



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:31 PM UTC

PDB ID : 6JLF / pdb_00006jlf
Title : Crystal structure of a bacterial Bestrophin homolog from *Klebsiella pneumoniae* D179A mutation - HR
Authors : Kittredge, A.; Chen, S.; Yang, T.
Deposited on : 2019-03-05
Resolution : 2.55 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

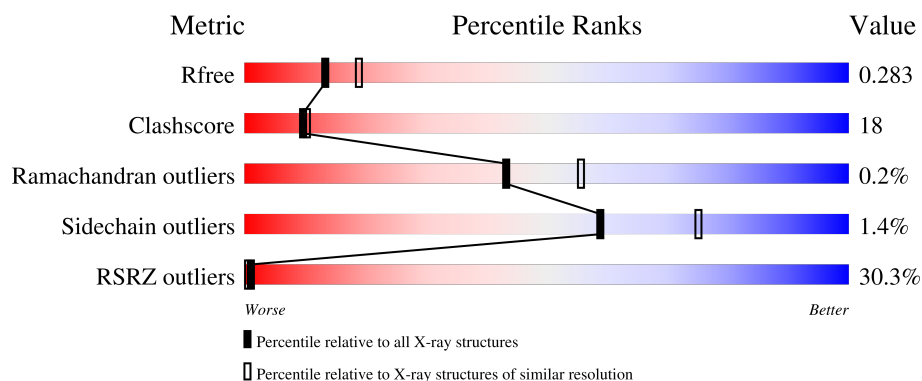
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	297	28% 59% 30% 10%
1	B	297	38% 62% 28% 10%
1	C	297	23% 70% 18% 10%
1	D	297	24% 58% 31% 10%
1	E	297	23% 63% 27% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10541 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	267	Total	C	N	O	S	0	0	0
			2102	1364	354	375	9			
1	B	266	Total	C	N	O	S	0	0	0
			2084	1357	346	372	9			
1	C	268	Total	C	N	O	S	0	0	0
			2100	1362	355	374	9			
1	D	268	Total	C	N	O	S	0	0	0
			2093	1358	351	375	9			
1	E	266	Total	C	N	O	S	0	0	0
			2098	1361	355	373	9			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP W1ELP7
A	-1	ASN	-	expression tag	UNP W1ELP7
A	0	ALA	-	expression tag	UNP W1ELP7
A	179	ALA	ASP	engineered mutation	UNP W1ELP7
B	-2	SER	-	expression tag	UNP W1ELP7
B	-1	ASN	-	expression tag	UNP W1ELP7
B	0	ALA	-	expression tag	UNP W1ELP7
B	179	ALA	ASP	engineered mutation	UNP W1ELP7
C	-2	SER	-	expression tag	UNP W1ELP7
C	-1	ASN	-	expression tag	UNP W1ELP7
C	0	ALA	-	expression tag	UNP W1ELP7
C	179	ALA	ASP	engineered mutation	UNP W1ELP7
D	-2	SER	-	expression tag	UNP W1ELP7
D	-1	ASN	-	expression tag	UNP W1ELP7
D	0	ALA	-	expression tag	UNP W1ELP7
D	179	ALA	ASP	engineered mutation	UNP W1ELP7
E	-2	SER	-	expression tag	UNP W1ELP7
E	-1	ASN	-	expression tag	UNP W1ELP7
E	0	ALA	-	expression tag	UNP W1ELP7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	179	ALA	ASP	engineered mutation	UNP W1ELP7

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

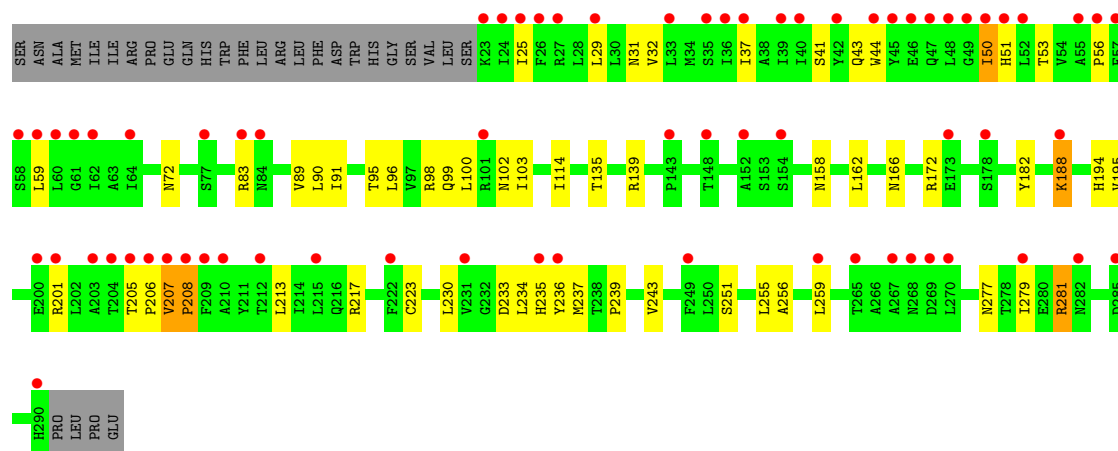
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Zn 3 3	0	0
2	B	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0
2	E	2	Total Zn 2 2	0	0

- Molecule 3 is water.

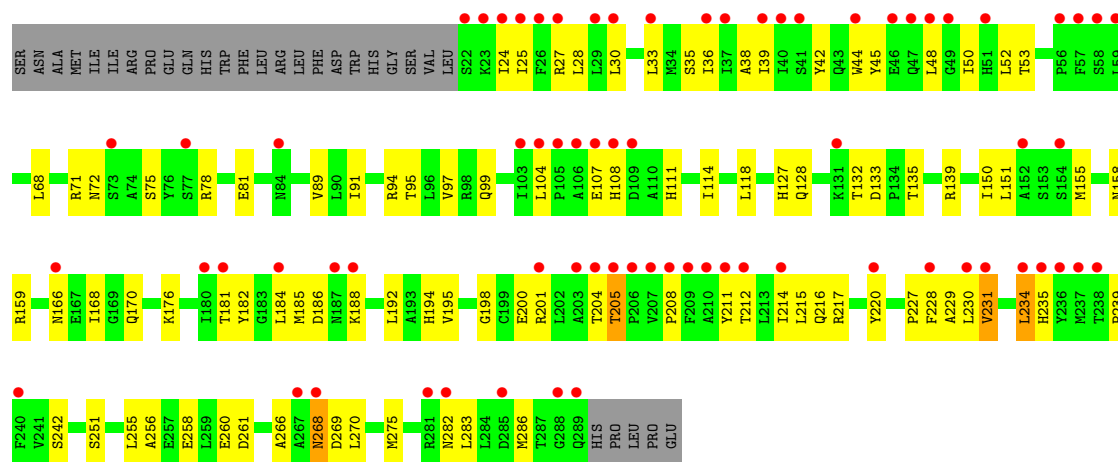
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	10	Total O 10 10	0	0
3	B	5	Total O 5 5	0	0
3	C	9	Total O 9 9	0	0
3	D	10	Total O 10 10	0	0
3	E	19	Total O 19 19	0	0

