WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:11 am GMT

PDB ID	:	3FD8
Title	:	Crystal Structure of an oxidoreductase from Enterococcus faecalis
Authors	:	Damodharan, L.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2008-11-25
Resolution	:	2.45 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
http://wwpdb.org/validation/2016/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:

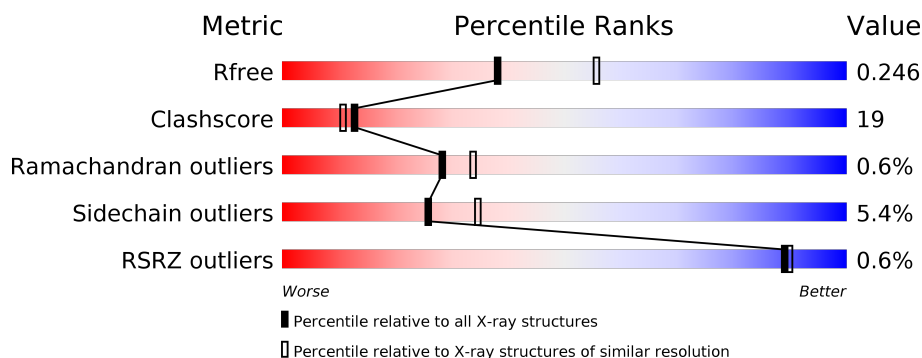|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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 2.45 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		0.246
Clashscore		19
Ramachandran outliers		0.6%
Sidechain outliers		5.4%
RSRZ outliers		0.6%

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}	100719	1119 (2.48-2.44)
Clashscore	112137	1193 (2.48-2.44)
Ramachandran outliers	110173	1185 (2.48-2.44)
Sidechain outliers	110143	1185 (2.48-2.44)
RSRZ outliers	101464	1126 (2.48-2.44)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	359	70% 26% • •
1	B	359	64% 30% • •
1	C	359	% 62% 32% • •
1	D	359	66% 28% • •
1	E	359	% 63% 30% • •
1	F	359	65% 29% • • •

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The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PGE	F	360	-	-	-	X

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 17472 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 Oxidoreductase, Gfo/Idh/MocA family.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	Se	0	0	0
			2767	1769	458	530	2	8			
1	B	348	Total	C	N	O	S	Se	0	0	0
			2767	1769	458	530	2	8			
1	C	347	Total	C	N	O	S	Se	0	0	0
			2758	1764	457	527	2	8			
1	D	349	Total	C	N	O	S	Se	0	0	0
			2773	1772	459	532	2	8			
1	E	349	Total	C	N	O	S	Se	0	0	0
			2775	1773	460	532	2	8			
1	F	349	Total	C	N	O	S	Se	0	0	0
			2773	1772	459	532	2	8			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	expression tag	UNP Q835X4
A	2	SER	-	expression tag	UNP Q835X4
A	3	LEU	-	expression tag	UNP Q835X4
A	352	GLU	-	expression tag	UNP Q835X4
A	353	GLY	-	expression tag	UNP Q835X4
A	354	HIS	-	expression tag	UNP Q835X4
A	355	HIS	-	expression tag	UNP Q835X4
A	356	HIS	-	expression tag	UNP Q835X4
A	357	HIS	-	expression tag	UNP Q835X4
A	358	HIS	-	expression tag	UNP Q835X4
A	359	HIS	-	expression tag	UNP Q835X4
B	1	MSE	-	expression tag	UNP Q835X4
B	2	SER	-	expression tag	UNP Q835X4
B	3	LEU	-	expression tag	UNP Q835X4
B	352	GLU	-	expression tag	UNP Q835X4
B	353	GLY	-	expression tag	UNP Q835X4
B	354	HIS	-	expression tag	UNP Q835X4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	355	HIS	-	expression tag	UNP Q835X4
B	356	HIS	-	expression tag	UNP Q835X4
B	357	HIS	-	expression tag	UNP Q835X4
B	358	HIS	-	expression tag	UNP Q835X4
B	359	HIS	-	expression tag	UNP Q835X4
C	1	MSE	-	expression tag	UNP Q835X4
C	2	SER	-	expression tag	UNP Q835X4
C	3	LEU	-	expression tag	UNP Q835X4
C	352	GLU	-	expression tag	UNP Q835X4
C	353	GLY	-	expression tag	UNP Q835X4
C	354	HIS	-	expression tag	UNP Q835X4
C	355	HIS	-	expression tag	UNP Q835X4
C	356	HIS	-	expression tag	UNP Q835X4
C	357	HIS	-	expression tag	UNP Q835X4
C	358	HIS	-	expression tag	UNP Q835X4
C	359	HIS	-	expression tag	UNP Q835X4
D	1	MSE	-	expression tag	UNP Q835X4
D	2	SER	-	expression tag	UNP Q835X4
D	3	LEU	-	expression tag	UNP Q835X4
D	352	GLU	-	expression tag	UNP Q835X4
D	353	GLY	-	expression tag	UNP Q835X4
D	354	HIS	-	expression tag	UNP Q835X4
D	355	HIS	-	expression tag	UNP Q835X4
D	356	HIS	-	expression tag	UNP Q835X4
D	357	HIS	-	expression tag	UNP Q835X4
D	358	HIS	-	expression tag	UNP Q835X4
D	359	HIS	-	expression tag	UNP Q835X4
E	1	MSE	-	expression tag	UNP Q835X4
E	2	SER	-	expression tag	UNP Q835X4
E	3	LEU	-	expression tag	UNP Q835X4
E	352	GLU	-	expression tag	UNP Q835X4
E	353	GLY	-	expression tag	UNP Q835X4
E	354	HIS	-	expression tag	UNP Q835X4
E	355	HIS	-	expression tag	UNP Q835X4
E	356	HIS	-	expression tag	UNP Q835X4
E	357	HIS	-	expression tag	UNP Q835X4
E	358	HIS	-	expression tag	UNP Q835X4
E	359	HIS	-	expression tag	UNP Q835X4
F	1	MSE	-	expression tag	UNP Q835X4
F	2	SER	-	expression tag	UNP Q835X4
F	3	LEU	-	expression tag	UNP Q835X4
F	352	GLU	-	expression tag	UNP Q835X4

