Full wwPDB X-ray Structure Validation Report ⓘ

Jun 2, 2022 – 06:10 PM JST

PDB ID	:	6JLF
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 following versions of software and data (see references ⓘ) were used in the production of this report:

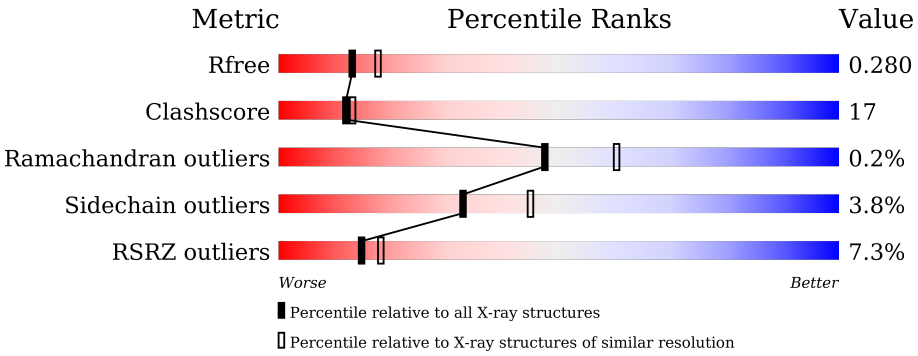
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

1 Overall quality at a glance (i)

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}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 <=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	7% 59% 29% • 10%
1	B	297	9% 61% 29% 10%
1	C	297	6% 69% 20% • 10%
1	D	297	7% 56% 33% • 10%
1	E	297	3% 64% 24% • 10%

2 Entry composition (i)

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 (three-letter code: 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.

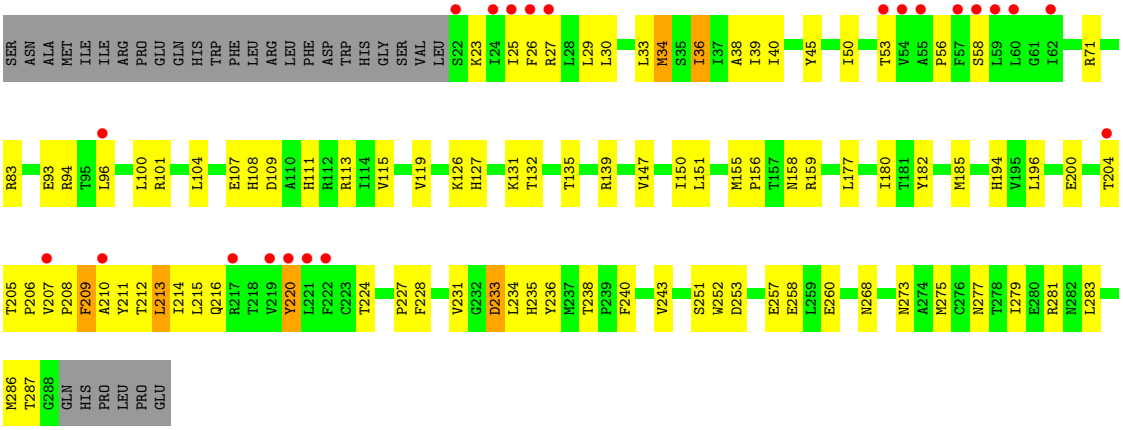
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	10	Total O 10 10	0	0
3	B	5	Total O 5 5	0	0
3	C	9	Total O 9 9	0	0
3	D	10	Total O 10 10	0	0
3	E	19	Total O 19 19	0	0

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.

