W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Oct 31, 2023 – 05:33 PM EDT

PDB ID	:	3IIO
Title	:	Evolutionary optimization of computationally designed enzymes: Kemp eliminases of the KE07 series
Authors	:	Khersonsky, O.; Dym, O.; Tawfik, D.S.
Deposited on	:	2009-08-03
Resolution	:	2.25 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

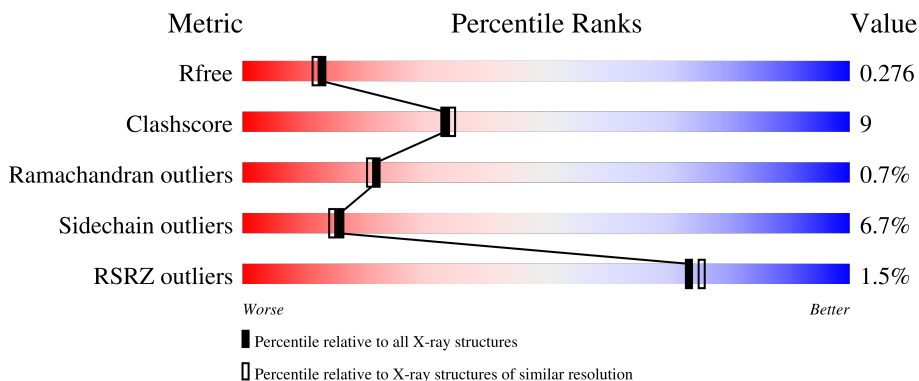|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.25 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.
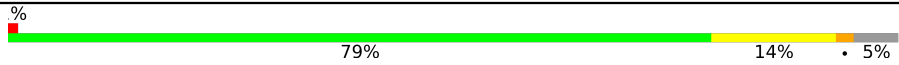
Metric	Percentile Ranks	Value
Rfree		0.276
Clashscore		9
Ramachandran outliers		0.7%
Sidechain outliers		6.7%
RSRZ outliers		1.5%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	262	79% 15% · 5%
1	B	262	.% 77% 16% · 5%
1	C	262	75% 15% · · 5%
1	D	262	.% 76% 16% · 5%
1	E	262	5% 67% 26% · 5%

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Mol	Chain	Length	Quality of chain
1	F	262	% 79% 14% · 5%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 11835 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 KE07.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total 1934	C 1232	N 332	O 366	S 4	0	0	0
1	B	250	Total 1947	C 1241	N 334	O 368	S 4	0	0	0
1	C	248	Total 1934	C 1232	N 332	O 366	S 4	0	0	0
1	D	250	Total 1947	C 1241	N 334	O 368	S 4	0	0	0
1	E	248	Total 1934	C 1232	N 332	O 366	S 4	0	0	0
1	F	248	Total 1934	C 1232	N 332	O 366	S 4	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	43	Total 43	O 43	0	0
2	B	36	Total 36	O 36	0	0
2	C	58	Total 58	O 58	0	0
2	D	41	Total 41	O 41	0	0
2	E	12	Total 12	O 12	0	0
2	F	15	Total 15	O 15	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: KE07