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Chain	Residue	Modelled	Actual	Comment	Reference
F	353	GLY	-	expression tag	UNP Q835X4
F	354	HIS	-	expression tag	UNP Q835X4
F	355	HIS	-	expression tag	UNP Q835X4
F	356	HIS	-	expression tag	UNP Q835X4
F	357	HIS	-	expression tag	UNP Q835X4
F	358	HIS	-	expression tag	UNP Q835X4
F	359	HIS	-	expression tag	UNP Q835X4

- Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).
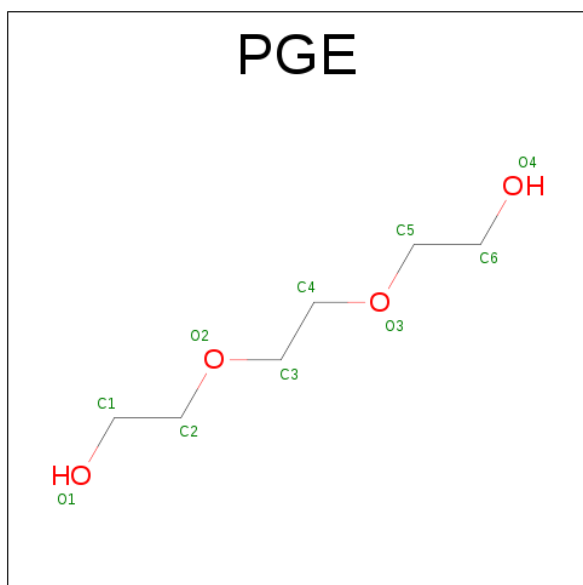
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total 10	C 6	O 4	0	0
2	C	1	Total 10	C 6	O 4	0	0
2	F	1	Total 10	C 6	O 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	132	Total 132	O 132	0	0
3	B	142	Total 142	O 142	0	0
3	C	112	Total 112	O 112	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	142	Total 142	O 142	0	0
3	E	137	Total 137	O 137	0	0
3	F	164	Total 164	O 164	0	0