- Molecule 1: Bestrophin homolog

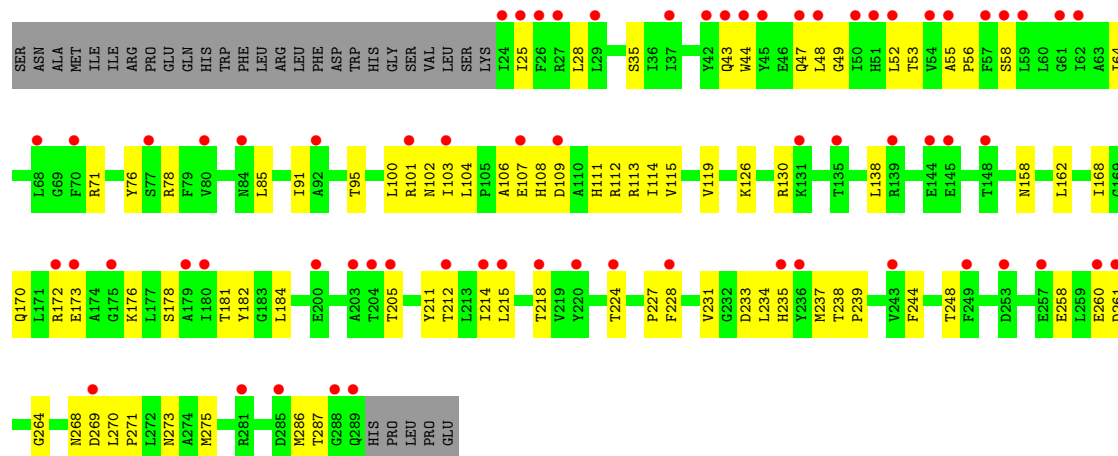




• Molecule 1: Bestrophin homolog



• 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	113.97Å 159.47Å 161.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.19 – 2.55 93.19 – 2.55	Depositor EDS
% Data completeness (in resolution range)	98.2 (93.19-2.55) 98.2 (93.19-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.55Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.230 , 0.276 0.238 , 0.283	Depositor DCC
R_{free} test set	1999 reflections (2.06%)	wwPDB-VP
Wilson B-factor (Å ²)	74.0	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 61.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for -h,l,k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10541	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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	0.52	0/2148	0.73	0/2927
1	B	0.49	0/2130	0.65	0/2905
1	C	0.57	0/2146	0.81	4/2926 (0.1%)
1	D	0.52	0/2138	0.70	1/2915 (0.0%)
1	E	0.55	0/2143	0.73	0/2920
All	All	0.53	0/10705	0.73	5/14593 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	206	PRO	CA-C-N	-9.86	114.03	120.24
1	C	206	PRO	C-N-CA	-9.86	114.03	120.24
1	C	206	PRO	N-CA-C	-8.86	97.39	111.03
1	C	235	HIS	N-CA-C	6.97	118.52	111.07
1	D	205	THR	CA-CB-OG1	5.14	117.31	109.60

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	2102	0	2133	92	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2084	0	2111	88	0
1	C	2100	0	2123	65	0
1	D	2093	0	2115	109	0
1	E	2098	0	2140	91	0
2	A	3	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
3	A	10	0	0	1	0
3	B	5	0	0	1	0
3	C	9	0	0	1	0
3	D	10	0	0	8	0
3	E	19	0	0	1	0
All	All	10541	0	10622	374	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 18.