Chain A:
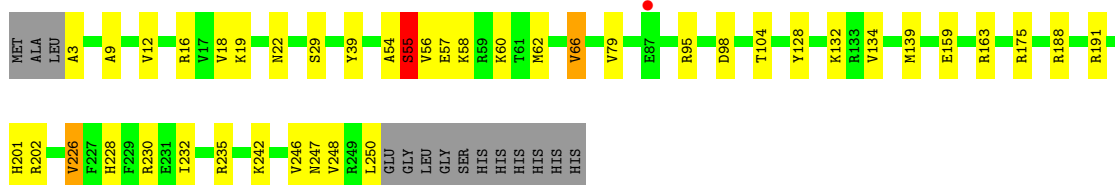
- Molecule 1: KE07

Chain B:
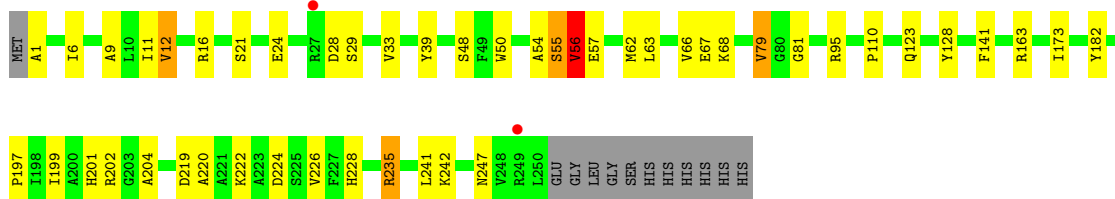
- Molecule 1: KE07

Chain C:

- Molecule 1: KE07

Chain D:

L153 R154 D155 W156 I173 D174 R175 K179 I199 A200 H201 R202 M207 E208 A220 A221 K222 A223 D224 S225 V226 E231 E236 L237 Y240 L250 GLU GLY LEU GLY SER HIS HIS HIS HIS HIS

• Molecule 1: KE07

Chain E:

5%

67%   26%   • 5%

MET ALA LEU A3 K4 D7 R16 N22 N25 L26 R27 K37 F38 I42 E46 L47 S48 F49 W50 A54 S55 V56 R59 V66 E67 K68 Q72 I73 P76 V79 H84 D85 S90 L94 R95 K99 N103 V107 E108 N109 P110

S111 L112 I113 T114 Q118 T119 F120 G121 S122 V125 Y128 K132 D135 Y143 S144 G145 E146 K147 L152 L153 R154 D155 W156 V157 G164 A165 G166 E167 I173 D174 R175 L176 G181 T184 I187 R188 I199 A200 H201 R202 G203 M207 E208 H209 F214

A220 A221 K222 A223 D224 S225 V226 F227 R230 D233 E236 L237 Y240 L241 V246 N247 V248 R249 L250 GLU GLY LEU GLY SER HIS HIS HIS HIS HIS

• Molecule 1: KE07

Chain F:

%

79%   14%   • 5%

MET ALA LEU A3 V12 K13 D14 G15 R16 R27 D28 S29 K37 F38 I42 G43 L47 S48 I52 T53 A54 S55 V56 E57 L63 V66 Q72 I73 D74 I75 V79 E91 R95 S111 Y128 K132 R175 L176 Y182 I199 A200 H201

R202 G203 A204 E208 E212 A213 A220 A221 K222 A223 D224 S225 V226 R235 K238 L250 GLU GLY LEU GLY SER HIS HIS HIS HIS HIS

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	106.58Å 106.58Å 128.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.25 49.24 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-2.25) 99.1 (49.24-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.215 , 0.278 0.214 , 0.276	Depositor DCC
R_{free} test set	3874 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	32.7	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 10.4	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l 0.328 for h,-h-k,-l 0.033 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11835	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

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	0.77	0/1965	0.80	3/2649 (0.1%)
1	B	0.71	0/1978	0.79	1/2667 (0.0%)
1	C	0.74	0/1965	0.80	1/2649 (0.0%)
1	D	0.68	1/1978 (0.1%)	0.73	0/2667
1	E	0.59	0/1965	0.68	1/2649 (0.0%)
1	F	0.67	0/1965	0.69	0/2649
All	All	0.70	1/11816 (0.0%)	0.75	6/15930 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	91	GLU	CG-CD	6.37	1.61	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	79	VAL	CB-CA-C	-7.06	97.98	111.40
1	A	188	ARG	NE-CZ-NH1	-6.63	116.98	120.30
1	A	188	ARG	NE-CZ-NH2	5.59	123.10	120.30
1	E	250	LEU	CA-CB-CG	5.26	127.40	115.30
1	A	191	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	C	79	VAL	CB-CA-C	-5.14	101.64	111.40

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	1934	0	1956	27	0
1	B	1947	0	1975	32	0
1	C	1934	0	1956	38	0
1	D	1947	0	1975	38	0
1	E	1934	0	1956	49	0
1	F	1934	0	1956	18	0
2	A	43	0	0	2	0
2	B	36	0	0	2	0
2	C	58	0	0	2	0
2	D	41	0	0	5	0
2	E	12	0	0	6	0
2	F	15	0	0	1	0
All	All	11835	0	11774	200	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 9.

