNP W1ELP7
B	-1	ASN	-	expression tag	UNP W1ELP7
B	0	ALA	-	expression tag	UNP W1ELP7
B	269	ALA	ASP	engineered mutation	UNP W1ELP7
C	-1	ASN	-	expression tag	UNP W1ELP7
C	0	ALA	-	expression tag	UNP W1ELP7
C	269	ALA	ASP	engineered mutation	UNP W1ELP7
D	-1	ASN	-	expression tag	UNP W1ELP7
D	0	ALA	-	expression tag	UNP W1ELP7
D	269	ALA	ASP	engineered mutation	UNP W1ELP7
E	-1	ASN	-	expression tag	UNP W1ELP7
E	0	ALA	-	expression tag	UNP W1ELP7
E	269	ALA	ASP	engineered mutation	UNP W1ELP7

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

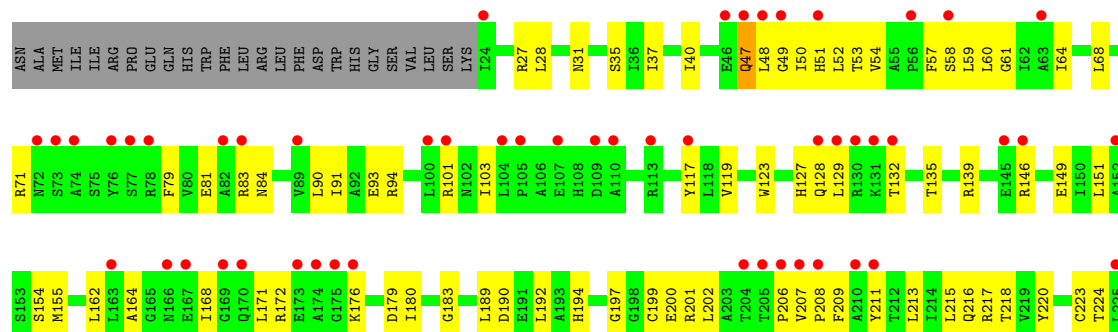
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total 3	Zn 3	0	0
2	B	1	Total 1	Zn 1	0	0
2	C	1	Total 1	Zn 1	0	0
2	D	2	Total 2	Zn 2	0	0
2	E	2	Total 2	Zn 2	0	0

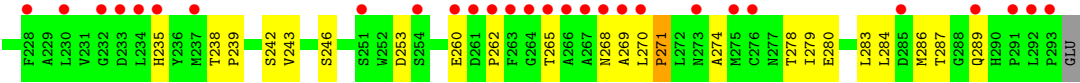


• Molecule 1: Bestrophin homolog



• 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	113.97Å 161.77Å 162.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.19 – 3.72 81.19 – 3.72	Depositor EDS
% Data completeness (in resolution range)	81.3 (81.19-3.72) 81.3 (81.19-3.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 3.67Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.289 , 0.351 0.292 , 0.355	Depositor DCC
R_{free} test set	1987 reflections (6.17%)	wwPDB-VP
Wilson B-factor (Å ²)	117.2	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 47.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.032 for -h,l,k	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	10562	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.20	0/2163	0.48	0/2946
1	B	0.23	0/2146	0.51	0/2925
1	C	0.20	0/2119	0.47	0/2887
1	D	0.21	0/2156	0.49	0/2937
1	E	0.21	0/2198	0.51	0/2995
All	All	0.21	0/10782	0.49	0/14690

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2117	0	2152	85	0
1	B	2100	0	2134	69	0
1	C	2076	0	2111	63	0
1	D	2111	0	2145	70	0
1	E	2149	0	2196	89	0
2	A	3	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2	0	0	0	0
2	E	2	0	0	0	0
All	All	10562	0	10738	311	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 15.