All (374) 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:207:VAL:HG21	1:E:76:TYR:CE1	1.64	1.32
1:B:211:TYR:CE1	1:D:255:LEU:HD21	1.66	1.29
1:B:211:TYR:CE1	1:D:255:LEU:CD2	2.23	1.20
1:C:83:ARG:HD3	1:D:201:ARG:CG	1.74	1.17
1:C:207:VAL:HG23	1:C:208:PRO:HD3	1.26	1.12
1:C:207:VAL:HG21	1:E:76:TYR:HE1	0.94	1.10
1:E:107:GLU:HG3	1:E:176:LYS:NZ	1.75	1.02
1:C:207:VAL:CG2	1:E:76:TYR:HE1	1.73	1.00
1:C:213:LEU:HD23	1:C:217:ARG:HH21	1.28	0.98
1:A:205:THR:HG21	1:B:83:ARG:HD2	1.46	0.98
1:C:83:ARG:HD3	1:D:201:ARG:HG3	1.46	0.97
1:D:270:LEU:HB3	1:D:275:MET:HE1	1.47	0.96
1:A:33:LEU:O	1:A:36:ILE:HG13	1.63	0.96
1:B:211:TYR:CD1	1:D:255:LEU:HD21	1.99	0.96
1:C:59:LEU:HD13	1:E:58:SER:HA	1.49	0.93
1:E:107:GLU:CG	1:E:176:LYS:NZ	2.31	0.91
1:E:211:TYR:O	1:E:215:LEU:HD23	1.72	0.90
1:B:211:TYR:CE1	1:D:255:LEU:HD23	2.04	0.89
1:B:210:ALA:O	1:B:214:ILE:HG12	1.71	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:VAL:CG2	1:C:208:PRO:HD3	2.05	0.85
1:E:107:GLU:CG	1:E:176:LYS:HZ1	1.89	0.84
1:B:254:SER:HA	1:B:257:GLU:HG2	1.58	0.83
1:B:211:TYR:CD1	1:D:255:LEU:CD2	2.60	0.82
1:D:104:LEU:HD13	1:D:107:GLU:HB2	1.63	0.81
1:A:234:LEU:HD21	1:E:56:PRO:HG2	1.63	0.80
1:E:258:GLU:OE2	1:E:268:ASN:ND2	2.16	0.79
1:B:71:ARG:HH12	1:B:212:THR:HG22	1.49	0.78
1:C:83:ARG:HD3	1:D:201:ARG:HG2	1.67	0.77
1:C:83:ARG:HD3	1:D:201:ARG:CD	2.13	0.77
1:B:71:ARG:NH2	1:B:253:ASP:OD1	2.19	0.76
1:D:155:MET:HG2	1:D:158:ASN:HB2	1.66	0.75
1:D:212:THR:O	1:D:216:GLN:N	2.18	0.75
1:A:33:LEU:HA	1:A:36:ILE:CG1	2.17	0.75
1:A:279:ILE:O	1:A:283:LEU:HD12	1.87	0.74
1:A:212:THR:HA	1:A:215:LEU:HD12	1.68	0.74
1:B:211:TYR:CZ	1:D:255:LEU:HD21	2.22	0.74
1:E:107:GLU:CD	1:E:176:LYS:HZ3	1.96	0.73
1:C:83:ARG:CD	1:D:201:ARG:HD2	2.18	0.73
1:B:27:ARG:NH2	1:B:224:THR:HG23	2.02	0.73
1:C:32:VAL:HG12	1:C:243:VAL:HG11	1.71	0.72
1:E:107:GLU:HG3	1:E:176:LYS:HZ1	1.46	0.72
1:E:107:GLU:CG	1:E:176:LYS:HZ3	2.03	0.71
1:C:91:ILE:O	1:C:95:THR:HG23	1.92	0.70
1:B:83:ARG:HG2	1:B:270:LEU:HD21	1.74	0.70
1:A:127:HIS:HD1	1:A:132:THR:HG1	1.38	0.70
1:C:59:LEU:HD13	1:E:58:SER:CA	2.22	0.70
1:E:231:VAL:HA	1:E:238:THR:HG21	1.74	0.69
1:D:198:GLY:HA2	1:D:201:ARG:NH1	2.06	0.69
1:A:101:ARG:HE	1:E:162:LEU:HD21	1.58	0.69
1:B:91:ILE:O	1:B:95:THR:HG23	1.92	0.68
1:C:53:THR:HG23	1:C:56:PRO:CD	2.23	0.67
1:B:44:TRP:O	1:B:46:GLU:N	2.27	0.67
1:A:216:GLN:HG2	1:A:253:ASP:OD2	1.94	0.67
1:D:211:TYR:OH	3:D:401:HOH:O	2.12	0.67
1:D:52:LEU:HB3	1:D:229:ALA:HA	1.76	0.67
1:E:112:ARG:NH1	1:E:287:THR:HB	2.10	0.67
1:B:127:HIS:ND1	1:B:132:THR:OG1	2.28	0.66
1:E:53:THR:HB	1:E:56:PRO:HD3	1.76	0.66
1:B:214:ILE:HD12	1:D:251:SER:HB3	1.76	0.66
1:D:186:ASP:OD2	3:D:402:HOH:O	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:ARG:CD	1:D:201:ARG:CD	2.73	0.65
1:E:107:GLU:HG3	1:E:176:LYS:CE	2.26	0.65
1:D:104:LEU:HD12	1:D:104:LEU:O	1.96	0.65
1:A:127:HIS:ND1	1:A:132:THR:OG1	2.29	0.65
1:D:91:ILE:O	1:D:95:THR:HG23	1.97	0.65
1:D:39:ILE:HD11	1:D:239:PRO:HD3	1.78	0.65
1:B:135:THR:HG22	1:B:151:LEU:HD21	1.79	0.64
1:B:211:TYR:HE1	1:D:255:LEU:HD23	1.55	0.64
1:D:104:LEU:HD12	1:D:111:HIS:HE2	1.61	0.64
1:A:33:LEU:HA	1:A:36:ILE:HG12	1.78	0.64
1:A:109:ASP:OD2	1:A:113:ARG:NH1	2.31	0.63
1:A:207:VAL:HG11	1:A:260:GLU:CD	2.23	0.63
1:C:90:LEU:HD22	1:C:279:ILE:HB	1.80	0.63
1:C:31:ASN:ND2	1:C:223:CYS:O	2.30	0.63
1:D:72:ASN:ND2	1:D:256:ALA:HB2	2.12	0.63
1:D:71:ARG:HD3	1:D:215:LEU:HD12	1.79	0.62
1:D:282:ASN:O	1:D:286:MET:HG3	1.99	0.62
1:D:42:TYR:HE2	1:D:235:HIS:CE1	2.18	0.62
1:C:83:ARG:HD2	1:D:201:ARG:HD2	1.80	0.61
1:C:102:ASN:ND2	1:D:166:ASN:OD1	2.33	0.61
1:A:210:ALA:C	1:A:211:TYR:HD1	2.07	0.61
1:A:100:LEU:HA	1:A:185:MET:HE1	1.82	0.61
1:D:266:ALA:HB3	1:D:269:ASP:OD2	2.01	0.61
1:A:126:LYS:NZ	1:A:273:ASN:OD1	2.34	0.61
1:A:33:LEU:C	1:A:36:ILE:HG13	2.26	0.61
1:A:233:ASP:HB3	1:E:53:THR:OG1	2.00	0.61
1:B:27:ARG:NH2	1:B:220:TYR:O	2.34	0.61
1:A:252:TRP:CE3	1:E:214:ILE:HD11	2.36	0.60
1:B:213:LEU:HD22	1:B:216:GLN:HB3	1.83	0.60
1:C:207:VAL:HG23	1:C:208:PRO:CD	2.18	0.60
1:A:23:LYS:O	1:A:27:ARG:NH1	2.34	0.60
1:C:51:HIS:CE1	1:E:235:HIS:CG	2.90	0.60
1:A:135:THR:HG23	1:A:151:LEU:HD11	1.84	0.59
1:A:212:THR:HG23	1:A:257:GLU:OE2	2.02	0.59