All (200) 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:B:55:SER:HB3	1:B:56:VAL:CA	1.71	1.18
1:B:55:SER:CB	1:B:56:VAL:HA	1.77	1.15
1:D:55:SER:HB3	1:D:56:VAL:HA	1.19	1.11
1:F:13:LYS:HG3	1:F:52:ILE:HG13	1.31	1.11
1:A:55:SER:HB2	1:A:56:VAL:HA	1.37	1.03
1:C:249:ARG:HG3	1:C:249:ARG:HH11	1.18	1.02
1:C:55:SER:HB2	1:C:56:VAL:HA	1.44	0.99
1:D:55:SER:CB	1:D:56:VAL:HA	2.00	0.92
1:E:114:THR:HG22	1:E:118:GLN:HE21	1.32	0.90
1:B:199:ILE:HD12	1:B:220:ALA:HB3	1.53	0.89
1:D:55:SER:HB3	1:D:56:VAL:CA	2.01	0.89
1:B:33:VAL:HG21	1:B:68:LYS:HG2	1.54	0.88
1:A:55:SER:CB	1:A:56:VAL:HA	2.05	0.85
1:B:235:ARG:HH11	1:B:235:ARG:HB2	1.41	0.85
1:E:122:SER:HB2	1:E:164:GLY:O	1.76	0.85
1:D:63:LEU:HD21	1:D:91:GLU:HG2	1.56	0.85
1:C:179:LYS:NZ	1:C:231:GLU:OE1	2.11	0.84
1:C:249:ARG:HH11	1:C:249:ARG:CG	1.91	0.83
1:B:55:SER:HB3	1:B:56:VAL:HA	0.87	0.83
1:C:249:ARG:HG3	1:C:249:ARG:NH1	1.90	0.80
1:D:66:VAL:HG12	1:D:79:VAL:HG11	1.64	0.79
1:F:63:LEU:HD21	1:F:91:GLU:HG3	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:GLU:HG2	2:D:275:HOH:O	1.82	0.78
1:C:207:MET:HE3	1:C:236:GLU:HB3	1.65	0.76
1:B:33:VAL:HG21	1:B:68:LYS:CG	2.15	0.76
1:B:9:ALA:HB2	1:B:222:LYS:HD3	1.67	0.76
1:E:246:VAL:HG12	1:E:248:VAL:HG13	1.66	0.76
1:F:54:ALA:O	1:F:57:GLU:HG2	1.85	0.76
1:E:122:SER:CB	1:E:164:GLY:O	2.33	0.75
1:D:63:LEU:HD11	1:D:91:GLU:CD	2.08	0.74
1:A:55:SER:HB2	1:A:56:VAL:CA	2.15	0.72
1:D:199:ILE:HD12	1:D:220:ALA:HB3	1.71	0.72
1:C:55:SER:CB	1:C:56:VAL:HA	2.19	0.72
2:A:269:HOH:O	1:B:1:ALA:HB2	1.90	0.71
1:D:16:ARG:NH2	1:D:28:ASP:OD2	2.22	0.70
1:B:62:MET:O	1:B:66:VAL:HG13	1.91	0.70
1:F:48:SER:OG	1:F:222:LYS:HE3	1.90	0.70
1:F:16:ARG:HH22	1:F:28:ASP:CG	1.96	0.69
1:E:184:THR:O	1:E:188:ARG:HG3	1.91	0.69
1:F:128:TYR:OH	1:F:201:HIS:HD2	1.76	0.69
1:D:128:TYR:OH	1:D:201:HIS:HD2	1.77	0.67
1:D:63:LEU:CD2	1:D:91:GLU:HG2	2.25	0.67
1:C:207:MET:CE	1:C:236:GLU:HB3	2.24	0.66
1:F:199:ILE:HD12	1:F:220:ALA:HB3	1.76	0.66
1:E:48:SER:HB2	2:E:273:HOH:O	1.95	0.66
1:E:128:TYR:OH	1:E:201:HIS:HD2	1.79	0.65
1:D:179:LYS:HE3	1:D:231:GLU:OE1	1.96	0.65
1:C:152:LEU:HD13	1:C:154:ARG:NH1	2.12	0.65
1:B:16:ARG:NH2	1:B:28:ASP:OD2	2.30	0.64
1:D:66:VAL:CG1	1:D:79:VAL:HG11	2.28	0.64
1:E:202:ARG:HG2	1:E:202:ARG:HH21	1.61	0.64