All (311) 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:D:271:PRO:HD2	1:D:275:MET:HE3	1.60	0.82
1:A:98:ARG:NH2	1:E:190:ASP:OD1	2.13	0.81
1:D:231:VAL:HG12	1:D:238:THR:OG1	1.79	0.81
1:D:42:TYR:OH	1:D:228:PHE:O	2.00	0.78
1:C:139:ARG:NH1	1:C:144:GLU:OE1	2.17	0.77
1:B:34:MET:SD	1:B:34:MET:N	2.57	0.76
1:B:50:ILE:HB	1:D:237:MET:HG2	1.66	0.76
1:D:235:HIS:HD1	1:D:236:TYR:HD1	1.34	0.76
1:E:155:MET:SD	1:E:155:MET:N	2.60	0.75
1:D:177:LEU:HD13	1:D:182:TYR:HB2	1.69	0.74
1:C:155:MET:SD	1:E:94:ARG:NH2	2.62	0.72
1:B:186:ASP:OD2	1:D:99:GLN:NE2	2.22	0.72
1:B:130:ARG:NH2	1:B:270:LEU:O	2.23	0.70
1:E:207:VAL:O	1:E:209:PHE:N	2.25	0.69
1:A:101:ARG:NH2	1:A:286:MET:O	2.25	0.69
1:C:31:ASN:ND2	1:C:246:SER:OG	2.26	0.69
1:B:180:ILE:HG13	1:D:180:ILE:HD12	1.74	0.69
1:C:54:VAL:HG21	1:D:55:ALA:HB1	1.73	0.68
1:E:68:LEU:HD23	1:E:215:LEU:HD13	1.75	0.68
1:D:270:LEU:HD22	1:D:275:MET:HE1	1.75	0.68
1:A:81:GLU:OE2	1:A:201:ARG:NH1	2.26	0.68
1:A:200:GLU:O	1:A:204:THR:OG1	2.11	0.67
1:D:31:ASN:HD21	1:D:243:VAL:HA	1.60	0.65
1:B:150:ILE:HD13	1:B:160:ILE:HG12	1.78	0.65
1:C:278:THR:O	1:C:282:ASN:ND2	2.28	0.65
1:E:172:ARG:NH2	1:E:179:ASP:OD1	2.30	0.65
1:C:78:ARG:NH2	1:C:202:LEU:O	2.29	0.64
1:E:117:TYR:OH	1:E:146:ARG:NH1	2.31	0.63
1:A:205:THR:HG21	1:B:83:ARG:HG3	1.80	0.63
1:E:128:GLN:NE2	1:E:200:GLU:OE2	2.29	0.63
1:A:186:ASP:OD2	1:B:99:GLN:NE2	2.31	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:LEU:HD22	1:A:275:MET:HE1	1.82	0.62
1:C:78:ARG:NH1	1:C:205:THR:O	2.33	0.62
1:A:146:ARG:NH2	1:A:149:GLU:OE1	2.25	0.61
1:A:237:MET:HG2	1:E:50:ILE:HB	1.81	0.61
1:C:194:HIS:HA	1:E:91:ILE:HD13	1.82	0.61
1:D:128:GLN:NE2	1:D:200:GLU:OE2	2.32	0.61
1:D:137:ASP:OD1	1:D:140:ARG:NH2	2.33	0.61
1:E:287:THR:OG1	1:E:289:GLN:OE1	2.14	0.61
1:C:165:GLY:O	1:C:169:GLY:N	2.32	0.61
1:A:236:TYR:HB2	1:E:50:ILE:HG22	1.82	0.61
1:A:96:LEU:HD23	1:A:118:LEU:HD11	1.82	0.61
1:A:211:TYR:OH	1:B:251:SER:O	2.12	0.61
1:B:31:ASN:ND2	1:B:223:CYS:O	2.33	0.61
1:E:101:ARG:NH2	1:E:286:MET:O	2.23	0.60
1:A:28:LEU:O	1:A:32:VAL:HG23	2.01	0.60
1:A:211:TYR:CE2	1:B:255:LEU:HB2	2.36	0.60
1:C:234:LEU:HD22	1:D:52:LEU:HD23	1.83	0.60
1:E:27:ARG:HH21	1:E:220:TYR:HA	1.66	0.60
1:C:25:ILE:HG12	1:C:28:LEU:HD22	1.85	0.59
1:B:232:GLY:O	1:B:235:HIS:NE2	2.35	0.59
1:A:282:ASN:ND2	1:E:155:MET:HE2	2.17	0.59
1:B:85:LEU:HB3	1:B:195:VAL:HG13	1.83	0.59
1:C:158:ASN:ND2	1:E:286:MET:SD	2.75	0.59
1:A:184:LEU:HD11	1:E:183:GLY:HA2	1.85	0.59
1:B:89:VAL:HG23	1:B:195:VAL:HG11	1.83	0.58
1:A:268:ASN:HD21	1:E:211:TYR:HE2	1.49	0.58
1:B:234:LEU:O	1:B:238:THR:OG1	2.20	0.58
1:D:107:GLU:OE2	1:D:176:LYS:NZ	2.32	0.58
1:C:156:PRO:O	1:C:160:ILE:HG13	2.04	0.58
1:A:23:LYS:O	1:A:27:ARG:NE	2.36	0.58
1:A:42:TYR:HA	1:A:45:TYR:CE1	2.39	0.57
1:A:231:VAL:HA	1:A:238:THR:HG21	1.85	0.57
1:A:234:LEU:HD22	1:E:51:HIS:O	2.03	0.57
1:B:127:HIS:NE2	1:B:137:ASP:OD2	2.37	0.57
1:A:85:LEU:HB3	1:A:195:VAL:HG13	1.87	0.57
1:E:239:PRO:O	1:E:243:VAL:HG12	2.05	0.57
1:B:262:PRO:O	1:B:270:LEU:HB2	2.05	0.57
1:C:43:GLN:HG3	1:C:44:TRP:CD1	2.40	0.57
1:C:201:ARG:NH1	1:E:84:ASN:OD1	2.38	0.57
1:A:126:LYS:NZ	1:A:273:ASN:OD1	2.36	0.57
1:C:155:MET:HG2	1:C:158:ASN:HB3	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:HIS:NE2	1:D:137:ASP:OD2	2.38	0.56
1:E:135:THR:HG22	1:E:151:LEU:CD1	2.34	0.56
1:B:200:GLU:OE2	1:D:94:ARG:NH2	2.28	0.56
1:C:91:ILE:HG12	1:D:197:GLY:HA3	1.87	0.55
1:C:236:TYR:HB2	1:D:50:ILE:HG22	1.89	0.55
1:A:89:VAL:HG23	1:A:195:VAL:HG11	1.87	0.55