1:C:277:ASN:O	1:C:281:ARG:HD3	2.02	0.59
1:E:107:GLU:HG2	1:E:176:LYS:HZ1	1.67	0.59
1:B:89:VAL:CG1	1:B:195:VAL:HG11	2.33	0.59
1:B:215:LEU:HA	1:B:218:THR:HG22	1.83	0.59
1:C:162:LEU:HD11	1:E:101:ARG:HG2	1.83	0.59
1:B:147:VAL:O	1:B:151:LEU:HD13	2.03	0.58
1:C:53:THR:HG21	1:E:233:ASP:OD2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:112:ARG:NH2	3:E:401:HOH:O	2.35	0.58
1:E:211:TYR:O	1:E:215:LEU:CD2	2.47	0.58
1:C:205:THR:O	1:C:205:THR:HG22	2.03	0.58
1:B:94:ARG:NH1	3:B:401:HOH:O	2.18	0.58
1:E:25:ILE:H	1:E:25:ILE:HD12	1.69	0.58
1:C:96:LEU:HB2	1:C:188:LYS:HG2	1.84	0.58
1:C:230:LEU:O	1:C:234:LEU:HD23	2.03	0.58
1:A:194:HIS:HA	1:B:91:ILE:HD13	1.86	0.58
1:B:71:ARG:C	1:B:71:ARG:HD2	2.29	0.58
1:E:47:GLN:CD	1:E:48:LEU:HD12	2.29	0.58
1:B:71:ARG:NH1	1:B:212:THR:HG22	2.18	0.57
1:C:53:THR:HG23	1:C:56:PRO:HD3	1.86	0.57
1:B:24:ILE:HD11	1:B:250:LEU:HB3	1.85	0.57
1:E:264:GLY:HA3	1:E:269:ASP:OD2	2.04	0.57
1:A:213:LEU:HG	1:A:214:ILE:H	1.70	0.57
1:B:53:THR:H	1:D:234:LEU:HD23	1.69	0.57
1:B:90:LEU:HD21	1:B:94:ARG:NH2	2.20	0.56
1:C:103:ILE:HD11	1:D:182:TYR:CE2	2.40	0.56
1:A:204:THR:O	1:A:206:PRO:HD3	2.05	0.56
1:A:252:TRP:CH2	1:E:215:LEU:HD21	2.41	0.56
1:B:37:ILE:O	1:B:41:SER:OG	2.23	0.56
1:B:194:HIS:HA	1:D:91:ILE:HD13	1.86	0.56
1:A:33:LEU:O	1:A:36:ILE:CG1	2.48	0.56
1:A:205:THR:CG2	1:B:83:ARG:HH11	2.19	0.56
1:B:72:ASN:OD1	1:B:256:ALA:HB2	2.05	0.56
1:B:100:LEU:HD11	1:B:114:ILE:HD13	1.88	0.56
1:A:155:MET:HE1	1:B:94:ARG:NH2	2.20	0.55
1:D:42:TYR:HA	1:D:45:TYR:CD1	2.41	0.55
1:A:212:THR:CA	1:A:215:LEU:HD12	2.37	0.55
1:C:91:ILE:HD13	1:D:194:HIS:HA	1.88	0.55
1:C:158:ASN:OD1	1:E:286:MET:HE2	2.07	0.55
1:E:91:ILE:O	1:E:95:THR:HG23	2.07	0.55
1:C:37:ILE:O	1:C:41:SER:OG	2.23	0.54
1:B:108:HIS:HA	1:B:111:HIS:CD2	2.42	0.54
1:E:100:LEU:HD11	1:E:114:ILE:HD13	1.88	0.54
1:D:78:ARG:NH2	1:D:205:THR:O	2.41	0.54
1:B:135:THR:HG22	1:B:151:LEU:CD2	2.38	0.54
1:B:31:ASN:ND2	1:B:223:CYS:O	2.38	0.54
1:D:201:ARG:O	3:D:404:HOH:O	2.18	0.54
1:D:258:GLU:OE1	1:D:268:ASN:CB	2.55	0.54
1:D:258:GLU:OE1	1:D:268:ASN:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:SER:HB2	1:E:214:ILE:HD12	1.90	0.54
1:B:44:TRP:C	1:B:46:GLU:H	2.16	0.54
1:D:38:ALA:HB2	1:D:228:PHE:CD1	2.43	0.54
1:D:135:THR:HG22	1:D:151:LEU:HD11	1.89	0.53
1:B:27:ARG:HD2	1:B:27:ARG:O	2.08	0.53
1:C:255:LEU:HD21	1:D:211:TYR:CD1	2.44	0.53
1:A:45:TYR:HB3	1:A:50:ILE:O	2.08	0.53
1:A:127:HIS:O	1:A:131:LYS:N	2.39	0.53
1:D:128:GLN:OE1	3:D:403:HOH:O	2.18	0.53
1:A:115:VAL:HG21	1:A:287:THR:HG21	1.91	0.53
1:A:205:THR:CG2	1:B:83:ARG:HD2	2.31	0.53
1:A:83:ARG:CZ	1:A:275:MET:HE3	2.39	0.52
1:D:35:SER:OG	1:D:239:PRO:HB3	2.09	0.52
1:C:237:MET:HE3	1:D:50:ILE:HG22	1.91	0.52
1:D:27:ARG:NH1	1:D:220:TYR:CZ	2.77	0.52
1:D:33:LEU:O	1:D:36:ILE:HG13	2.10	0.52
1:D:201:ARG:HA	3:D:404:HOH:O	2.09	0.52
1:E:271:PRO:O	1:E:275:MET:HG3	2.10	0.52
1:D:42:TYR:HE2	1:D:235:HIS:HE1	1.57	0.52
1:D:45:TYR:CD1	1:D:50:ILE:HD11	2.45	0.52
1:D:168:ILE:HG22	1:D:182:TYR:CE1	2.44	0.52
1:D:208:PRO:O	1:D:211:TYR:HB2	2.10	0.52
1:A:39:ILE:HD13	1:A:236:TYR:HD1	1.73	0.52
1:D:38:ALA:HB2	1:D:228:PHE:HD1	1.74	0.52
1:A:209:PHE:HD2	1:A:209:PHE:O	1.92	0.52
1:A:224:THR:O	1:A:227:PRO:HD2	2.10	0.52
1:B:44:TRP:C	1:B:46:GLU:N	2.67	0.52
1:D:158:ASN:ND2	3:D:407:HOH:O	2.44	0.51
1:D:231:VAL:HA	1:D:234:LEU:O	2.10	0.51
1:D:27:ARG:NH1	1:D:220:TYR:OH	2.43	0.51
1:D:97:VAL:HG21	1:D:283:LEU:HD22	1.92	0.51
1:B:239:PRO:O	1:B:243:VAL:HG12	2.10	0.51
1:D:200:GLU:O	1:D:204:THR:HG23	2.11	0.51
1:B:42:TYR:HA	1:B:45:TYR:CE1	2.46	0.51
1:C:51:HIS:HE1	1:E:235:HIS:CG	2.27	0.51
1:C:166:ASN:OD1	1:E:102:ASN:ND2	2.44	0.51
1:B:200:GLU:O	1:B:204:THR:HG23	2.11	0.51
1:A:26:PHE:CE1	1:A:30:LEU:HD11	2.46	0.51
1:D:42:TYR:CE2	1:D:235:HIS:CE1	2.99	0.51
1:E:107:GLU:HG3	1:E:176:LYS:HZ3	1.65	0.51
1:B:183:GLY:HA2	1:D:184:LEU:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:LEU:HD21	1:D:208:PRO:HG3	1.94	0.50
1:A:158:ASN:OD1	1:B:286:MET:HE2	2.11	0.50
1:E:234:LEU:HB3	1:E:237:MET:HB3	1.93	0.50
1:A:38:ALA:HB2	1:A:228:PHE:CD1	2.47	0.50
1:C:236:TYR:O	1:C:236:TYR:CD1	2.65	0.50
1:D:94:ARG:NH1	3:D:405:HOH:O	2.25	0.50