3 Residue-property plots ⓘ

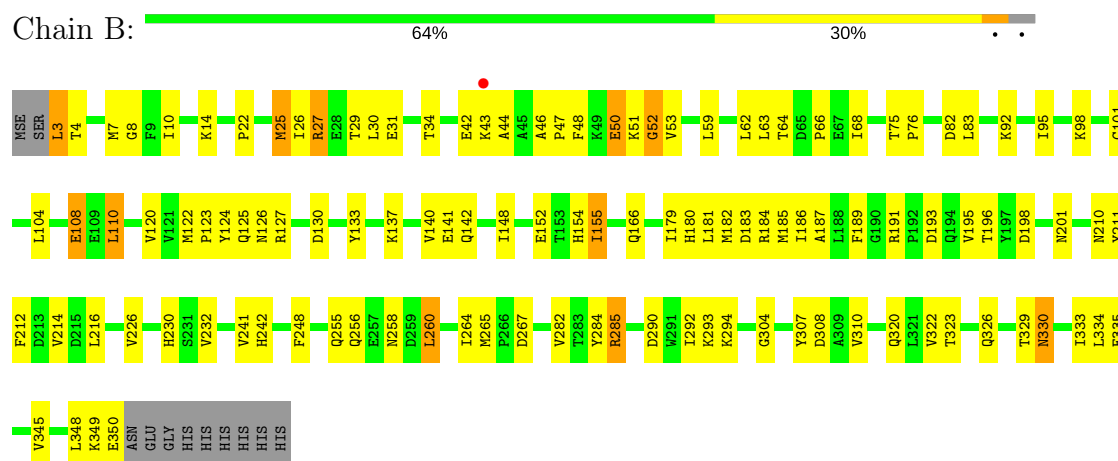These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.
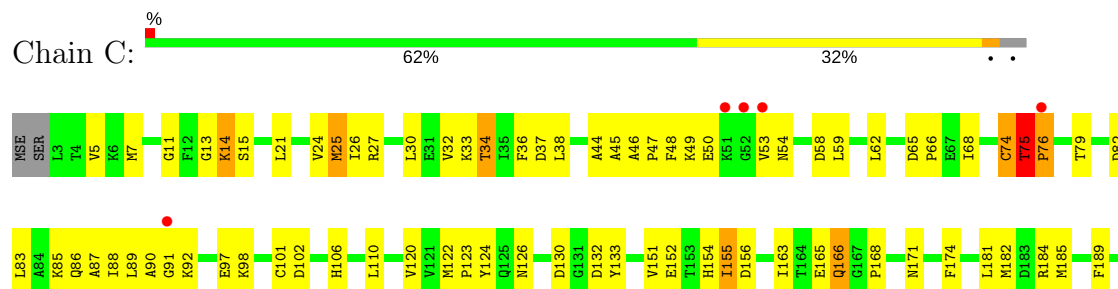
- Molecule 1: Oxidoreductase, Gfo/Idh/MocA family

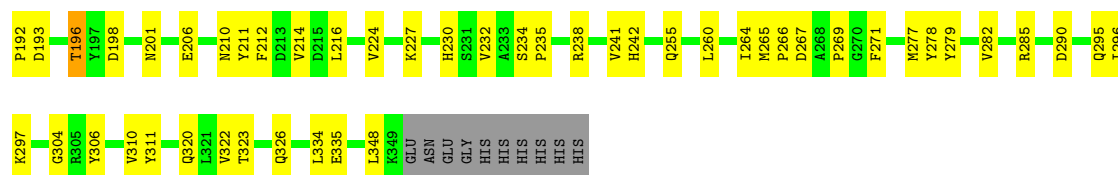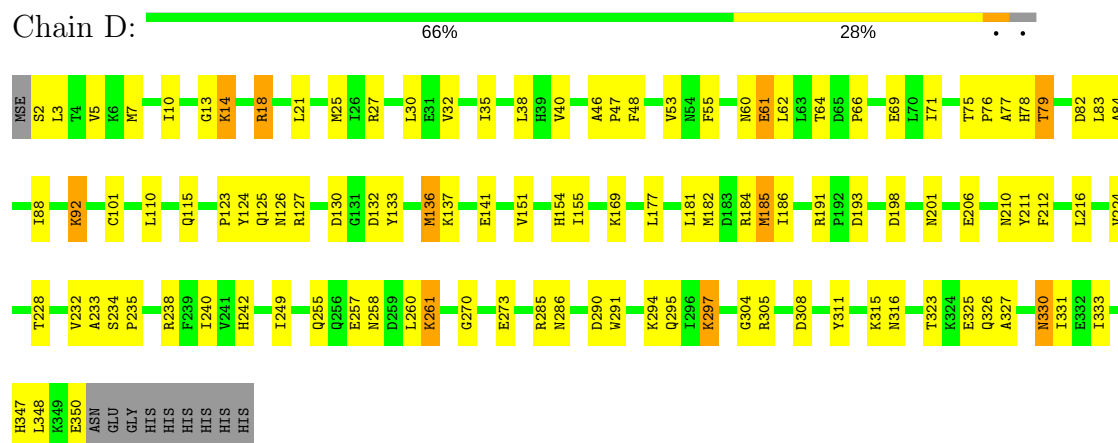Chain A:

- Molecule 1: Oxidoreductase, Gfo/Idh/MocA family

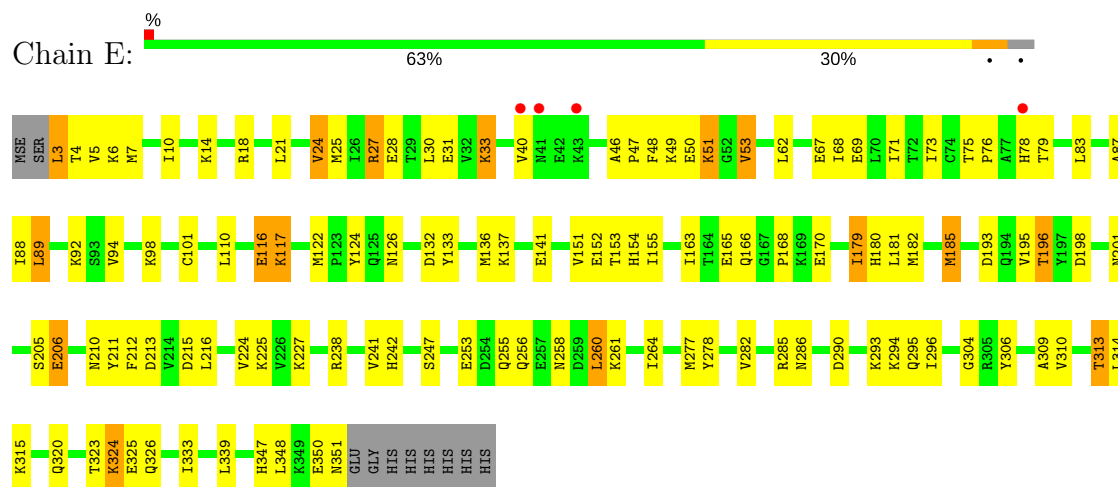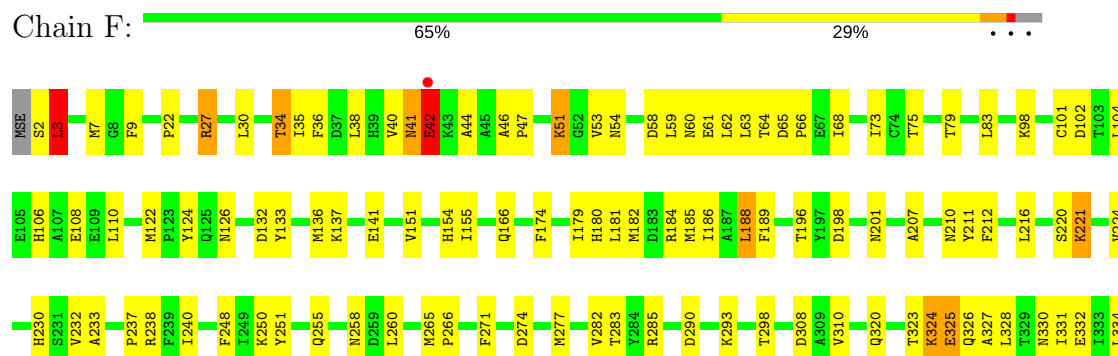Chain B:

- Molecule 1: Oxidoreductase, Gfo/Idh/MocA family

Chain C:

P192 D193 T196 Y197 D198 N201 E206 N210 Y211 F212 D213 V214 D215 L216 V224 K227 H230 S231 V232 A233 S234 P235 R238 V241 H242 Q255 L260 I264 M265 P266 D267 A268 P269 G270 F271 M277 Y278 Y279 V282 R285 D290 Q295 I296

K297 G304 R305 Y306 V310 Y311 Q320 L321 V322 T323 Q326 L334 E335 L348 K349 GLU ASN GLU GLY HIS HIS HIS HIS HIS HIS

• Molecule 1: Oxidoreductase, Gfo/Idh/MocA family

Chain D:

66% 28%

MSE S2 L3 T4 V5 K6 M7 I10 G13 K14 R18 L21 M25 I26 R27 L30 E31 V32 I35 L38 H39 V40 A46 P47 F48 V53 N54 F55 N60 E61 L62 L63 T64 D65 P66 E69 L70 I71 T75 P76 A77 H78 T79 D82 L83 A84

I88 K92 C101 L110 Q115 P123 Y124 Q125 N126 R127 D130 G131 D132 Y133 M136 K137 E141 V151 H154 I155 K169 L177 L181 M182 D183 R184 M185 I186 R191 P192 D193 D198 N201 E206 N210 Y211 F212 L216 V224

T228 V232 A233 S234 P235 R238 F239 I240 V241 H242 I249 Q255 Q256 E257 N258 D259 L260 K261 G270 E273 R285 N286 D290 W291 K294 Q295 K297 G304 R305 A327 D308 Y311 K315 N316 T323 K324 E325 Q326 A327 N330 I331 E332 I333

H347 L348 K349 E350 ASN GLU GLY HIS HIS HIS HIS HIS HIS

• Molecule 1: Oxidoreductase, Gfo/Idh/MocA family

Chain E:

%
63% 30%

MSE SER L3 T4 V5 K6 M7 I10 K14 R18 L21 V24 M25 I26 R27 E28 T29 L30 E31 V32 K33 V40 N41 E42 K43 A46 P47 F48 K49 E50 K51 G52 V53 L62 E67 I68 E69 L70 I71 I72 I73 C74 T75 P76 A77 H78 T79 L83 A87

I88 L89 K92 S93 V94 K98 C101 L110 E116 K117 M122 P123 Y124 Q125 N126 D132 Y133 M136 K137 E141 V151 E152 T153 H154 I155 I163 T164 E165 Q166 G167 P168 K169 E170 I179 H180 L181 M182 M185 D193 Q194 V195 T196 Y197 D198 N201