1:B:49:GLY:O	1:D:235:HIS:HB3	2.06	0.55
1:A:211:TYR:CZ	1:B:255:LEU:HB2	2.42	0.55
1:E:27:ARG:NH2	1:E:224:THR:HG23	2.22	0.55
1:E:213:LEU:HD13	1:E:217:ARG:HD3	1.89	0.54
1:B:153:SER:OG	1:D:285:ASP:OD2	2.23	0.54
1:D:24:ILE:HD12	1:D:250:LEU:O	2.07	0.54
1:A:91:ILE:HD13	1:E:194:HIS:HA	1.89	0.53
1:B:34:MET:HA	1:B:37:ILE:HB	1.90	0.53
1:E:27:ARG:NE	1:E:220:TYR:HD1	2.06	0.53
1:E:79:PHE:CZ	1:E:269:ALA:HB3	2.44	0.53
1:E:90:LEU:HA	1:E:279:ILE:HD13	1.89	0.53
1:A:236:TYR:CD2	1:E:48:LEU:HB2	2.43	0.53
1:C:150:ILE:HD13	1:C:160:ILE:HG12	1.89	0.53
1:A:127:HIS:ND1	1:A:132:THR:OG1	2.38	0.52
1:A:138:LEU:HB3	1:A:147:VAL:HG22	1.90	0.52
1:D:155:MET:SD	1:D:155:MET:N	2.82	0.52
1:E:127:HIS:ND1	1:E:132:THR:OG1	2.33	0.52
1:D:108:HIS:HE1	1:D:287:THR:HB	1.74	0.52
1:A:217:ARG:NH2	1:B:247:TYR:OH	2.43	0.52
1:E:216:GLN:NE2	1:E:253:ASP:OD2	2.42	0.52
1:C:270:LEU:HD22	1:C:275:MET:HE1	1.92	0.52
1:E:28:LEU:HB3	1:E:243:VAL:HG23	1.92	0.51
1:E:260:GLU:N	1:E:260:GLU:OE1	2.43	0.51
1:C:28:LEU:HD23	1:C:29:LEU:HD22	1.91	0.51
1:C:127:HIS:ND1	1:C:132:THR:OG1	2.37	0.51
1:A:113:ARG:HE	1:A:167:GLU:CD	2.18	0.51
1:D:127:HIS:ND1	1:D:132:THR:OG1	2.37	0.51
1:E:135:THR:HG22	1:E:151:LEU:HD11	1.91	0.51
1:E:135:THR:O	1:E:139:ARG:HG3	2.09	0.51
1:A:103:ILE:HD12	1:A:185:MET:HE3	1.91	0.51
1:C:43:GLN:HG3	1:C:44:TRP:HD1	1.75	0.51
1:C:31:ASN:HA	1:C:34:MET:HB2	1.91	0.51
1:A:83:ARG:HE	1:E:201:ARG:HG3	1.77	0.50
1:D:80:VAL:HG13	1:D:83:ARG:HH21	1.74	0.50
1:A:108:HIS:HA	1:A:111:HIS:CG	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:THR:HG22	1:E:54:VAL:H	1.76	0.50
1:A:104:LEU:HD11	1:A:177:LEU:HG	1.92	0.50
1:B:127:HIS:ND1	1:B:132:THR:OG1	2.32	0.50
1:E:53:THR:HG22	1:E:54:VAL:N	2.27	0.50
1:A:133:ASP:OD2	1:A:135:THR:OG1	2.18	0.50
1:B:82:ALA:HB1	1:B:263:PHE:CE1	2.46	0.50
1:D:24:ILE:HG23	1:D:25:ILE:HD12	1.93	0.50
1:E:129:LEU:HD11	1:E:199:CYS:HB3	1.94	0.50
1:A:154:SER:HB3	1:B:285:ASP:OD1	2.13	0.49
1:E:189:LEU:HD23	1:E:192:LEU:HD12	1.94	0.49
1:A:113:ARG:NH2	1:A:167:GLU:OE1	2.40	0.49
1:A:135:THR:HG23	1:A:151:LEU:HD11	1.94	0.49
1:D:271:PRO:HB2	1:D:274:ALA:HB3	1.94	0.49
1:A:68:LEU:HB3	1:A:252:TRP:HD1	1.77	0.49
1:A:270:LEU:HD22	1:A:275:MET:CE	2.43	0.49
1:D:231:VAL:HG13	1:D:238:THR:HG21	1.95	0.49
1:A:22:SER:OG	1:A:23:LYS:N	2.41	0.49
1:C:50:ILE:O	1:C:51:HIS:HD2	1.95	0.49
1:D:165:GLY:O	1:D:169:GLY:N	2.35	0.49
1:C:31:ASN:O	1:C:35:SER:N	2.41	0.49
1:A:183:GLY:HA2	1:A:186:ASP:HB3	1.95	0.49
1:B:41:SER:HB2	1:B:45:TYR:CE2	2.48	0.48
1:A:154:SER:OG	1:A:155:MET:N	2.47	0.48
1:C:81:GLU:O	1:C:85:LEU:HG	2.12	0.48
1:B:213:LEU:O	1:B:217:ARG:HD3	2.13	0.48
1:E:37:ILE:HA	1:E:40:ILE:HG12	1.95	0.48
1:C:91:ILE:HD13	1:D:194:HIS:HA	1.95	0.48
1:E:48:LEU:HD23	1:E:48:LEU:H	1.79	0.48
1:E:93:GLU:HB2	1:E:279:ILE:HD11	1.95	0.48
1:A:104:LEU:HD12	1:A:171:LEU:HD13	1.96	0.48
1:C:180:ILE:HD13	1:E:180:ILE:HG13	1.96	0.48
1:A:32:VAL:O	1:A:35:SER:OG	2.25	0.48
1:A:153:SER:HB2	1:A:159:ARG:HE	1.77	0.48
1:B:52:LEU:HB3	1:B:229:ALA:HA	1.95	0.47
1:B:150:ILE:HD11	1:B:163:LEU:HD12	1.95	0.47
1:E:270:LEU:HA	1:E:270:LEU:HD23	1.50	0.47
1:D:125:LEU:O	1:D:129:LEU:HG	2.15	0.47
1:B:179:ASP:HA	1:B:182:TYR:HB3	1.96	0.47
1:C:262:PRO:O	1:C:270:LEU:HB2	2.14	0.47
1:D:177:LEU:CD1	1:D:182:TYR:HB2	2.41	0.47
1:A:45:TYR:HD2	1:A:50:ILE:HG13	1.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:PHE:O	1:C:27:ARG:HG2	2.14	0.47
1:A:211:TYR:O	1:A:215:LEU:N	2.47	0.47
1:B:108:HIS:HA	1:B:111:HIS:ND1	2.30	0.47
1:A:216:GLN:O	1:A:220:TYR:HD2	1.97	0.47