1:B:30:LEU:HD23	1:B:34:MET:HG2	1.94	0.50
1:D:270:LEU:HB3	1:D:275:MET:CE	2.31	0.50
1:E:64:ILE:HG12	1:E:218:THR:CG2	2.42	0.50
1:A:205:THR:HG22	1:B:83:ARG:HH11	1.75	0.50
1:D:45:TYR:CE1	1:D:50:ILE:HD11	2.47	0.50
1:D:107:GLU:OE2	1:D:176:LYS:NZ	2.28	0.50
1:E:43:GLN:HG3	1:E:44:TRP:CD1	2.46	0.50
1:E:52:LEU:HD12	1:E:228:PHE:HB3	1.94	0.49
1:A:237:MET:HE3	1:E:52:LEU:HD21	1.93	0.49
1:C:158:ASN:OD1	1:E:286:MET:CE	2.61	0.49
1:B:271:PRO:O	1:B:275:MET:HG3	2.13	0.49
1:A:27:ARG:HB3	1:A:220:TYR:CE1	2.48	0.49
1:C:201:ARG:O	1:C:205:THR:HB	2.12	0.49
1:E:53:THR:HB	1:E:56:PRO:CD	2.42	0.49
1:A:39:ILE:HD13	1:A:236:TYR:CD1	2.47	0.49
1:A:252:TRP:CZ3	1:E:215:LEU:HD21	2.48	0.49
1:B:94:ARG:HG2	1:B:286:MET:HE1	1.94	0.49
1:D:68:LEU:HD23	1:D:215:LEU:HD13	1.94	0.49
1:C:100:LEU:HD11	1:C:114:ILE:HD13	1.95	0.49
1:D:261:ASP:O	1:D:269:ASP:OD1	2.29	0.49
1:A:139:ARG:HA	1:A:147:VAL:HG21	1.95	0.48
1:A:231:VAL:HA	1:A:238:THR:OG1	2.13	0.48
1:C:59:LEU:HB2	1:E:58:SER:HB2	1.95	0.48
1:C:158:ASN:ND2	3:C:401:HOH:O	2.45	0.48
1:C:29:LEU:O	1:C:32:VAL:HG22	2.13	0.48
1:A:33:LEU:HA	1:A:36:ILE:HG13	1.95	0.48
1:B:25:ILE:O	1:B:29:LEU:HD12	2.13	0.48
1:E:71:ARG:HH11	1:E:212:THR:HG22	1.79	0.48
1:A:94:ARG:HG2	1:A:286:MET:HE1	1.95	0.48
1:D:133:ASP:OD1	1:D:135:THR:HG23	2.14	0.48
1:A:212:THR:HA	1:A:215:LEU:HB2	1.96	0.48
1:D:114:ILE:O	1:D:118:LEU:HG	2.13	0.48
1:D:188:LYS:HA	1:D:188:LYS:HD3	1.59	0.48
1:E:107:GLU:HG3	1:E:176:LYS:HE2	1.95	0.48
1:A:209:PHE:O	1:A:211:TYR:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:VAL:CG2	1:C:195:VAL:HG11	2.42	0.48
1:D:227:PRO:HA	1:D:230:LEU:HB2	1.95	0.48
1:E:231:VAL:HA	1:E:238:THR:CG2	2.40	0.48
1:A:101:ARG:HD2	1:A:286:MET:O	2.14	0.47
1:E:78:ARG:NH1	1:E:205:THR:O	2.47	0.47
1:B:138:LEU:HD13	1:B:151:LEU:HD11	1.97	0.47
1:D:44:TRP:O	1:D:48:LEU:N	2.38	0.47
1:A:155:MET:SD	1:A:200:GLU:OE2	2.72	0.47
1:D:75:SER:HB3	1:D:260:GLU:HG3	1.96	0.47
1:D:78:ARG:NH1	1:D:260:GLU:O	2.47	0.47
1:E:108:HIS:HB3	1:E:112:ARG:NH2	2.30	0.47
1:E:109:ASP:HB3	1:E:113:ARG:HH12	1.78	0.47
1:E:270:LEU:HD22	1:E:275:MET:HE1	1.97	0.47
1:B:79:PHE:O	1:B:83:ARG:HG3	2.14	0.47
1:D:269:ASP:O	1:D:270:LEU:C	2.56	0.47
1:D:150:ILE:HA	1:D:159:ARG:HG2	1.97	0.46
1:D:166:ASN:O	1:D:170:GLN:HG3	2.15	0.46
1:A:93:GLU:HB3	1:A:283:LEU:HD21	1.96	0.46
1:A:211:TYR:O	1:A:215:LEU:N	2.31	0.46
1:A:234:LEU:O	1:A:238:THR:OG1	2.27	0.46
1:E:271:PRO:HD2	1:E:275:MET:HE3	1.96	0.46
1:D:104:LEU:CD1	1:D:111:HIS:HE2	2.28	0.46
1:E:258:GLU:CD	1:E:268:ASN:HD22	2.20	0.46
1:B:146:ARG:HA	1:B:146:ARG:HD3	1.57	0.46
1:D:24:ILE:HG12	1:D:28:LEU:HD11	1.97	0.46
1:A:209:PHE:O	1:A:212:THR:N	2.48	0.46
1:A:258:GLU:OE1	1:A:268:ASN:HB2	2.15	0.46
1:C:43:GLN:OE1	1:C:44:TRP:CZ2	2.69	0.46
1:B:52:LEU:HD12	1:B:228:PHE:O	2.15	0.46
1:B:151:LEU:HD12	1:B:151:LEU:N	2.31	0.46
1:E:106:ALA:O	1:E:108:HIS:CD2	2.69	0.46
1:A:26:PHE:O	1:A:30:LEU:HD13	2.16	0.46
1:A:53:THR:HG23	1:A:56:PRO:HD3	1.98	0.46
1:B:53:THR:H	1:D:234:LEU:CD2	2.29	0.46
1:A:273:ASN:ND2	3:A:401:HOH:O	2.23	0.45
1:E:108:HIS:O	1:E:112:ARG:HG2	2.15	0.45
1:B:214:ILE:O	1:B:217:ARG:HG2	2.16	0.45
1:C:32:VAL:CG1	1:C:243:VAL:HG11	2.44	0.45
1:E:126:LYS:C	1:E:126:LYS:HD2	2.41	0.45
1:A:200:GLU:O	1:A:204:THR:OG1	2.34	0.45
1:B:52:LEU:HA	1:D:234:LEU:CD2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:LEU:HA	1:B:216:GLN:HB3	1.99	0.45
1:E:115:VAL:O	1:E:119:VAL:HG23	2.16	0.45
1:B:51:HIS:O	1:D:234:LEU:HB3	2.15	0.45
1:B:210:ALA:HB3	1:D:255:LEU:HD13	1.98	0.45
1:B:138:LEU:CD1	1:B:151:LEU:HD11	2.46	0.45
1:E:130:ARG:HH12	1:E:273:ASN:HD21	1.65	0.45
1:A:158:ASN:ND2	1:B:94:ARG:HD3	2.31	0.45
1:C:99:GLN:NE2	3:D:402:HOH:O	2.49	0.45
1:A:220:TYR:CE2	1:A:224:THR:HG23	2.51	0.45
1:C:50:ILE:O	1:C:50:ILE:HG13	2.17	0.45
1:C:98:ARG:HH11	1:C:98:ARG:HG2	1.82	0.45
1:E:170:GLN:HA	1:E:173:GLU:HG2	1.98	0.45
1:A:213:LEU:H	1:A:213:LEU:HD23	1.81	0.44
1:B:254:SER:HA	1:B:257:GLU:CG	2.38	0.44
1:D:95:THR:O	1:D:99:GLN:HG3	2.17	0.44
1:A:25:ILE:O	1:A:29:LEU:HG	2.17	0.44
1:A:53:THR:HG22	1:B:234:LEU:HD21	1.97	0.44
1:B:103:ILE:HG13	1:B:104:LEU:HG	1.98	0.44
1:C:72:ASN:HD22	1:C:256:ALA:HB2	1.82	0.44
1:B:275:MET:HE2	1:B:275:MET:HB3	1.70	0.44
1:A:235:HIS:HB3	1:E:49:GLY:O	2.17	0.44