S205 E206 N210 Y211 F212 D213 V214 D215 L216 V224 K225 V226 K227 R238 V241 H242 S247 E253 D254 Q255 Q256 E257 N258 D259 L260 K261 I264 M277 Y278 V282 R285 N286 D290 K293 K294 Q295 I296 G304 R305 Y306 A309 V310 T313 L314

K315 Q320 T323 K324 E325 Q326 I333 L339 H347 L348 H347 K349 E350 N351 GLU GLY HIS HIS HIS HIS HIS

• Molecule 1: Oxidoreductase, Gfo/Idh/MocA family

Chain F:

65% 29%

MSE S2 L3 M7 G8 F9 P22 R27 L30 T34 I35 F36 D37 L38 H39 V40 N41 E42 K43 A44 A45 A46 P47 K51 G52 V53 N54 D58 L59 N60 E61 L62 L63 T64 D65 P66 E67 I68 I73 C74 T75 T79 L83 K98 C101 D102 T103 L104

E105 H106 A107 E108 E109 L110 M122 P123 Y124 Q125 N126 D132 Y133 M136 K137 E141 V151 H154 I155 Q166 F174 I179 H180 L181 M182 D183 R184 M185 I186 A187 L188 F189 T196 Y197 D198 N201 A207 N210 Y211 F212 L216 S220 K221 V224

H230 S231 V232 A233 P237 R238 F239 I240 F248 I249 K250 Y251 Q255 N258 D259 L260 M265 P266 F271 D274 M277 V282 T283 Y284 R285 D290 K293 T298 D308 A309 V310 Q320 T323 K324 E325 Q326 A327 L328 T329 N330 I331 E332 I333 L334

H347 L348 K349 E350 ASN GLU GLY HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.57Å 151.32Å 161.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.14 – 2.45 48.80 – 2.45	Depositor EDS
% Data completeness (in resolution range)	91.4 (48.14-2.45) 95.2 (48.80-2.45)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.57 (at 2.45Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.196 , 0.240 0.202 , 0.246	Depositor DCC
R_{free} test set	4539 reflections (5.03%)	DCC
Wilson B-factor (Å^2)	23.6	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 40.1	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	17472	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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 (i)

5.1   Standard geometry (i)

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

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	0.35	0/2826	0.64	0/3815
1	B	0.36	0/2826	0.65	1/3815 (0.0%)
1	C	0.35	0/2817	0.69	1/3803 (0.0%)
1	D	0.36	0/2832	0.66	0/3823
1	E	0.37	0/2834	0.67	0/3826
1	F	0.38	0/2832	0.68	0/3823
All	All	0.36	0/16967	0.66	2/22905 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	75	THR	N-CA-C	7.36	130.86	111.00
1	B	52	GLY	N-CA-C	5.03	125.69	113.10

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	2767	0	2692	82	0
1	B	2767	0	2692	102	0
1	C	2758	0	2686	111	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2773	0	2697	105	0
1	E	2775	0	2698	129	0
1	F	2773	0	2697	100	0
2	B	10	0	14	1	0
2	C	10	0	14	5	0
2	F	10	0	14	2	0
3	A	132	0	0	5	0
3	B	142	0	0	8	0
3	C	112	0	0	9	0
3	D	142	0	0	10	0
3	E	137	0	0	7	0
3	F	164	0	0	5	0
All	All	17472	0	16204	608	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 19.