1:A:221:LEU:HB3	1:B:244:PHE:CZ	2.50	0.47
1:B:283:LEU:O	1:B:286:MET:HG3	2.15	0.47
1:D:64:ILE:HD11	1:D:218:THR:HG22	1.97	0.47
1:E:81:GLU:HB3	1:E:202:LEU:HD11	1.96	0.47
1:A:180:ILE:HG12	1:E:180:ILE:HD11	1.97	0.47
1:A:236:TYR:HD2	1:E:48:LEU:HB2	1.80	0.47
1:E:27:ARG:HH22	1:E:224:THR:HG23	1.80	0.47
1:E:60:LEU:O	1:E:64:ILE:HG13	2.15	0.47
1:E:79:PHE:HZ	1:E:269:ALA:HB3	1.80	0.47
1:A:42:TYR:HA	1:A:45:TYR:HE1	1.79	0.46
1:D:99:GLN:HB3	1:D:185:MET:HE2	1.98	0.46
1:E:31:ASN:ND2	1:E:242:SER:OG	2.48	0.46
1:E:274:ALA:O	1:E:278:THR:OG1	2.25	0.46
1:A:58:SER:HA	1:E:59:LEU:HD13	1.98	0.46
1:B:32:VAL:HG22	1:B:243:VAL:HG11	1.98	0.46
1:C:25:ILE:HG23	1:C:27:ARG:H	1.81	0.46
1:D:189:LEU:O	1:D:193:ALA:N	2.49	0.46
1:D:260:GLU:C	1:D:262:PRO:HD3	2.40	0.46
1:C:135:THR:HG22	1:C:139:ARG:HE	1.81	0.46
1:A:180:ILE:HG13	1:B:180:ILE:HG21	1.98	0.46
1:B:214:ILE:HD13	1:D:251:SER:HB3	1.97	0.46
1:D:71:ARG:NH1	1:D:212:THR:HA	2.31	0.46
1:B:239:PRO:O	1:B:243:VAL:HG22	2.16	0.46
1:B:280:GLU:O	1:B:284:LEU:HB2	2.15	0.46
1:D:214:ILE:O	1:D:218:THR:OG1	2.19	0.46
1:E:262:PRO:O	1:E:270:LEU:HD12	2.16	0.46
1:A:190:ASP:OD1	1:B:98:ARG:NH2	2.50	0.46
1:B:86:TRP:CE2	1:B:272:LEU:HD22	2.50	0.45
1:B:190:ASP:OD2	1:D:188:LYS:NZ	2.39	0.45
1:E:206:PRO:HD2	1:E:209:PHE:CE1	2.52	0.45
1:A:91:ILE:HD11	1:E:197:GLY:HA3	1.99	0.45
1:D:188:LYS:HD3	1:D:188:LYS:HA	1.76	0.45
1:C:172:ARG:HE	1:E:103:ILE:HG23	1.82	0.45
1:C:214:ILE:O	1:C:218:THR:OG1	2.25	0.45
1:A:155:MET:SD	1:B:94:ARG:NH2	2.90	0.45
1:A:245:ILE:HG12	1:E:60:LEU:HB2	1.98	0.45
1:B:52:LEU:HD12	1:B:228:PHE:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:VAL:HG21	1:C:283:LEU:HD22	1.99	0.45
1:A:115:VAL:HG21	1:A:287:THR:HG21	1.98	0.45
1:B:103:ILE:HD13	1:B:181:THR:HB	1.99	0.45
1:B:74:ALA:HB1	1:D:76:TYR:CE2	2.52	0.45
1:C:31:ASN:OD1	1:C:32:VAL:N	2.49	0.44
1:C:200:GLU:O	1:C:204:THR:OG1	2.33	0.44
1:D:89:VAL:HG23	1:D:195:VAL:HG11	1.98	0.44
1:A:268:ASN:ND2	1:E:211:TYR:HE2	2.15	0.44
1:B:166:ASN:OD1	1:D:102:ASN:ND2	2.50	0.44
1:D:27:ARG:HD3	1:D:27:ARG:HA	1.70	0.44
1:E:206:PRO:C	1:E:208:PRO:HD2	2.42	0.44
1:A:129:LEU:HD13	1:A:263:PHE:CD2	2.53	0.44
1:A:180:ILE:HG12	1:E:180:ILE:CD1	2.46	0.44
1:E:280:GLU:O	1:E:284:LEU:HG	2.18	0.44
1:D:52:LEU:HD12	1:D:228:PHE:HB3	1.99	0.44
1:A:201:ARG:HG3	1:B:83:ARG:HD2	2.00	0.44
1:D:262:PRO:O	1:D:270:LEU:HB2	2.18	0.44
1:E:154:SER:HB2	1:E:155:MET:SD	2.58	0.44
1:B:133:ASP:OD1	1:B:135:THR:OG1	2.28	0.44
1:E:90:LEU:HD12	1:E:279:ILE:HD13	1.99	0.44
1:A:32:VAL:HG22	1:A:243:VAL:HG21	1.99	0.43
1:B:79:PHE:CD1	1:B:262:PRO:HB3	2.53	0.43
1:E:146:ARG:HA	1:E:149:GLU:HG2	2.01	0.43
1:A:244:PHE:CE1	1:E:218:THR:HG23	2.53	0.43
1:D:184:LEU:HD23	1:D:184:LEU:HA	1.74	0.43
1:C:90:LEU:O	1:C:94:ARG:HB2	2.17	0.43
1:C:128:GLN:HE22	1:C:155:MET:HE1	1.83	0.43
1:C:155:MET:HG2	1:C:158:ASN:CB	2.47	0.43
1:C:90:LEU:HD13	1:C:279:ILE:HG12	2.00	0.43
1:D:37:ILE:HA	1:D:40:ILE:HG12	1.99	0.43
1:D:81:GLU:O	1:D:85:LEU:HG	2.18	0.43
1:B:159:ARG:NH2	1:D:285:ASP:O	2.51	0.43
1:E:269:ALA:O	1:E:271:PRO:HD3	2.18	0.43
1:D:208:PRO:O	1:D:211:TYR:HB2	2.18	0.43
1:E:119:VAL:O	1:E:123:TRP:HD1	2.01	0.43
1:B:156:PRO:O	1:B:160:ILE:HG13	2.19	0.42
1:A:234:LEU:HD21	1:E:53:THR:H	1.84	0.42
1:A:236:TYR:O	1:A:239:PRO:HD2	2.19	0.42
1:D:42:TYR:CE1	1:D:45:TYR:CE2	3.07	0.42
1:A:180:ILE:HG21	1:E:180:ILE:HD13	2.00	0.42
1:B:41:SER:O	1:B:44:TRP:N	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:LEU:HG	1:D:250:LEU:HD12	2.00	0.42
1:E:71:ARG:NH2	1:E:253:ASP:OD1	2.48	0.42