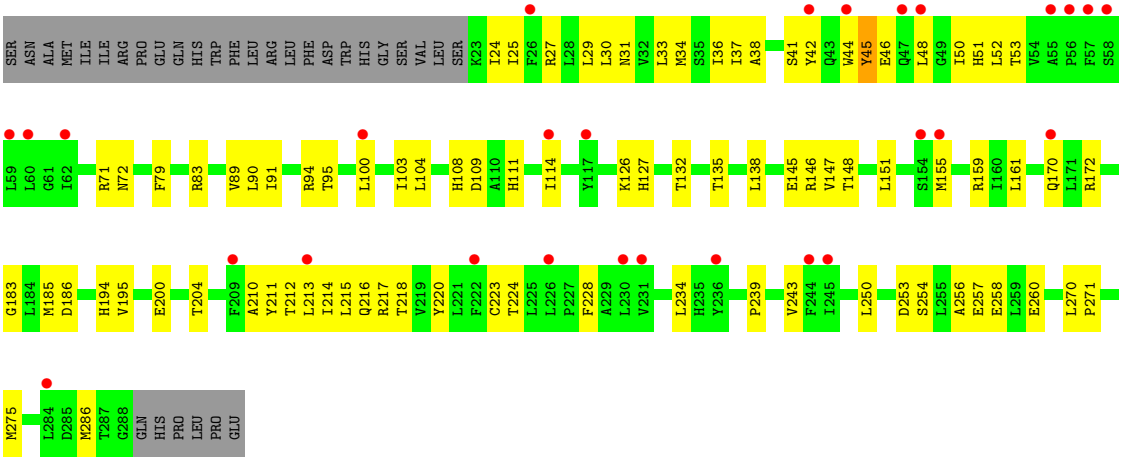
• Molecule 1: Bestrophin homolog

Chain A:



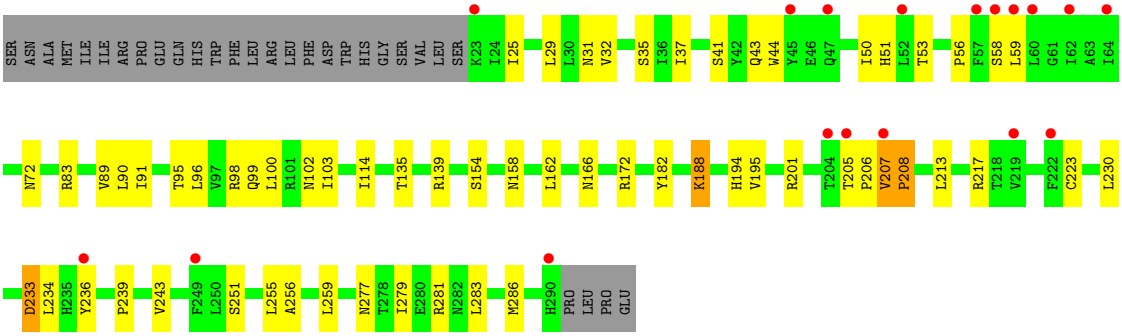
• Molecule 1: Bestrophin homolog

Chain B:



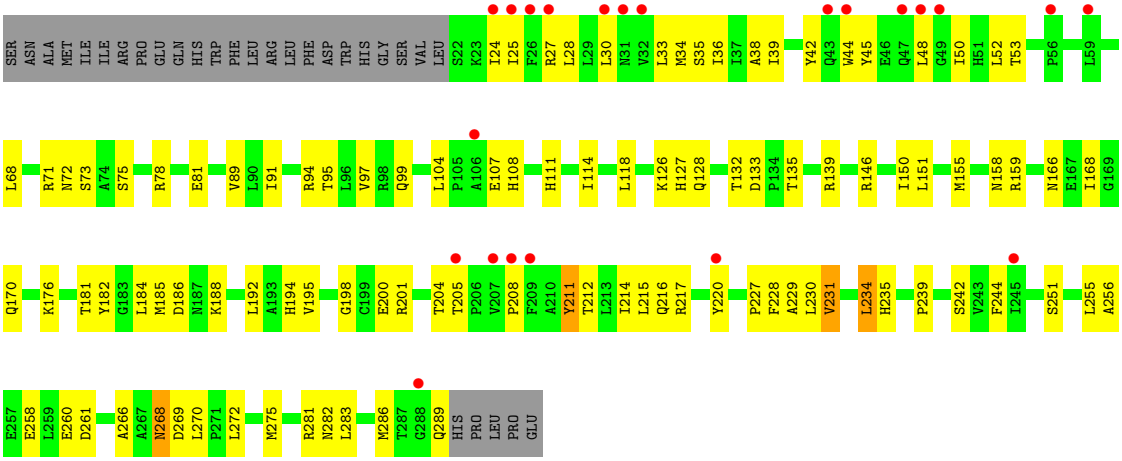
• Molecule 1: Bestrophin homolog

Chain C:



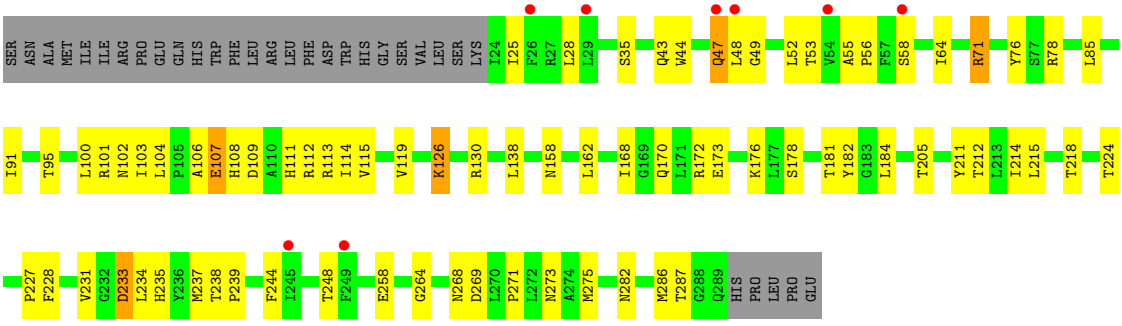
• Molecule 1: Bestrophin homolog

Chain D:



• Molecule 1: Bestrophin homolog

Chain E:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.43 (at 2.55Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.230 , 0.276 0.233 , 0.280	Depositor DCC
R_{free} test set	1998 reflections (2.10%)	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)	0.30 , 64.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.53	0/2148	0.69	0/2927
1	B	0.49	0/2130	0.66	0/2905
1	C	0.55	0/2146	0.69	1/2926 (0.0%)
1	D	0.52	0/2138	0.65	0/2915
1	E	0.57	0/2143	0.70	0/2920
All	All	0.53	0/10705	0.68	1/14593 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	206	PRO	N-CA-C	-5.66	97.39	112.10

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	2102	0	2133	85	0
1	B	2084	0	2111	83	0
1	C	2100	0	2123	65	0
1	D	2093	0	2115	110	0
1	E	2098	0	2140	87	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	364	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 17.

All (364) 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: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
1:E:107:GLU:CG	1:E:176:LYS:HZ1	1.87	0.86
1:C:207:VAL:CG2	1:C:208:PRO:HD3	2.05	0.85
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:83:ARG:CD	1:D:201:ARG:HD2	2.18	0.73
1:E:107:GLU:HG3	1:E:176:LYS:HZ1	1.44	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:A:127:HIS:HD1	1:A:132:THR:HG1	1.36	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:C:59:LEU:HD13	1:E:58:SER:CA	2.22	0.70
1:E:107:GLU:CG	1:E:176:LYS:HZ3	2.05	0.69
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:E:107:GLU:CD	1:E:176:LYS:HZ3	1.97	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:D:270:LEU:HB3	1:D:275:MET:CE	2.31	0.60
1:E:107:GLU:HG2	1:E:176:LYS:HZ1	1.66	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:A:207:VAL:HG11	1:A:260:GLU:CD	2.23	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:HIS:HA	1:B:91:ILE:HD13	1.86	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:A:210:ALA:C	1:A:211:TYR:HD1	2.07	0.56
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:33:LEU:C	1:A:36:ILE:HG13	2.26	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:D:270:LEU:HB3	1:D:275:MET:HE3	1.88	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: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:E:91:ILE:O	1:E:95:THR:HG23	2.07	0.55
1:A:83:ARG:CZ	1:A:275:MET:HE3	2.37	0.54
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
1:A:251:SER:HB2	1:E:214:ILE:HD12	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:ARG:C	1:B:71:ARG:HD2	2.29	0.53
1:D:128:GLN:OE1	3:D:403:HOH:O	2.18	0.53
1:E:47:GLN:CD	1:E:48:LEU:HD12	2.29	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:D:35:SER:OG	1:D:239:PRO:HB3	2.09	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:A:100:LEU:HA	1:A:185:MET:HE1	1.90	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: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:B:183:GLY:HA2	1:D:184:LEU:HD11	1.93	0.50
1:C:259:LEU:HD21	1:D:208:PRO:HG3	1.94	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:43:GLN:HG3	1:E:44:TRP:CD1	2.46	0.50
1:E:107:GLU:HG3	1:E:176:LYS:HZ3	1.66	0.49
1:E:52:LEU:HD12	1:E:228:PHE:HB3	1.94	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:44:TRP:C	1:B:46:GLU:H	2.16	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: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
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:D:272:LEU:HD23	1:D:275:MET:HE3	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:TRP:C	1:B:46:GLU:N	2.67	0.47
1:B:79:PHE:O	1:B:83:ARG:HG3	2.14	0.47
1:D:107:GLU:OE2	1:D:176:LYS:NZ	2.28	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:D:104:LEU:CD1	1:D:111:HIS:HE2	2.28	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:D:133:ASP:OD2	1:D:135:THR:OG1	2.22	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:C:283:LEU:HD23	1:C:286:MET:HE3	1.98	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: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
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:D:270:LEU:HB3	1:D:275:MET:HE1	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:SER:HA	1:B:257:GLU:CG	2.38	0.44
1:C:158:ASN:OD1	1:E:286:MET:HE1	2.18	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: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
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:B:38:ALA:O	1:B:42:TYR:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:168:ILE:HG22	1:E:182:TYR:CE1	2.54	0.42
1:E:286:MET:HE3	1:E:286:MET:HB2	1.93	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:D:269:ASP:O	1:D:270:LEU:C	2.56	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:B:94:ARG:HG2	1:B:286:MET:HE1	2.02	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:E:258:GLU:CD	1:E:268:ASN:HD22	2.20	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
1:A:33:LEU:CA	1:A:36:ILE:HG13	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:126:LYS:C	1:E:126:LYS:HD2	2.41	0.41
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