1:C:207:MET:HE1	1:C:236:GLU:C	2.18	0.63
1:E:22:ASN:HB2	1:E:230:ARG:HG3	1.80	0.63
1:F:66:VAL:HG12	1:F:79:VAL:HG11	1.78	0.63
1:A:98:ASP:OD2	1:B:1:ALA:HB1	1.99	0.63
1:E:114:THR:HG22	1:E:118:GLN:NE2	2.10	0.62
1:A:55:SER:CB	1:A:56:VAL:CA	2.76	0.62
1:E:37:LYS:HD2	1:E:72:GLN:HB3	1.82	0.62
1:D:63:LEU:CD1	1:D:91:GLU:OE2	2.48	0.61
1:C:55:SER:HB2	1:C:56:VAL:CA	2.21	0.61
1:E:56:VAL:HG23	2:E:262:HOH:O	1.99	0.61
1:C:67:GLU:O	1:C:71:GLU:HG3	2.01	0.61
1:C:226:VAL:CG1	1:C:232:ILE:HD12	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:LEU:HD13	1:D:91:GLU:OE2	2.01	0.60
1:C:84:HIS:HD2	2:C:307:HOH:O	1.85	0.60
1:C:54:ALA:O	1:C:55:SER:O	2.20	0.60
1:C:233:ASP:HB3	1:C:236:GLU:HB2	1.83	0.59
1:E:208:GLU:HG3	1:E:240:TYR:OH	2.02	0.59
1:D:207:MET:HE2	1:D:237:LEU:N	2.18	0.59
1:C:226:VAL:HG11	1:C:232:ILE:HD12	1.84	0.58
1:D:54:ALA:O	1:D:55:SER:O	2.23	0.57
1:D:55:SER:CB	1:D:56:VAL:CA	2.73	0.57
1:E:103:ASN:O	1:E:107:VAL:HG23	2.05	0.57
1:B:55:SER:C	1:B:57:GLU:H	2.08	0.56
1:E:128:TYR:OH	1:E:201:HIS:CD2	2.58	0.56
1:E:199:ILE:HD13	1:E:199:ILE:N	2.20	0.56
1:D:12:VAL:HG13	2:D:294:HOH:O	2.06	0.56
1:C:139:MET:SD	1:C:152:LEU:HD23	2.47	0.55
1:E:202:ARG:HH21	1:E:202:ARG:CG	2.18	0.55
1:B:54:ALA:O	1:B:55:SER:O	2.23	0.55
1:E:94:LEU:HD21	1:E:120:PHE:HE1	1.72	0.55
1:E:176:LEU:HB2	1:E:202:ARG:HD3	1.89	0.54
1:B:235:ARG:HH11	1:B:235:ARG:CB	2.17	0.54
1:A:226:VAL:HG11	1:A:232:ILE:HD12	1.90	0.54
1:F:43:GLY:O	1:F:238:LYS:HE3	2.07	0.54
1:C:87:GLU:O	1:C:91:GLU:HG3	2.07	0.54
1:C:122:SER:HB2	1:C:164:GLY:O	2.09	0.53
1:A:226:VAL:CG1	1:A:232:ILE:HD12	2.39	0.53
1:E:122:SER:HB3	1:E:164:GLY:O	2.08	0.52
1:C:39:TYR:OH	1:C:228:HIS:HD2	1.93	0.52
1:B:128:TYR:OH	1:B:201:HIS:HD2	1.92	0.52
1:F:182:TYR:CZ	1:F:204:ALA:HB2	2.45	0.52
1:A:242:LYS:HD3	2:A:278:HOH:O	2.09	0.52
1:B:55:SER:CB	1:B:56:VAL:CA	2.55	0.52
1:B:197:PRO:HA	1:B:219:ASP:OD2	2.10	0.51
1:B:242:LYS:NZ	1:B:247:ASN:OD1	2.43	0.51
1:D:55:SER:C	1:D:57:GLU:H	2.14	0.51
1:E:99:LYS:NZ	1:E:167:GLU:OE1	2.38	0.51
1:A:55:SER:C	1:A:57:GLU:H	2.13	0.51
1:A:54:ALA:O	1:A:55:SER:O	2.29	0.50
1:C:199:ILE:HG13	1:C:220:ALA:HB3	1.91	0.50
1:E:153:LEU:O	1:E:157:VAL:HG23	2.11	0.50
1:A:9:ALA:O	1:A:228:HIS:HE1	1.94	0.50
1:C:55:SER:CB	1:C:56:VAL:CA	2.86	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:TYR:OH	1:A:228:HIS:HD2	1.95	0.50