1:E:164:ALA:O	1:E:168:ILE:HG12	2.19	0.42
1:E:223:CYS:SG	1:E:246:SER:HA	2.59	0.42
1:E:265:THR:O	1:E:268:ASN:ND2	2.51	0.42
1:B:52:LEU:HD23	1:B:52:LEU:HA	1.69	0.42
1:B:189:LEU:HD23	1:B:189:LEU:HA	1.88	0.42
1:B:254:SER:O	1:B:257:GLU:HG2	2.19	0.42
1:C:190:ASP:OD1	1:C:191:GLU:N	2.53	0.42
1:C:208:PRO:C	1:C:210:ALA:H	2.27	0.42
1:A:52:LEU:HD21	1:B:237:MET:HE2	2.02	0.42
1:C:35:SER:HA	1:C:227:PRO:HB2	2.01	0.42
1:D:209:PHE:C	1:D:211:TYR:H	2.26	0.42
1:A:50:ILE:HB	1:B:237:MET:HG2	2.02	0.42
1:A:155:MET:HE1	1:A:200:GLU:OE2	2.20	0.42
1:C:284:LEU:HA	1:C:287:THR:HG23	2.01	0.42
1:B:140:ARG:HH22	1:B:280:GLU:CD	2.26	0.42
1:E:57:PHE:O	1:E:61:GLY:N	2.41	0.42
1:A:37:ILE:O	1:A:41:SER:OG	2.22	0.42
1:A:89:VAL:CG2	1:A:195:VAL:HG11	2.50	0.42
1:B:180:ILE:HD12	1:B:180:ILE:H	1.84	0.42
1:C:234:LEU:HD11	1:D:56:PRO:HG2	2.02	0.42
1:C:244:PHE:CE1	1:D:221:LEU:HD23	2.55	0.42
1:C:119:VAL:HG22	1:C:283:LEU:HD12	2.02	0.42
1:C:282:ASN:O	1:C:286:MET:HG3	2.20	0.42
1:E:83:ARG:CD	1:E:270:LEU:HD21	2.50	0.42
1:A:81:GLU:O	1:A:85:LEU:HG	2.20	0.41
1:D:24:ILE:HG13	1:D:250:LEU:HB3	2.01	0.41
1:D:209:PHE:C	1:D:211:TYR:N	2.78	0.41
1:E:93:GLU:HB3	1:E:283:LEU:HD11	2.01	0.41
1:E:207:VAL:C	1:E:209:PHE:N	2.78	0.41
1:C:172:ARG:NH2	1:C:179:ASP:OD1	2.53	0.41
1:C:230:LEU:HD22	1:D:56:PRO:HG3	2.02	0.41
1:C:252:TRP:CH2	1:D:215:LEU:HD21	2.56	0.41
1:E:135:THR:HG22	1:E:151:LEU:HD13	2.01	0.41
1:A:82:ALA:HB1	1:A:263:PHE:CE1	2.55	0.41
1:E:171:LEU:HD22	1:E:176:LYS:HD2	2.02	0.41
1:E:213:LEU:O	1:E:217:ARG:HB2	2.20	0.41
1:A:36:ILE:O	1:A:40:ILE:HG23	2.21	0.41
1:A:183:GLY:HA3	1:B:184:LEU:HD21	2.02	0.41
1:C:36:ILE:O	1:C:40:ILE:HG23	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:CYS:SG	1:C:246:SER:OG	2.79	0.41
1:D:172:ARG:NH2	1:D:179:ASP:OD2	2.53	0.41
1:A:180:ILE:H	1:A:180:ILE:HD12	1.85	0.41
1:D:150:ILE:HD13	1:D:160:ILE:HG12	2.03	0.41
1:E:35:SER:OG	1:E:239:PRO:HB3	2.20	0.41
1:C:137:ASP:OD1	1:C:140:ARG:NH2	2.46	0.41
1:E:83:ARG:HD3	1:E:270:LEU:HD21	2.03	0.41
1:A:272:LEU:HD23	1:A:275:MET:SD	2.61	0.41
1:B:97:VAL:HG21	1:B:283:LEU:HG	2.03	0.41
1:A:200:GLU:OE2	1:B:94:ARG:NH2	2.46	0.41
1:B:28:LEU:HG	1:B:247:TYR:HD1	1.85	0.41
1:C:41:SER:C	1:C:43:GLN:N	2.79	0.41
1:C:126:LYS:HD3	1:C:130:ARG:HG3	2.02	0.41
1:C:172:ARG:HA	1:C:177:LEU:HD11	2.03	0.41
1:C:234:LEU:O	1:C:235:HIS:C	2.64	0.41
1:E:47:GLN:HB2	1:E:48:LEU:H	1.73	0.41
1:A:98:ARG:HG3	1:E:162:LEU:HD12	2.02	0.41
1:C:59:LEU:HD13	1:E:58:SER:HA	2.02	0.41
1:C:234:LEU:O	1:C:237:MET:N	2.54	0.41
1:D:42:TYR:CZ	1:D:45:TYR:CE2	3.09	0.41
1:E:52:LEU:HD23	1:E:52:LEU:HA	1.85	0.41
1:E:238:THR:N	1:E:239:PRO:HD2	2.36	0.41
1:A:60:LEU:HD21	1:B:244:PHE:CD2	2.56	0.40
1:B:126:LYS:HG3	1:B:127:HIS:N	2.36	0.40
1:D:95:THR:HB	1:D:98:ARG:HH21	1.86	0.40
1:A:134:PRO:O	1:A:138:LEU:HD13	2.20	0.40
1:B:125:LEU:O	1:B:129:LEU:HG	2.20	0.40
1:C:42:TYR:O	1:C:45:TYR:HD2	2.03	0.40
1:D:89:VAL:CG2	1:D:195:VAL:HG11	2.51	0.40
1:B:207:VAL:HG22	1:B:260:GLU:OE2	2.21	0.40
1:D:95:THR:HA	1:D:98:ARG:HB3	2.03	0.40
1:D:115:VAL:O	1:D:119:VAL:HG23	2.21	0.40
1:B:89:VAL:CG2	1:B:195:VAL:HG11	2.48	0.40
1:D:237:MET:SD	1:D:240:PHE:HD1	2.45	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%)	256 (96%)	8 (3%)	2 (1%)	16	47
1	B	264/296 (89%)	251 (95%)	13 (5%)	0	100	100
1	C	263/296 (89%)	250 (95%)	7 (3%)	6 (2%)	5	30
1	D	266/296 (90%)	254 (96%)	9 (3%)	3 (1%)	11	41
1	E	268/296 (90%)	252 (94%)	12 (4%)	4 (2%)	8	36
All	All	1327/1480 (90%)	1263 (95%)	49 (4%)	15 (1%)	11	41