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	265/297 (89%)	257 (97%)	7 (3%)	1 (0%)	34	46
1	B	264/297 (89%)	255 (97%)	8 (3%)	1 (0%)	34	46
1	C	266/297 (90%)	258 (97%)	7 (3%)	1 (0%)	34	46
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%)	47	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	45	TYR

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Mol	Chain	Res	Type
1	C	208	PRO
1	A	208	PRO

5.3.2 Protein sidechains (i)

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%)	215 (95%)	11 (5%)	25	34
1	B	223/259 (86%)	217 (97%)	6 (3%)	44	59
1	C	224/259 (86%)	217 (97%)	7 (3%)	40	54
1	D	224/259 (86%)	212 (95%)	12 (5%)	22	29
1	E	226/259 (87%)	219 (97%)	7 (3%)	40	54
All	All	1123/1295 (87%)	1080 (96%)	43 (4%)	33	45

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	MET
1	A	36	ILE
1	A	40	ILE
1	A	58	SER
1	A	107	GLU
1	A	156	PRO
1	A	180	ILE
1	A	209	PHE
1	A	213	LEU
1	A	220	TYR
1	A	233	ASP
1	B	109	ASP
1	B	126	LYS
1	B	155	MET
1	B	159	ARG
1	B	170	GLN
1	B	172	ARG