1:C:16:ARG:NH2	1:C:28:ASP:OD2	2.45	0.49
1:E:207:MET:HE3	1:E:236:GLU:HB3	1.94	0.49
1:C:242:LYS:HG2	1:C:250:LEU:HD12	1.93	0.49
1:D:141:PHE:HB2	1:D:173:ILE:HD11	1.94	0.49
1:E:4:LYS:HB3	1:E:214:PHE:CE1	2.48	0.49
1:E:207:MET:HE2	1:E:240:TYR:HB2	1.93	0.49
1:F:47:LEU:HG	1:F:75:ILE:HD11	1.94	0.49
1:A:9:ALA:O	1:A:228:HIS:CE1	2.66	0.49
1:B:110:PRO:HB2	1:B:163:ARG:CZ	2.42	0.49
1:D:63:LEU:CD1	1:D:91:GLU:CD	2.81	0.48
1:A:104:THR:HG21	1:C:143:TYR:HE1	1.77	0.48
1:F:37:LYS:HD2	1:F:72:GLN:HB3	1.94	0.48
1:C:128:TYR:OH	1:C:201:HIS:HD2	1.95	0.48
1:E:7:ASP:O	1:E:222:LYS:HA	2.12	0.48
1:E:110:PRO:CG	2:E:271:HOH:O	2.62	0.48
1:E:199:ILE:HG23	1:E:220:ALA:HB3	1.96	0.48
1:E:181:GLY:O	1:E:203:GLY:HA3	2.13	0.47
1:D:13:LYS:HB2	1:D:52:ILE:HG13	1.96	0.47
1:B:39:TYR:OH	1:B:228:HIS:HD2	1.97	0.47
1:C:91:GLU:O	1:C:95:ARG:HB2	2.14	0.47
1:B:12:VAL:HG13	2:B:294:HOH:O	2.15	0.47
1:B:29:SER:HB3	2:B:273:HOH:O	2.14	0.47
1:E:184:THR:HA	1:E:187:ILE:HD12	1.97	0.47
1:E:173:ILE:HG13	2:E:270:HOH:O	2.15	0.47
1:E:66:VAL:CG1	1:E:79:VAL:HG11	2.44	0.46
1:C:175:ARG:NH1	2:C:310:HOH:O	1.97	0.46
1:D:207:MET:CE	2:D:292:HOH:O	2.62	0.46
1:E:233:ASP:OD2	1:E:236:GLU:N	2.46	0.46
1:E:223:ALA:HB3	1:E:227:PHE:CE2	2.51	0.46
1:D:5:ARG:HG2	1:D:45:ASP:HB2	1.97	0.46
1:A:55:SER:HA	1:A:58:LYS:H	1.82	0.45
1:D:208:GLU:HG3	1:D:240:TYR:OH	2.17	0.45
1:E:122:SER:O	1:E:166:GLY:HA3	2.16	0.45
1:E:110:PRO:HG2	2:E:271:HOH:O	2.16	0.45
1:F:63:LEU:HD22	1:F:95:ARG:NH1	2.32	0.45
1:B:6:ILE:HD11	1:B:241:LEU:CD1	2.47	0.45
1:F:175:ARG:NH1	2:F:268:HOH:O	2.50	0.44
1:C:14:ASP:HA	1:C:61:THR:HG21	1.98	0.44
1:B:182:TYR:CZ	1:B:204:ALA:HB2	2.52	0.44
1:E:132:LYS:HG3	1:E:174:ASP:OD1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:202:ARG:CG	1:E:202:ARG:NH2	2.77	0.44
1:C:56:VAL:HG12	1:C:56:VAL:O	2.17	0.44
1:E:241:LEU:HB3	1:E:246:VAL:HB	2.00	0.44
1:A:159:GLU:OE1	1:A:163:ARG:NE	2.44	0.44
1:E:237:LEU:O	1:E:241:LEU:HG	2.18	0.44
1:B:11:ILE:HD12	1:B:11:ILE:H	1.83	0.43
1:A:62:MET:O	1:A:66:VAL:HG13	2.17	0.43
1:B:33:VAL:HG21	1:B:68:LYS:HG3	1.99	0.43
1:D:63:LEU:HD11	1:D:91:GLU:OE2	2.16	0.43
1:E:113:ILE:HG23	1:E:125:VAL:HG11	2.00	0.43
1:E:110:PRO:CB	2:E:271:HOH:O	2.66	0.43
1:A:57:GLU:HA	1:A:57:GLU:OE1	2.18	0.43