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	235	HIS
1	D	266	ALA
1	E	235	HIS
1	E	271	PRO
1	C	28	LEU
1	C	42	TYR
1	C	173	GLU
1	E	47	GLN
1	E	49	GLY
1	A	235	HIS
1	C	174	ALA
1	D	210	ALA
1	A	48	LEU
1	C	206	PRO
1	D	288	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	228/258 (88%)	228 (100%)	0	100	100
1	B	226/258 (88%)	222 (98%)	4 (2%)	51	67
1	C	222/258 (86%)	221 (100%)	1 (0%)	81	80
1	D	227/258 (88%)	226 (100%)	1 (0%)	84	81
1	E	234/258 (91%)	234 (100%)	0	100	100
All	All	1137/1290 (88%)	1131 (100%)	6 (0%)	81	80

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	48	LEU
1	B	177	LEU
1	B	270	LEU
1	B	284	LEU
1	C	213	LEU
1	D	259	LEU

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

Mol	Chain	Res	Type
1	C	51	HIS
1	C	216	GLN
1	C	235	HIS
1	D	43	GLN
1	D	51	HIS
1	D	108	HIS
1	E	51	HIS
1	E	268	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](#)

Of 9 ligands modelled in this entry, 9 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%)	1.62	62 (23%) 2 3	82, 114, 155, 182	0
1	B	266/296 (89%)	1.55	74 (27%) 1 2	74, 105, 153, 172	0
1	C	265/296 (89%)	1.32	45 (16%) 4 6	73, 107, 150, 175	0
1	D	268/296 (90%)	1.25	51 (19%) 3 4	78, 105, 147, 186	0
1	E	270/296 (91%)	1.81	80 (29%) 1 2	81, 116, 164, 193	0
All	All	1337/1480 (90%)	1.51	312 (23%) 2 3	73, 110, 155, 193	0