1:D:231:VAL:O	1:D:234:LEU:O	2.36	0.44
1:E:28:LEU:HD23	1:E:28:LEU:HA	1.79	0.44
1:E:138:LEU:HD23	1:E:138:LEU:HA	1.85	0.44
1:C:182:TYR:CE2	1:E:103:ILE:HD11	2.52	0.44
1:C:25:ILE:O	1:C:29:LEU:HG	2.18	0.44
1:D:227:PRO:O	1:D:231:VAL:HG22	2.18	0.44
1:A:277:ASN:O	1:A:281:ARG:HG3	2.18	0.43
1:D:108:HIS:HA	1:D:111:HIS:ND1	2.33	0.43
1:D:230:LEU:HD12	1:D:242:SER:HB2	1.99	0.43
1:E:224:THR:O	1:E:227:PRO:HD2	2.17	0.43
1:D:24:ILE:O	1:D:28:LEU:HD12	2.18	0.43
1:E:244:PHE:O	1:E:248:THR:HG23	2.18	0.43
1:A:115:VAL:O	1:A:119:VAL:HG23	2.18	0.43
1:A:252:TRP:HE3	1:E:214:ILE:HD11	1.81	0.43
1:C:103:ILE:HG23	1:C:103:ILE:HD12	1.72	0.43
1:A:182:TYR:OH	1:B:103:ILE:HG22	2.17	0.43
1:D:181:THR:O	1:D:185:MET:HG3	2.19	0.43
1:E:184:LEU:HA	1:E:184:LEU:HD23	1.79	0.43
1:E:215:LEU:HD13	1:E:215:LEU:HA	1.88	0.43
1:B:100:LEU:HG	1:B:185:MET:CE	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:GLU:O	1:B:260:GLU:N	2.51	0.43
1:C:135:THR:O	1:C:139:ARG:HG3	2.19	0.43
1:B:50:ILE:O	1:B:50:ILE:HG13	2.17	0.43
1:B:254:SER:O	1:B:257:GLU:HB2	2.18	0.43
1:D:217:ARG:HA	1:D:217:ARG:NE	2.34	0.43
1:D:25:ILE:HA	1:D:28:LEU:HD13	2.01	0.42
1:C:233:ASP:HB3	1:D:53:THR:OG1	2.19	0.42
1:E:64:ILE:CD1	1:E:218:THR:HG22	2.49	0.42
1:A:34:MET:SD	1:A:34:MET:N	2.92	0.42
1:E:35:SER:HA	1:E:227:PRO:HB2	2.00	0.42
1:E:178:SER:OG	1:E:181:THR:HG23	2.18	0.42
1:E:238:THR:N	1:E:239:PRO:HD2	2.34	0.42
1:E:286:MET:HB2	1:E:286:MET:HE3	1.77	0.42
1:B:38:ALA:O	1:B:42:TYR:HB2	2.18	0.42
1:C:207:VAL:N	1:C:208:PRO:CD	2.82	0.42
1:D:198:GLY:HA2	1:D:201:ARG:HH12	1.81	0.42
1:B:33:LEU:HA	1:B:36:ILE:HG13	2.00	0.42
1:B:48:LEU:HD12	1:B:48:LEU:HA	1.75	0.42
1:D:192:LEU:HA	1:D:192:LEU:HD23	1.84	0.42
1:E:260:GLU:O	1:E:261:ASP:C	2.62	0.42
1:E:168:ILE:HG22	1:E:182:TYR:CE1	2.54	0.42
1:A:53:THR:HG23	1:A:56:PRO:CD	2.50	0.42
1:A:71:ARG:HG3	1:A:71:ARG:HH11	1.84	0.42
1:A:94:ARG:HD3	1:E:158:ASN:OD1	2.20	0.42
1:E:47:GLN:OE1	1:E:48:LEU:N	2.42	0.42
1:E:130:ARG:HH11	1:E:130:ARG:HD2	1.72	0.42
1:B:145:GLU:O	1:B:148:THR:OG1	2.33	0.42
1:E:107:GLU:OE1	1:E:176:LYS:NZ	2.33	0.42
1:E:130:ARG:HH12	1:E:273:ASN:ND2	2.18	0.42
1:A:53:THR:HG22	1:B:234:LEU:CD2	2.50	0.42
1:A:196:LEU:O	1:A:200:GLU:HG3	2.20	0.42
1:D:89:VAL:CG2	1:D:195:VAL:HG11	2.50	0.42
1:D:127:HIS:ND1	1:D:132:THR:OG1	2.46	0.41
1:D:24:ILE:HG12	1:D:28:LEU:CD1	2.50	0.41
1:B:161:LEU:HD23	1:B:161:LEU:HA	1.70	0.41
1:B:186:ASP:OD2	1:D:99:GLN:NE2	2.51	0.41
1:C:53:THR:HG21	1:E:233:ASP:HB3	2.03	0.41
1:D:30:LEU:HD12	1:D:30:LEU:H	1.85	0.41
1:A:96:LEU:CD1	1:A:185:MET:HB3	2.50	0.41
1:A:108:HIS:HA	1:A:111:HIS:ND1	2.34	0.41
1:C:194:HIS:HA	1:E:91:ILE:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LEU:CA	1:A:36:ILE:HG13	2.50	0.41
1:B:155:MET:HE2	1:D:282:ASN:ND2	2.36	0.41
1:C:207:VAL:CG2	1:E:76:TYR:CE1	2.57	0.41
1:A:23:LYS:O	1:A:27:ARG:CZ	2.69	0.41
1:A:45:TYR:HA	1:A:50:ILE:HG12	2.03	0.41
1:B:108:HIS:HA	1:B:111:HIS:CG	2.56	0.41
1:B:217:ARG:HG3	1:B:218:THR:N	2.36	0.41
1:C:72:ASN:ND2	1:C:256:ALA:HB2	2.36	0.41
1:C:239:PRO:O	1:C:243:VAL:HG13	2.21	0.41
1:A:240:PHE:O	1:A:243:VAL:HG12	2.21	0.41
1:E:53:THR:HG22	1:E:55:ALA:H	1.85	0.41
1:E:85:LEU:HD23	1:E:85:LEU:HA	1.83	0.41
1:A:23:LYS:O	1:A:27:ARG:NH2	2.53	0.41
1:A:213:LEU:HG	1:A:214:ILE:N	2.34	0.41
1:D:104:LEU:O	1:D:104:LEU:CD1	2.68	0.41
1:A:104:LEU:HD11	1:A:177:LEU:HD21	2.03	0.41
1:E:104:LEU:O	1:E:111:HIS:NE2	2.52	0.41
1:A:207:VAL:CG1	1:A:260:GLU:CD	2.94	0.40
1:D:216:GLN:HG3	1:D:220:TYR:CE2	2.56	0.40
1:E:64:ILE:HG12	1:E:218:THR:HG21	2.02	0.40
1:B:215:LEU:HA	1:B:218:THR:CG2	2.49	0.40
1:C:251:SER:HB3	1:D:214:ILE:HG12	2.04	0.40
1:D:81:GLU:OE2	1:D:201:ARG:NH2	2.53	0.40
1:D:39:ILE:HD11	1:D:239:PRO:CD	2.48	0.40
1:A:150:ILE:HA	1:A:159:ARG:HG2	2.03	0.40
1:A:231:VAL:O	1:A:232:GLY:C	2.65	0.40
1:B:44:TRP:O	1:B:45:TYR:C	2.63	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	265/297 (89%)	257 (97%)	7 (3%)	1 (0%)	30	39
1	B	264/297 (89%)	255 (97%)	8 (3%)	1 (0%)	30	39
1	C	266/297 (90%)	258 (97%)	7 (3%)	1 (0%)	30	39
1	D	266/297 (90%)	258 (97%)	8 (3%)	0	100	100
1	E	264/297 (89%)	261 (99%)	3 (1%)	0	100	100
All	All	1325/1485 (89%)	1289 (97%)	33 (2%)	3 (0%)	43	56