1:C:59:ARG:NH2	1:C:91:GLU:OE2	2.52	0.43
1:E:152:LEU:HB2	1:E:155:ASP:OD1	2.18	0.43
1:D:156:TRP:HA	1:D:156:TRP:CE3	2.53	0.42
1:D:175:ARG:HA	1:D:175:ARG:HD3	1.89	0.42
1:E:90:SER:O	1:E:94:LEU:HG	2.19	0.42
1:A:18:VAL:O	1:A:19:LYS:HB2	2.20	0.42
1:A:39:TYR:OH	1:A:228:HIS:CD2	2.73	0.42
1:D:141:PHE:HB2	1:D:173:ILE:CD1	2.49	0.42
1:F:182:TYR:CD2	1:F:213:ALA:HB2	2.54	0.42
1:C:178:THR:C	1:C:179:LYS:HG2	2.40	0.42
1:E:181:GLY:HA2	1:E:209:HIS:CG	2.54	0.42
1:B:11:ILE:HD12	1:B:11:ILE:N	2.34	0.42
1:A:134:VAL:HB	1:A:139:MET:HG3	2.02	0.42
1:A:55:SER:C	1:A:57:GLU:N	2.74	0.42
1:B:21:SER:O	1:B:29:SER:OG	2.38	0.42
1:B:50:TRP:CZ2	1:B:81:GLY:HA2	2.54	0.42
1:C:68:LYS:NZ	1:C:72:GLN:HE22	2.17	0.42
1:D:207:MET:HE1	1:D:236:GLU:HB3	2.02	0.42
1:A:22:ASN:HB2	1:A:230:ARG:HG3	2.02	0.41
1:C:206:LYS:HG2	1:C:209:HIS:CE1	2.55	0.41
1:E:46:GLU:HG2	1:E:76:PRO:HD2	2.02	0.41
1:A:242:LYS:HG2	1:A:250:LEU:HD12	2.03	0.41
1:E:201:HIS:O	1:E:202:ARG:HB2	2.19	0.41
1:D:199:ILE:HD13	1:D:199:ILE:N	2.35	0.41
1:D:28:ASP:HB3	2:D:295:HOH:O	2.21	0.41
1:D:67:GLU:O	1:D:71:GLU:HG2	2.21	0.41
1:B:141:PHE:HB2	1:B:173:ILE:CD1	2.50	0.41
1:D:70:ALA:HA	2:D:279:HOH:O	2.20	0.41
1:A:128:TYR:OH	1:A:201:HIS:HD2	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:38:PHE:O	1:F:42:ILE:HG13	2.20	0.41
1:A:3:ALA:HA	1:A:247:ASN:O	2.21	0.41
1:B:63:LEU:O	1:B:67:GLU:HB2	2.21	0.41
1:D:39:TYR:HA	1:D:42:ILE:HG12	2.03	0.41
1:A:246:VAL:HG12	1:A:248:VAL:HG13	2.03	0.41
1:C:207:MET:CE	1:C:237:LEU:N	2.83	0.41
1:C:249:ARG:CG	1:C:249:ARG:NH1	2.61	0.41
1:E:26:LEU:HD21	1:E:38:PHE:HB2	2.03	0.41
1:D:48:SER:OG	1:D:222:LYS:HE3	2.21	0.41
1:D:152:LEU:HD13	1:D:154:ARG:NH1	2.36	0.40
1:F:208:GLU:O	1:F:212:GLU:HG3	2.21	0.40
1:F:66:VAL:CG1	1:F:79:VAL:HG11	2.48	0.40
1:C:7:ASP:O	1:C:222:LYS:HA	2.21	0.40
1:E:27:ARG:NH1	1:E:27:ARG:HB3	2.36	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	246/262 (94%)	236 (96%)	8 (3%)	2 (1%)	19	17
1	B	248/262 (95%)	240 (97%)	5 (2%)	3 (1%)	13	9
1	C	246/262 (94%)	237 (96%)	7 (3%)	2 (1%)	19	17
1	D	248/262 (95%)	233 (94%)	13 (5%)	2 (1%)	19	17
1	E	246/262 (94%)	230 (94%)	15 (6%)	1 (0%)	34	37
1	F	246/262 (94%)	232 (94%)	13 (5%)	1 (0%)	34	37
All	All	1480/1572 (94%)	1408 (95%)	61 (4%)	11 (1%)	22	21