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Mol	Chain	Res	Type
1	C	35	SER
1	C	58	SER
1	C	154	SER
1	C	172	ARG
1	C	188	LYS
1	C	207	VAL
1	C	233	ASP
1	D	34	MET
1	D	73	SER
1	D	126	LYS
1	D	139	ARG
1	D	146	ARG
1	D	211	TYR
1	D	231	VAL
1	D	234	LEU
1	D	244	PHE
1	D	268	ASN
1	D	281	ARG
1	D	289	GLN
1	E	47	GLN
1	E	71	ARG
1	E	107	GLU
1	E	126	LYS
1	E	172	ARG
1	E	233	ASP
1	E	282	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) 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	290	HIS
1	D	72	ASN
1	D	235	HIS
1	E	235	HIS
1	E	273	ASN
1	E	289	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.58	22 (8%) 11 14	56, 83, 112, 127	0
1	B	266/297 (89%)	0.75	28 (10%) 6 8	59, 89, 122, 143	0
1	C	268/297 (90%)	0.77	18 (6%) 17 21	49, 75, 114, 134	0
1	D	268/297 (90%)	0.62	22 (8%) 11 14	52, 81, 120, 140	0
1	E	266/297 (89%)	0.67	8 (3%) 50 57	51, 75, 115, 137	0
All	All	1335/1485 (89%)	0.68	98 (7%) 15 18	49, 81, 117, 143	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	204	THR	8.8
1	E	47	GLN	7.0
1	A	220	TYR	7.0
1	A	59	LEU	6.7
1	B	48	LEU	6.7
1	E	48	LEU	6.6
1	C	60	LEU	5.7
1	B	47	GLN	5.6
1	D	48	LEU	5.6
1	B	236	TYR	5.5
1	E	26	PHE	5.0
1	C	205	THR	4.6
1	B	154	SER	4.6
1	C	59	LEU	4.5
1	B	62	ILE	4.5
1	D	44	TRP	4.5
1	B	226	LEU	4.4
1	A	22	SER	4.4
1	A	24	ILE	4.3
1	B	44	TRP	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	24	ILE	4.2
1	D	47	GLN	4.2
1	D	27	ARG	3.9
1	A	210	ALA	3.8
1	A	217	ARG	3.8
1	B	58	SER	3.8
1	D	207	VAL	3.8
1	B	245	ILE	3.5
1	C	23	LYS	3.5
1	A	55	ALA	3.5
1	E	245	ILE	3.4
1	C	236	TYR	3.3
1	B	59	LEU	3.3
1	B	57	PHE	3.2
1	A	222	PHE	3.2
1	B	222	PHE	3.2
1	A	62	ILE	3.2
1	B	114	ILE	3.2
1	C	47	GLN	3.1
1	D	208	PRO	3.1
1	A	219	VAL	3.1
1	B	56	PRO	3.1
1	A	54	VAL	3.0
1	C	249	PHE	3.0
1	D	209	PHE	3.0
1	B	100	LEU	3.0
1	C	52	LEU	3.0
1	B	213	LEU	2.9
1	B	284	LEU	2.9
1	C	290	HIS	2.8
1	D	32	VAL	2.8
1	A	221	LEU	2.8
1	D	30	LEU	2.8
1	C	58	SER	2.8
1	D	59	LEU	2.8
1	D	220	TYR	2.8
1	A	27	ARG	2.7
1	B	26	PHE	2.7
1	D	43	GLN	2.7
1	C	207	VAL	2.7
1	B	244	PHE	2.7
1	B	55	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	56	PRO	2.6
1	B	60	LEU	2.6
1	D	49	GLY	2.6
1	D	106	ALA	2.6
1	E	54	VAL	2.5
1	C	57	PHE	2.5
1	D	31	ASN	2.5
1	B	230	LEU	2.5
1	A	26	PHE	2.5
1	A	204	THR	2.5
1	C	64	ILE	2.4
1	D	245	ILE	2.4
1	C	62	ILE	2.4
1	A	207	VAL	2.3
1	B	231	VAL	2.3
1	D	26	PHE	2.3
1	C	45	TYR	2.3
1	C	219	VAL	2.2
1	A	53	THR	2.2
1	D	25	ILE	2.2
1	D	288	GLY	2.2
1	B	117	TYR	2.2
1	A	25	ILE	2.2
1	E	29	LEU	2.2
1	B	42	TYR	2.2
1	E	249	PHE	2.2
1	D	205	THR	2.1
1	C	222	PHE	2.1
1	A	57	PHE	2.1
1	A	60	LEU	2.1
1	A	96	LEU	2.1
1	A	58	SER	2.1
1	B	209	PHE	2.1
1	E	58	SER	2.0
1	B	155	MET	2.0
1	B	170	GLN	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 monosaccharides 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, 95^{th} 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	E	302	1/1	0.92	0.29	83,83,83,83	0
2	ZN	D	301	1/1	0.93	0.15	149,149,149,149	0
2	ZN	B	302	1/1	0.93	0.26	102,102,102,102	0
2	ZN	C	301	1/1	0.94	0.31	77,77,77,77	0
2	ZN	A	303	1/1	0.95	0.29	98,98,98,98	0
2	ZN	D	302	1/1	0.96	0.28	85,85,85,85	0
2	ZN	C	302	1/1	0.97	0.33	76,76,76,76	0
2	ZN	A	302	1/1	0.98	0.23	78,78,78,78	0
2	ZN	A	301	1/1	0.98	0.23	71,71,71,71	0
2	ZN	B	301	1/1	0.99	0.28	73,73,73,73	0
2	ZN	E	301	1/1	1.00	0.23	70,70,70,70	0

6.5 Other polymers (i)

There are no such residues in this entry.