All (608) 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:E:185:MSE:HG2	1:E:224:VAL:HG11	1.23	1.18
1:D:185:MSE:HG2	1:D:224:VAL:HG11	1.30	1.13
1:E:182:MSE:HE1	1:E:333:ILE:HG21	1.33	1.11
1:C:182:MSE:HE2	1:C:216:LEU:HD21	1.19	1.10
1:F:155:ILE:HD13	1:F:181:LEU:HD21	1.22	1.10
1:D:182:MSE:CE	1:D:216:LEU:HD21	1.83	1.08
1:F:182:MSE:HE2	1:F:216:LEU:HD21	1.38	1.06
1:C:48:PHE:HB3	1:C:53:VAL:HG11	1.42	1.02
1:B:182:MSE:HE2	1:B:216:LEU:HD11	1.42	0.98
1:E:31:GLU:HB3	1:E:33:LYS:HZ1	1.28	0.98
1:D:182:MSE:HE2	1:D:216:LEU:HD21	1.43	0.98
1:E:6:LYS:HD2	1:E:67:GLU:HG3	1.48	0.95
1:E:25:MSE:HA	1:E:25:MSE:HE2	1.49	0.94
1:E:182:MSE:CE	1:E:216:LEU:HD21	1.99	0.93
1:D:7:MSE:CE	1:D:30:LEU:HB3	2.01	0.91
1:B:7:MSE:HE1	1:B:30:LEU:HD23	1.53	0.90
1:F:155:ILE:CD1	1:F:181:LEU:HD21	2.03	0.89
1:C:7:MSE:HE2	1:C:30:LEU:HD12	1.55	0.89
1:A:136:MSE:HE1	1:A:188:LEU:HD22	1.55	0.88
1:D:155:ILE:HD13	1:D:181:LEU:HD21	1.52	0.88
1:C:182:MSE:CE	1:C:216:LEU:HD21	2.04	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:349:LYS:O	1:F:350:GLU:HB2	1.70	0.87
1:B:182:MSE:CE	1:B:216:LEU:HD21	2.05	0.86
1:F:7:MSE:HE3	1:F:30:LEU:HB3	1.58	0.86
1:D:185:MSE:HE3	1:D:185:MSE:HA	1.57	0.85
1:F:7:MSE:CE	1:F:30:LEU:HD12	2.08	0.82
1:A:350:GLU:HG2	1:A:350:GLU:O	1.80	0.81
1:E:75:THR:HG21	1:E:83:LEU:HD12	1.61	0.81
1:B:3:LEU:HD13	1:B:4:THR:H	1.45	0.81
1:D:132:ASP:OD1	1:D:238:ARG:HG2	1.81	0.81
1:B:98:LYS:HE3	1:B:180:HIS:NE2	1.96	0.81
1:E:7:MSE:HE3	1:E:30:LEU:HB3	1.61	0.80
1:D:115:GLN:HG3	3:D:415:HOH:O	1.81	0.80
1:C:14:LYS:H	1:C:14:LYS:HE2	1.45	0.80
1:C:25:MSE:HA	1:C:25:MSE:HE3	1.61	0.80
1:E:255:GLN:HE22	1:E:258:ASN:HD22	1.31	0.79
1:E:7:MSE:HE2	1:E:30:LEU:HD12	1.64	0.79
1:B:182:MSE:HE1	1:B:216:LEU:HD21	1.65	0.79
1:B:7:MSE:CE	1:B:30:LEU:HB3	2.14	0.78
1:E:132:ASP:OD1	1:E:238:ARG:HG2	1.84	0.77
1:E:75:THR:HG23	1:E:79:THR:HG23	1.67	0.77
1:F:34:THR:HG21	3:F:716:HOH:O	1.85	0.77
1:D:7:MSE:HE2	1:D:30:LEU:HD12	1.68	0.76
1:F:182:MSE:CE	1:F:216:LEU:HD21	2.14	0.76
1:F:237:PRO:HG2	1:F:240:ILE:HD11	1.66	0.76
1:F:154:HIS:O	1:F:155:ILE:HD12	1.85	0.76
1:B:182:MSE:HE1	1:B:333:ILE:HG21	1.67	0.76
1:B:25:MSE:HE3	1:B:25:MSE:HA	1.67	0.75
1:C:14:LYS:H	1:C:14:LYS:CE	2.00	0.75
1:F:42:GLU:H	1:F:42:GLU:CD	1.89	0.75
1:A:101:CYS:SG	1:A:110:LEU:HD22	2.25	0.75
1:D:185:MSE:CG	1:D:224:VAL:HG11	2.13	0.75
1:E:25:MSE:HA	1:E:25:MSE:CE	2.17	0.75
1:D:101:CYS:SG	1:D:110:LEU:HD22	2.26	0.75
1:E:48:PHE:O	1:E:53:VAL:HG13	1.87	0.75
1:E:185:MSE:HA	1:E:185:MSE:CE	2.16	0.74
1:C:48:PHE:O	1:C:53:VAL:HG12	1.88	0.74
1:E:7:MSE:CE	1:E:30:LEU:HD12	2.17	0.74
1:F:75:THR:HG21	1:F:83:LEU:HD12	1.69	0.74
1:C:185:MSE:HG3	1:C:224:VAL:HG11	1.69	0.74