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	45	TYR
1	C	208	PRO
1	A	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	226/259 (87%)	222 (98%)	4 (2%)	51	70
1	B	223/259 (86%)	221 (99%)	2 (1%)	70	82
1	C	224/259 (86%)	219 (98%)	5 (2%)	45	64
1	D	224/259 (86%)	220 (98%)	4 (2%)	51	70
1	E	226/259 (87%)	225 (100%)	1 (0%)	84	90
All	All	1123/1295 (87%)	1107 (99%)	16 (1%)	59	75

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ILE
1	A	40	ILE
1	A	180	ILE
1	A	287	THR
1	B	170	GLN

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Mol	Chain	Res	Type
1	B	172	ARG
1	C	50	ILE
1	C	172	ARG
1	C	188	LYS
1	C	207	VAL
1	C	281	ARG
1	D	139	ARG
1	D	231	VAL
1	D	234	LEU
1	D	268	ASN
1	E	172	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	B	111	HIS
1	B	282	ASN
1	C	51	HIS
1	C	72	ASN
1	C	84	ASN
1	C	99	GLN
1	C	268	ASN
1	C	290	HIS
1	D	31	ASN
1	D	72	ASN
1	D	235	HIS
1	E	31	ASN
1	E	84	ASN
1	E	235	HIS
1	E	273	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 11 ligands modelled in this entry, 11 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	267/297 (89%)	1.79	84 (31%) 1 0	56, 83, 112, 127	0
1	B	266/297 (89%)	2.01	112 (42%) 0 0	59, 89, 122, 143	0
1	C	268/297 (90%)	1.44	69 (25%) 1 1	49, 75, 114, 134	0
1	D	268/297 (90%)	1.53	72 (26%) 1 1	52, 81, 120, 140	0
1	E	266/297 (89%)	1.36	67 (25%) 1 1	51, 75, 115, 137	0
All	All	1335/1485 (89%)	1.63	404 (30%) 1 0	49, 81, 117, 143	0