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	SER
1	B	55	SER
1	C	14	ASP
1	C	55	SER
1	D	55	SER
1	E	55	SER
1	F	202	ARG
1	B	202	ARG
1	D	202	ARG
1	A	202	ARG
1	B	56	VAL

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	204/215 (95%)	192 (94%)	12 (6%)	19	19
1	B	205/215 (95%)	195 (95%)	10 (5%)	25	27
1	C	204/215 (95%)	186 (91%)	18 (9%)	10	8
1	D	205/215 (95%)	190 (93%)	15 (7%)	14	12
1	E	204/215 (95%)	190 (93%)	14 (7%)	15	14
1	F	204/215 (95%)	191 (94%)	13 (6%)	17	16
All	All	1226/1290 (95%)	1144 (93%)	82 (7%)	16	15

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	16	ARG
1	A	29	SER
1	A	55	SER
1	A	60	LYS
1	A	66	VAL
1	A	79	VAL
1	A	95	ARG

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Mol	Chain	Res	Type
1	A	132	LYS
1	A	175	ARG
1	A	226	VAL
1	A	235	ARG
1	B	12	VAL
1	B	24	GLU
1	B	48	SER
1	B	56	VAL
1	B	79	VAL
1	B	95	ARG
1	B	123	GLN
1	B	224	ASP
1	B	226	VAL
1	B	235	ARG
1	C	12	VAL
1	C	14	ASP
1	C	16	ARG
1	C	24	GLU
1	C	29	SER
1	C	48	SER
1	C	55	SER
1	C	68	LYS
1	C	71	GLU
1	C	73	ILE
1	C	79	VAL
1	C	91	GLU
1	C	95	ARG
1	C	99	LYS
1	C	154	ARG
1	C	226	VAL
1	C	249	ARG
1	C	250	LEU
1	D	12	VAL
1	D	16	ARG
1	D	27	ARG
1	D	29	SER
1	D	48	SER
1	D	55	SER
1	D	56	VAL
1	D	74	ASP
1	D	85	ASP
1	D	95	ARG