1:C:75:THR:HG23	1:C:79:THR:CG2	2.18	0.74
1:D:182:MSE:HE2	1:D:216:LEU:CD2	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:152:GLU:OE2	1:E:154:HIS:HE1	1.71	0.73
1:B:3:LEU:CD1	1:B:4:THR:H	2.01	0.73
1:E:185:MSE:HG2	1:E:224:VAL:CG1	2.12	0.72
1:C:7:MSE:HE3	1:C:30:LEU:HB3	1.71	0.72
1:D:136:MSE:HE3	1:D:137:LYS:N	2.05	0.72
1:D:206:GLU:H	1:D:206:GLU:CD	1.93	0.71
1:C:14:LYS:N	1:C:14:LYS:HE2	2.06	0.71
1:C:265:MSE:HE3	3:C:389:HOH:O	1.91	0.71
1:D:14:LYS:NZ	1:D:14:LYS:H	1.88	0.71
1:C:34:THR:HG23	1:C:68:ILE:HD11	1.72	0.70
1:D:46:ALA:HB3	1:D:47:PRO:HD3	1.72	0.70
1:C:27:ARG:NH2	1:C:304:GLY:HA3	2.06	0.70
1:B:26:ILE:HD13	1:B:267:ASP:HB3	1.74	0.69
1:D:18:ARG:NH1	1:D:261:LYS:HB3	2.07	0.69
1:A:255:GLN:HE21	1:D:294:LYS:HD3	1.57	0.68
1:D:182:MSE:O	1:D:186:ILE:HG12	1.94	0.68
1:C:14:LYS:H	1:C:14:LYS:CD	2.06	0.68
1:D:347:HIS:HB2	3:D:518:HOH:O	1.92	0.68
1:D:155:ILE:CD1	1:D:181:LEU:HD21	2.23	0.68
1:E:6:LYS:HD3	1:E:33:LYS:CD	2.23	0.68
1:C:201:ASN:HA	1:C:210:ASN:OD1	1.93	0.68
1:E:163:ILE:HD12	1:E:210:ASN:HB2	1.76	0.67
1:A:255:GLN:NE2	1:D:294:LYS:HD3	2.10	0.67
1:C:76:PRO:O	1:C:79:THR:HG22	1.94	0.67
1:E:31:GLU:CB	1:E:33:LYS:HZ1	2.06	0.67
1:B:195:VAL:HG21	1:B:333:ILE:HD12	1.77	0.66
1:B:82:ASP:HB3	3:B:410:HOH:O	1.95	0.66
1:D:10:ILE:HG21	1:D:83:LEU:HD13	1.76	0.66
1:D:48:PHE:O	1:D:53:VAL:HG22	1.96	0.66
1:F:182:MSE:O	1:F:186:ILE:HG12	1.96	0.66
1:F:122:MSE:HE1	1:F:310:VAL:HG22	1.79	0.65
1:B:46:ALA:HB3	1:B:47:PRO:HD3	1.77	0.65
1:D:27:ARG:NH2	1:D:304:GLY:HA3	2.11	0.65
1:A:205:SER:HB3	3:A:824:HOH:O	1.97	0.65
1:B:30:LEU:HD21	1:B:307:TYR:HB3	1.79	0.65
1:B:3:LEU:HD13	1:B:4:THR:N	2.12	0.65
1:C:46:ALA:HB3	1:C:47:PRO:HD3	1.78	0.65
1:D:76:PRO:O	1:D:79:THR:HG22	1.96	0.65
1:E:255:GLN:NE2	1:E:258:ASN:HD22	1.95	0.65
2:C:360:PGE:H42	1:E:293:LYS:NZ	2.12	0.65
1:F:2:SER:O	1:F:3:LEU:HB2	1.98	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:7:MSE:HE2	1:F:30:LEU:HD12	1.79	0.65
1:C:58:ASP:O	1:C:59:LEU:HB3	1.98	0.64
1:B:10:ILE:HG21	1:B:83:LEU:HD13	1.80	0.64
1:C:323:THR:OG1	1:C:326:GLN:HG3	1.97	0.64
1:D:7:MSE:HE3	1:D:30:LEU:HB3	1.78	0.63
1:B:155:ILE:HG13	1:B:181:LEU:HD21	1.78	0.63
1:B:27:ARG:HD3	1:B:308:ASP:OD1	1.97	0.63
1:B:294:LYS:HD3	1:C:255:GLN:HE21	1.63	0.63
1:E:50:GLU:O	1:E:51:LYS:HB2	1.97	0.63
1:C:285:ARG:HG3	1:C:285:ARG:HH11	1.64	0.63
1:B:123:PRO:HB2	1:B:125:GLN:HE21	1.62	0.63
1:A:18:ARG:NH1	1:A:261:LYS:NZ	2.46	0.63
1:E:206:GLU:H	1:E:206:GLU:CD	2.02	0.62
1:A:295:GLN:HG3	1:E:277:MSE:HE2	1.80	0.62
1:B:210:ASN:O	1:B:230:HIS:HD2	1.82	0.62
1:C:152:GLU:OE2	1:C:154:HIS:HE1	1.81	0.62
1:A:201:ASN:HA	1:A:210:ASN:OD1	1.99	0.62
1:C:101:CYS:SG	1:C:110:LEU:HD22	2.39	0.62