All (404) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	204	THR	21.9
1	C	205	THR	12.5
1	A	59	LEU	11.1
1	D	204	THR	11.0
1	E	47	GLN	10.2
1	A	58	SER	10.1
1	A	204	THR	9.2
1	A	55	ALA	9.1
1	D	209	PHE	8.6
1	D	205	THR	8.6
1	B	204	THR	8.5
1	D	207	VAL	8.2
1	E	58	SER	8.2
1	E	26	PHE	8.1
1	B	154	SER	8.0
1	B	58	SER	7.7
1	A	22	SER	7.6
1	B	236	TYR	7.6
1	D	47	GLN	7.5
1	D	48	LEU	7.5

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Mol	Chain	Res	Type	RSRZ
1	C	58	SER	7.2
1	E	48	LEU	7.2
1	B	215	LEU	7.0
1	C	203	ALA	6.8
1	A	210	ALA	6.7
1	D	59	LEU	6.7
1	A	207	VAL	6.7
1	D	208	PRO	6.7
1	C	209	PHE	6.6
1	B	24	ILE	6.4
1	A	48	LEU	6.3
1	B	214	ILE	6.3
1	E	25	ILE	6.3
1	D	106	ALA	6.2
1	E	204	THR	6.0
1	B	44	TRP	5.9
1	D	206	PRO	5.8
1	B	117	TYR	5.8
1	B	48	LEU	5.8
1	A	47	GLN	5.6
1	D	46	GLU	5.6
1	C	290	HIS	5.5
1	C	61	GLY	5.4
1	A	288	GLY	5.4
1	E	175	GLY	5.4
1	E	24	ILE	5.3
1	C	206	PRO	5.3
1	B	55	ALA	5.3
1	E	203	ALA	5.3
1	C	59	LEU	5.3
1	A	62	ILE	5.3
1	A	49	GLY	5.2
1	B	268	ASN	5.2
1	B	288	GLY	5.2
1	C	207	VAL	5.1
1	B	211	TYR	5.1
1	A	54	VAL	5.0
1	A	37	ILE	5.0
1	A	220	TYR	5.0
1	A	205	THR	5.0
1	E	144	GLU	4.9
1	D	184	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	222	PHE	4.9
1	B	174	ALA	4.8
1	B	205	THR	4.8
1	A	209	PHE	4.8
1	C	236	TYR	4.8
1	A	53	THR	4.7
1	C	60	LEU	4.7
1	A	235	HIS	4.7
1	B	166	ASN	4.7
1	D	210	ALA	4.7
1	B	50	ILE	4.6
1	C	23	LYS	4.6
1	A	183	GLY	4.6
1	B	77	SER	4.6
1	B	47	GLN	4.5
1	B	131	LYS	4.5
1	D	268	ASN	4.5
1	C	77	SER	4.4
1	C	268	ASN	4.4
1	A	50	ILE	4.4
1	E	80	VAL	4.4
1	E	235	HIS	4.4
1	A	208	PRO	4.4
1	B	130	ARG	4.4
1	E	145	GLU	4.3
1	B	46	GLU	4.3
1	A	57	PHE	4.3
1	D	211	TYR	4.3
1	B	45	TYR	4.2
1	B	129	LEU	4.2
1	A	60	LEU	4.1
1	D	234	LEU	4.1
1	A	206	PRO	4.1
1	B	255	LEU	4.1
1	C	267	ALA	4.1
1	D	44	TRP	4.1
1	C	25	ILE	4.1
1	B	265	THR	4.0
1	A	51	HIS	4.0
1	B	32	VAL	4.0
1	A	56	PRO	4.0
1	A	151	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	215	LEU	4.0
1	C	215	LEU	4.0
1	B	173	GLU	4.0
1	B	23	LYS	4.0
1	D	37	ILE	4.0
1	C	47	GLN	4.0
1	B	209	PHE	4.0
1	A	32	VAL	4.0
1	E	54	VAL	4.0
1	B	43	GLN	4.0
1	C	210	ALA	3.9
1	D	281	ARG	3.9
1	B	264	GLY	3.9
1	D	58	SER	3.9
1	D	105	PRO	3.9
1	A	231	VAL	3.9
1	A	26	PHE	3.8
1	E	57	PHE	3.8
1	E	289	GLN	3.8
1	D	240	PHE	3.8
1	B	213	LEU	3.8
1	C	269	ASP	3.8
1	A	213	LEU	3.7
1	D	285	ASP	3.7
1	B	219	VAL	3.7
1	C	42	TYR	3.7
1	D	57	PHE	3.7
1	A	77	SER	3.7
1	B	207	VAL	3.7
1	E	148	THR	3.7
1	B	163	LEU	3.7
1	C	235	HIS	3.6
1	E	51	HIS	3.6
1	B	266	ALA	3.6
1	A	46	GLU	3.6
1	A	192	LEU	3.6
1	A	41	SER	3.6
1	B	261	ASP	3.6
1	B	167	GLU	3.6
1	B	68	LEU	3.6
1	B	267	ALA	3.6
1	B	145	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	40	ILE	3.5
1	D	40	ILE	3.5
1	B	155	MET	3.5
1	E	45	TYR	3.5
1	D	56	PRO	3.5
1	E	288	GLY	3.5
1	A	39	ILE	3.5
1	B	235	HIS	3.5
1	B	269	ASP	3.4
1	E	84	ASN	3.4
1	D	238	THR	3.4
1	A	184	LEU	3.4
1	B	182	TYR	3.4
1	D	26	PHE	3.4
1	A	217	ARG	3.4
1	A	24	ILE	3.4
1	C	24	ILE	3.4
1	D	201	ARG	3.4
1	E	220	TYR	3.4
1	B	228	PHE	3.4
1	C	44	TRP	3.4
1	B	36	ILE	3.4
1	C	50	ILE	3.4
1	C	249	PHE	3.3
1	B	133	ASP	3.3
1	B	51	HIS	3.3
1	E	61	GLY	3.3
1	A	63	ALA	3.3
1	B	263	PHE	3.3
1	E	236	TYR	3.3
1	A	221	LEU	3.3
1	C	212	THR	3.3
1	D	51	HIS	3.3
1	A	180	ILE	3.3
1	D	104	LEU	3.3
1	B	25	ILE	3.3
1	C	83	ARG	3.3
1	B	37	ILE	3.2
1	A	274	ALA	3.2
1	D	267	ALA	3.2
1	B	146	ARG	3.2
1	C	173	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	185	MET	3.2
1	B	245	ILE	3.2
1	E	257	GLU	3.2
1	B	203	ALA	3.2
1	E	44	TRP	3.2
1	B	116	SER	3.2
1	C	57	PHE	3.2
1	D	230	LEU	3.2
1	B	199	CYS	3.2
1	E	212	THR	3.2
1	B	244	PHE	3.1
1	C	154	SER	3.1
1	C	285	ASP	3.1
1	E	109	ASP	3.1
1	C	45	TYR	3.1
1	D	24	ILE	3.1
1	C	52	LEU	3.1
1	B	175	GLY	3.1
1	D	103	ILE	3.1
1	E	42	TYR	3.1
1	B	26	PHE	3.1
1	B	33	LEU	3.1
1	A	23	LYS	3.0
1	B	57	PHE	3.0
1	D	109	ASP	3.0
1	E	285	ASP	3.0
1	D	231	VAL	3.0
1	B	110	ALA	3.0
1	D	203	ALA	3.0
1	D	228	PHE	3.0
1	E	261	ASP	3.0
1	B	27	ARG	3.0
1	B	49	GLY	3.0
1	C	26	PHE	3.0
1	E	77	SER	3.0
1	D	49	GLY	3.0
1	E	37	ILE	3.0
1	E	62	ILE	3.0
1	A	238	THR	3.0
1	B	252	TRP	3.0
1	D	27	ARG	3.0
1	A	186	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	289	GLN	3.0
1	C	279	ILE	2.9
1	D	212	THR	2.9
1	D	77	SER	2.9
1	B	170	GLN	2.9
1	D	166	ASN	2.9
1	C	62	ILE	2.9
1	B	71	ARG	2.9
1	C	152	ALA	2.9
1	C	46	GLU	2.9
1	B	172	ARG	2.9
1	C	265	THR	2.9
1	E	224	THR	2.9
1	E	92	ALA	2.9
1	A	228	PHE	2.9
1	E	260	GLU	2.9
1	B	59	LEU	2.9
1	C	222	PHE	2.9
1	B	251	SER	2.8
1	A	30	LEU	2.8
1	C	48	LEU	2.8
1	B	113	ARG	2.8
1	D	180	ILE	2.8
1	E	180	ILE	2.8
1	A	44	TRP	2.8
1	E	27	ARG	2.8
1	D	214	ILE	2.8
1	C	29	LEU	2.8
1	E	55	ALA	2.8
1	E	59	LEU	2.8
1	A	71	ARG	2.8
1	A	61	GLY	2.7
1	D	288	GLY	2.7
1	B	62	ILE	2.7
1	A	35	SER	2.7
1	D	73	SER	2.7
1	A	287	THR	2.7
1	E	68	LEU	2.7
1	B	179	ALA	2.7
1	C	55	ALA	2.7
1	E	101	ARG	2.7
1	E	139	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	37	ILE	2.7
1	D	25	ILE	2.7
1	A	34	MET	2.7
1	A	96	LEU	2.7
1	A	27	ARG	2.7
1	C	148	THR	2.7
1	D	188	LYS	2.7
1	A	33	LEU	2.7
1	D	236	TYR	2.7
1	C	36	ILE	2.6
1	D	23	LYS	2.6
1	B	158	ASN	2.6
1	B	106	ALA	2.6
1	E	218	THR	2.6
1	D	220	TYR	2.6
1	B	143	PRO	2.6
1	B	237	MET	2.6
1	C	40	ILE	2.6
1	C	64	ILE	2.6
1	B	61	GLY	2.6
1	E	50	ILE	2.6
1	B	164	ALA	2.6
1	B	256	ALA	2.6
1	C	51	HIS	2.6
1	A	286	MET	2.5
1	C	143	PRO	2.5
1	D	107	GLU	2.5
1	D	22	SER	2.5
1	A	25	ILE	2.5
1	A	29	LEU	2.5
1	E	70	PHE	2.5
1	A	92	ALA	2.5
1	B	83	ARG	2.5
1	A	236	TYR	2.5
1	B	186	ASP	2.5
1	B	79	PHE	2.5
1	E	228	PHE	2.5
1	A	140	ARG	2.5
1	E	107	GLU	2.5
1	D	30	LEU	2.5
1	A	212	THR	2.5
1	B	218	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	208	PRO	2.4
1	B	233	ASP	2.4
1	C	39	ILE	2.4
1	E	131	LYS	2.4
1	E	214	ILE	2.4
1	E	253	ASP	2.4
1	D	152	ALA	2.4
1	B	149	GLU	2.4
1	E	200	GLU	2.4
1	C	188	LYS	2.4
1	A	190	ASP	2.4
1	E	269	ASP	2.4
1	A	189	LEU	2.4
1	C	259	LEU	2.4
1	C	231	VAL	2.4
1	C	200	GLU	2.4
1	B	30	LEU	2.4
1	B	220	TYR	2.4
1	A	225	LEU	2.4
1	A	265	THR	2.3
1	B	148	THR	2.3
1	A	101	ARG	2.3
1	B	253	ASP	2.3
1	B	270	LEU	2.3
1	B	54	VAL	2.3
1	B	144	GLU	2.3
1	B	112	ARG	2.3
1	B	260	GLU	2.3
1	D	181	THR	2.3
1	C	101	ARG	2.3
1	C	201	ARG	2.3
1	E	179	ALA	2.3
1	A	218	THR	2.3
1	B	250	LEU	2.3
1	A	65	ALA	2.2
1	E	135	THR	2.2
1	E	43	GLN	2.2
1	B	40	ILE	2.2
1	B	100	LEU	2.2
1	D	33	LEU	2.2
1	D	41	SER	2.2
1	E	215	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	262	PRO	2.2
1	D	187	ASN	2.2
1	C	49	GLY	2.2
1	A	214	ILE	2.2
1	A	239	PRO	2.2
1	D	84	ASN	2.2
1	E	205	THR	2.2
1	B	284	LEU	2.2
1	B	240	PHE	2.2
1	C	56	PRO	2.2
1	D	282	ASN	2.2
1	D	237	MET	2.2
1	B	28	LEU	2.2
1	A	73	SER	2.2
1	D	108	HIS	2.1
1	A	43	GLN	2.1
1	D	29	LEU	2.1
1	E	52	LEU	2.1
1	A	154	SER	2.1
1	B	73	SER	2.1
1	E	281	ARG	2.1
1	C	84	ASN	2.1
1	C	33	LEU	2.1
1	D	36	ILE	2.1
1	D	39	ILE	2.1
1	E	103	ILE	2.1
1	E	172	ARG	2.1
1	D	154	SER	2.1
1	E	173	GLU	2.1
1	A	45	TYR	2.1
1	E	249	PHE	2.1
1	A	136	ALA	2.1
1	B	258	GLU	2.1
1	A	188	LYS	2.1
1	B	41	SER	2.1
1	C	178	SER	2.1
1	D	235	HIS	2.1
1	E	243	VAL	2.0
1	C	282	ASN	2.0
1	E	29	LEU	2.0
1	B	287	THR	2.0
1	C	27	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	259	LEU	2.0
1	C	270	LEU	2.0
1	B	72	ASN	2.0
1	D	131	LYS	2.0
1	B	212	THR	2.0
1	C	35	SER	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	D	301	1/1	0.90	0.13	149,149,149,149	0
2	ZN	C	301	1/1	0.92	0.16	77,77,77,77	0
2	ZN	C	302	1/1	0.92	0.15	76,76,76,76	0
2	ZN	B	302	1/1	0.92	0.15	102,102,102,102	0
2	ZN	E	302	1/1	0.93	0.14	83,83,83,83	0
2	ZN	D	302	1/1	0.95	0.15	85,85,85,85	0
2	ZN	A	303	1/1	0.96	0.15	98,98,98,98	0
2	ZN	B	301	1/1	0.98	0.11	73,73,73,73	0
2	ZN	A	301	1/1	0.99	0.04	71,71,71,71	0
2	ZN	A	302	1/1	0.99	0.06	78,78,78,78	0
2	ZN	E	301	1/1	1.00	0.04	70,70,70,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.