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Mol	Chain	Res	Type
1	D	111	SER
1	D	123	GLN
1	D	154	ARG
1	D	224	ASP
1	D	226	VAL
1	E	16	ARG
1	E	73	ILE
1	E	79	VAL
1	E	85	ASP
1	E	95	ARG
1	E	107	VAL
1	E	111	SER
1	E	146	GLU
1	E	147	LYS
1	E	199	ILE
1	E	224	ASP
1	E	226	VAL
1	E	230	ARG
1	E	250	LEU
1	F	12	VAL
1	F	13	LYS
1	F	14	ASP
1	F	16	ARG
1	F	29	SER
1	F	57	GLU
1	F	73	ILE
1	F	95	ARG
1	F	111	SER
1	F	132	LYS
1	F	224	ASP
1	F	226	VAL
1	F	235	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	HIS
1	A	115	GLN
1	A	201	HIS
1	A	228	HIS
1	B	118	GLN
1	B	201	HIS

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Mol	Chain	Res	Type
1	B	228	HIS
1	C	72	GLN
1	C	84	HIS
1	C	118	GLN
1	C	201	HIS
1	C	228	HIS
1	D	72	GLN
1	D	118	GLN
1	D	123	GLN
1	D	201	HIS
1	D	228	HIS
1	E	118	GLN
1	E	201	HIS
1	E	228	HIS
1	F	84	HIS
1	F	201	HIS
1	F	228	HIS

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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

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	248/262 (94%)	-0.34	1 (0%)	92	93	13, 26, 41, 51	0
1	B	250/262 (95%)	-0.33	2 (0%)	86	87	16, 28, 44, 59	0
1	C	248/262 (94%)	-0.41	0	100	100	14, 25, 38, 49	0
1	D	250/262 (95%)	-0.26	3 (1%)	79	81	17, 30, 48, 64	0
1	E	248/262 (94%)	0.26	13 (5%)	27	30	32, 49, 72, 79	0
1	F	248/262 (94%)	-0.11	3 (1%)	79	81	27, 41, 58, 75	0
All	All	1492/1572 (94%)	-0.20	22 (1%)	73	75	13, 33, 60, 79	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	135	ASP	4.1
1	E	54	ALA	4.0
1	B	249	ARG	4.0
1	E	25	ASN	3.6
1	F	56	VAL	3.3
1	E	68	LYS	2.9
1	F	27	ARG	2.9
1	D	91	GLU	2.8
1	F	176	LEU	2.6
1	E	84	HIS	2.6
1	E	145	GLY	2.5
1	E	56	VAL	2.5
1	D	27	ARG	2.3
1	E	59	ARG	2.3
1	E	109	ASN	2.3
1	E	42	ILE	2.3
1	B	27	ARG	2.2
1	E	143	TYR	2.1
1	D	50	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	87	GLU	2.1
1	E	50	TRP	2.1
1	E	26	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.