All (312) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	210	ALA	14.0
1	C	49	GLY	12.5
1	C	47	GLN	11.8
1	E	175	GLY	8.9
1	E	145	GLU	8.9
1	A	212	THR	8.4
1	A	209	PHE	8.3
1	E	173	GLU	8.3
1	A	24	ILE	8.0
1	E	113	ARG	8.0
1	E	76	TYR	7.5
1	E	109	ASP	7.5
1	E	232	GLY	7.2
1	C	48	LEU	7.0
1	C	53	THR	7.0
1	E	170	GLN	7.0
1	A	211	TYR	7.0
1	E	131	LYS	6.8
1	A	51	HIS	6.6
1	C	217	ARG	6.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	26	PHE	6.4
1	E	167	GLU	6.4
1	C	220	TYR	6.4
1	C	46	GLU	6.2
1	E	146	ARG	5.9
1	E	132	THR	5.8
1	B	267	ALA	5.7
1	E	176	LYS	5.6
1	E	77	SER	5.5
1	E	174	ALA	5.4
1	A	73	SER	5.4
1	D	145	GLU	5.4
1	A	52	LEU	5.4
1	E	130	ARG	5.3
1	A	262	PRO	5.3
1	E	204	THR	5.2
1	C	216	GLN	5.2
1	D	281	ARG	5.2
1	A	53	THR	5.2
1	C	51	HIS	5.1
1	E	269	ALA	5.1
1	A	33	LEU	5.0
1	D	46	GLU	5.0
1	E	233	ASP	5.0
1	B	92	ALA	5.0
1	D	77	SER	4.9
1	E	211	TYR	4.9
1	A	76	TYR	4.8
1	D	188	LYS	4.8
1	A	208	PRO	4.7
1	B	95	THR	4.7
1	E	292	LEU	4.7
1	E	117	TYR	4.7
1	A	101	ARG	4.7
1	C	54	VAL	4.7
1	E	234	LEU	4.6
1	E	208	PRO	4.5
1	B	167	GLU	4.5
1	B	97	VAL	4.5
1	B	165	GLY	4.5
1	A	77	SER	4.5
1	D	51	HIS	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	293	PRO	4.4
1	A	45	TYR	4.4
1	E	291	PRO	4.4
1	C	98	ARG	4.4
1	A	22	SER	4.4
1	E	276	CYS	4.4
1	A	235	HIS	4.4
1	A	25	ILE	4.3
1	B	203	ALA	4.3
1	B	81	GLU	4.3
1	E	110	ALA	4.3
1	A	44	TRP	4.2
1	D	88	THR	4.2
1	B	265	THR	4.2
1	D	81	GLU	4.2
1	E	74	ALA	4.2
1	C	288	GLY	4.2
1	B	211	TYR	4.2
1	C	50	ILE	4.2
1	D	253	ASP	4.1
1	B	197	GLY	4.1
1	D	235	HIS	4.1
1	B	48	LEU	4.1
1	A	57	PHE	4.0
1	A	258	GLU	4.0
1	D	144	GLU	4.0
1	B	236	TYR	4.0
1	B	269	ALA	4.0
1	D	260	GLU	3.9
1	A	55	ALA	3.9
1	B	210	ALA	3.9
1	B	283	LEU	3.9
1	C	260	GLU	3.9
1	C	106	ALA	3.9
1	D	84	ASN	3.8
1	B	258	GLU	3.8
1	E	48	LEU	3.7
1	B	112	ARG	3.7
1	E	72	ASN	3.7
1	C	188	LYS	3.7
1	E	235	HIS	3.7
1	E	166	ASN	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	207	VAL	3.6
1	D	203	ALA	3.6
1	A	102	ASN	3.6
1	D	191	GLU	3.6
1	A	32	VAL	3.6
1	A	106	ALA	3.6
1	B	240	PHE	3.6
1	E	237	MET	3.5
1	E	163	LEU	3.5
1	C	233	ASP	3.5
1	D	72	ASN	3.5
1	C	77	SER	3.5
1	D	186	ASP	3.4
1	E	51	HIS	3.4
1	E	266	ALA	3.4
1	A	93	GLU	3.4
1	E	104	LEU	3.4
1	C	70	PHE	3.4
1	E	73	SER	3.3
1	E	101	ARG	3.3
1	E	261	ASP	3.3
1	A	288	GLY	3.3
1	D	90	LEU	3.3
1	B	205	THR	3.2
1	B	268	ASN	3.2
1	A	75	SER	3.2
1	B	204	THR	3.2
1	A	260	GLU	3.2
1	B	235	HIS	3.2
1	E	264	GLY	3.2
1	B	266	ALA	3.2
1	E	267	ALA	3.2
1	A	213	LEU	3.2
1	A	270	LEU	3.1
1	D	194	HIS	3.1
1	A	204	THR	3.1
1	E	128	GLN	3.1
1	E	275	MET	3.1
1	B	40	ILE	3.1
1	B	36	ILE	3.1
1	D	209	PHE	3.1
1	C	94	ARG	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	152	ALA	3.0
1	B	247	TYR	3.0
1	B	233	ASP	3.0
1	B	61	GLY	3.0
1	A	207	VAL	3.0
1	C	276	CYS	3.0
1	D	213	LEU	3.0
1	E	78	ARG	3.0
1	D	248	THR	3.0
1	B	207	VAL	3.0
1	A	267	ALA	3.0
1	D	259	LEU	2.9
1	C	210	ALA	2.9
1	E	263	PHE	2.9
1	D	190	ASP	2.9
1	A	273	ASN	2.9
1	D	256	ALA	2.9
1	B	52	LEU	2.9
1	B	282	ASN	2.9
1	E	47	GLN	2.9
1	E	49	GLY	2.9
1	C	267	ALA	2.9
1	A	29	LEU	2.9
1	C	28	LEU	2.9
1	D	279	ILE	2.8
1	D	204	THR	2.8
1	A	105	PRO	2.8
1	B	162	LEU	2.8
1	A	179	ASP	2.8
1	C	174	ALA	2.8
1	B	260	GLU	2.8
1	E	273	ASN	2.8
1	B	287	THR	2.8
1	D	276	CYS	2.8
1	B	200	GLU	2.8
1	E	210	ALA	2.8
1	D	255	LEU	2.8
1	D	154	SER	2.8
1	E	206	PRO	2.8
1	B	274	ALA	2.8
1	B	90	LEU	2.7
1	D	234	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	155	MET	2.7
1	B	96	LEU	2.7
1	E	225	LEU	2.7
1	A	214	ILE	2.7
1	B	185	MET	2.7
1	D	87	GLY	2.7
1	E	270	LEU	2.7
1	E	63	ALA	2.7
1	C	204	THR	2.7
1	E	82	ALA	2.7
1	B	54	VAL	2.7
1	A	112	ARG	2.7
1	A	66	ILE	2.7
1	A	74	ALA	2.7
1	A	184	LEU	2.7
1	E	56	PRO	2.6
1	E	205	THR	2.6
1	E	46	GLU	2.6
1	E	105	PRO	2.6
1	C	26	PHE	2.6
1	B	100	LEU	2.6
1	B	170	GLN	2.6
1	E	289	GLN	2.6
1	E	89	VAL	2.6
1	B	173	GLU	2.6
1	A	275	MET	2.6
1	D	92	ALA	2.6
1	B	195	VAL	2.5
1	C	66	ILE	2.5
1	A	98	ARG	2.5
1	E	285	ASP	2.5
1	B	288	GLY	2.5
1	B	51	HIS	2.5
1	C	172	ARG	2.5
1	C	235	HIS	2.5
1	A	118	LEU	2.5
1	D	173	GLU	2.5
1	C	227	PRO	2.5
1	B	44	TRP	2.5
1	C	176	LYS	2.5
1	A	193	ALA	2.5
1	E	254	SER	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	131	LYS	2.4
1	D	166	ASN	2.4
1	B	49	GLY	2.4
1	C	44	TRP	2.4
1	C	103	ILE	2.4
1	B	166	ASN	2.4
1	C	219	VAL	2.4
1	C	109	ASP	2.4
1	B	91	ILE	2.4
1	B	270	LEU	2.4
1	A	84	ASN	2.4
1	C	102	ASN	2.4
1	E	265	THR	2.4
1	A	109	ASP	2.3
1	A	216	GLN	2.3
1	C	208	PRO	2.3
1	E	260	GLU	2.3
1	B	271	PRO	2.3
1	E	129	LEU	2.3
1	B	180	ILE	2.3
1	E	228	PHE	2.3
1	D	233	ASP	2.3
1	B	208	PRO	2.3
1	E	169	GLY	2.3
1	E	262	PRO	2.3
1	A	268	ASN	2.3
1	B	248	THR	2.3
1	C	107	GLU	2.3
1	B	239	PRO	2.3
1	D	86	TRP	2.3
1	D	55	ALA	2.3
1	D	95	THR	2.2
1	D	180	ILE	2.2
1	B	47	GLN	2.2
1	B	50	ILE	2.2
1	D	200	GLU	2.2
1	D	175	GLY	2.2
1	B	249	PHE	2.2
1	D	102	ASN	2.2
1	E	24	ILE	2.2
1	A	257	GLU	2.2
1	B	214	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	257	GLU	2.2
1	C	25	ILE	2.2
1	A	155	MET	2.1
1	A	42	TYR	2.1
1	D	117	TYR	2.1
1	D	78	ARG	2.1
1	B	79	PHE	2.1
1	C	182	TYR	2.1
1	D	182	TYR	2.1
1	D	197	GLY	2.1
1	A	110	ALA	2.1
1	B	72	ASN	2.1
1	D	89	VAL	2.1
1	A	163	LEU	2.1
1	B	253	ASP	2.1
1	E	230	LEU	2.1
1	B	144	GLU	2.1
1	B	218	THR	2.1
1	E	152	ALA	2.1
1	B	45	TYR	2.1
1	A	206	PRO	2.1
1	A	233	ASP	2.1
1	C	206	PRO	2.1
1	D	53	THR	2.1
1	B	281	ARG	2.1
1	E	83	ARG	2.1
1	E	58	SER	2.1
1	E	251	SER	2.1
1	C	207	VAL	2.1
1	E	268	ASN	2.1
1	C	213	LEU	2.1
1	E	100	LEU	2.1
1	B	155	MET	2.1
1	A	150	ILE	2.0
1	E	107	GLU	2.0
1	B	101	ARG	2.0
1	D	187	ASN	2.0
1	B	169	GLY	2.0
1	A	205	THR	2.0
1	B	259	LEU	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($\text{\AA}^2$)	Q<0.9
2	ZN	A	303	1/1	0.89	0.11	134,134,134,134	0
2	ZN	C	301	1/1	0.89	0.11	104,104,104,104	0
2	ZN	A	301	1/1	0.93	0.12	119,119,119,119	0
2	ZN	D	301	1/1	0.93	0.09	101,101,101,101	0
2	ZN	E	301	1/1	0.95	0.09	104,104,104,104	0
2	ZN	E	302	1/1	0.96	0.06	150,150,150,150	0
2	ZN	B	301	1/1	0.97	0.05	108,108,108,108	0
2	ZN	A	302	1/1	0.98	0.04	96,96,96,96	0
2	ZN	D	302	1/1	0.98	0.15	123,123,123,123	0

6.5 Other polymers [i](#)

There are no such residues in this entry.