1:C:75:THR:HG23	1:C:79:THR:HG23	1.79	0.62
1:D:154:HIS:O	1:D:155:ILE:HD12	2.00	0.62
1:D:10:ILE:HD13	1:D:71:ILE:CG2	2.30	0.62
1:F:327:ALA:O	1:F:331:ILE:HD13	2.00	0.61
1:B:255:GLN:HE22	1:B:258:ASN:HD22	1.48	0.61
1:A:75:THR:HB	1:A:76:PRO:HD2	1.82	0.61
1:B:63:LEU:O	1:B:92:LYS:HE2	2.00	0.61
1:C:75:THR:HG21	1:C:83:LEU:CD1	2.30	0.61
1:D:155:ILE:O	1:D:155:ILE:HG22	1.99	0.61
1:F:132:ASP:OD1	1:F:238:ARG:HG2	2.01	0.61
1:D:13:GLY:HA3	1:D:14:LYS:HZ1	1.66	0.61
1:E:3:LEU:HD12	1:E:315:LYS:HZ1	1.65	0.61
1:F:210:ASN:O	1:F:230:HIS:HD2	1.83	0.61
1:A:85:LYS:O	1:A:89:LEU:HG	2.01	0.61
1:E:225:LYS:HD3	1:E:227:LYS:HD2	1.82	0.60
1:C:85:LYS:O	1:C:89:LEU:HD13	2.01	0.60
1:F:133:TYR:CE1	1:F:136:MSE:HE1	2.36	0.60
1:F:151:VAL:HG11	1:F:185:MSE:CE	2.32	0.60
1:C:168:PRO:HD2	1:C:171:ASN:ND2	2.16	0.60
1:A:276:PRO:HA	1:A:279:TYR:CD1	2.37	0.60
1:C:25:MSE:HB2	3:C:470:HOH:O	2.03	0.59
1:E:50:GLU:O	1:E:51:LYS:CB	2.50	0.59
1:F:75:THR:HG21	1:F:83:LEU:CD1	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:PHE:CE2	1:C:334:LEU:HD12	2.37	0.59
1:D:27:ARG:HD3	1:D:308:ASP:OD1	2.03	0.59
1:D:2:SER:HA	1:D:315:LYS:HE3	1.83	0.59
1:F:324:LYS:HD2	1:F:328:LEU:HD12	1.85	0.59
1:B:133:TYR:CE1	1:B:184:ARG:HB2	2.37	0.59
1:E:201:ASN:HA	1:E:210:ASN:OD1	2.03	0.59
1:F:104:LEU:O	1:F:108:GLU:HG3	2.01	0.59
1:F:237:PRO:CG	1:F:240:ILE:HD11	2.32	0.59
1:E:185:MSE:HA	1:E:185:MSE:HE3	1.84	0.59
1:C:7:MSE:CE	1:C:30:LEU:HB3	2.32	0.58
1:C:44:ALA:O	1:C:47:PRO:HD2	2.03	0.58
1:D:84:ALA:O	1:D:88:ILE:HG12	2.03	0.58
1:F:185:MSE:HE1	1:F:189:PHE:HE2	1.67	0.58
1:F:75:THR:HG23	1:F:79:THR:OG1	2.03	0.58
1:A:27:ARG:HD3	1:A:308:ASP:OD1	2.03	0.58
1:F:185:MSE:CE	1:F:189:PHE:HE2	2.16	0.58
1:C:36:PHE:CZ	1:C:59:LEU:HB2	2.38	0.58
1:B:201:ASN:HA	1:B:210:ASN:OD1	2.03	0.58
1:C:122:MSE:SE	1:C:320:GLN:HB2	2.53	0.58
1:D:18:ARG:HH12	1:D:261:LYS:NZ	2.01	0.58
1:E:196:THR:HB	1:E:215:ASP:HB2	1.86	0.58
1:F:201:ASN:HA	1:F:210:ASN:OD1	2.04	0.58
1:A:136:MSE:HE3	1:A:137:LYS:CA	2.34	0.58
1:E:286:ASN:ND2	1:E:290:ASP:HB2	2.19	0.58
1:C:25:MSE:HA	1:C:25:MSE:CE	2.33	0.58
1:D:185:MSE:CE	1:D:185:MSE:HA	2.31	0.58
1:D:182:MSE:HE1	1:D:333:ILE:HG21	1.85	0.58
1:D:216:LEU:HD23	1:D:216:LEU:N	2.18	0.57
1:E:182:MSE:CE	1:E:333:ILE:HG21	2.21	0.57
1:D:182:MSE:HE3	1:D:216:LEU:HD21	1.79	0.57
1:D:75:THR:HB	1:D:79:THR:HG21	1.85	0.57
1:E:27:ARG:NH2	3:E:512:HOH:O	2.38	0.57
1:F:182:MSE:HE2	1:F:216:LEU:CD2	2.24	0.57
1:A:136:MSE:HE1	1:A:188:LEU:CD2	2.33	0.57
1:B:152:GLU:OE2	1:B:154:HIS:HE1	1.87	0.57
1:C:26:ILE:O	1:C:26:ILE:HG22	2.05	0.57
1:B:182:MSE:O	1:B:186:ILE:HG12	2.03	0.57
1:E:309:ALA:O	1:E:313:THR:HG22	2.05	0.57
2:C:360:PGE:H42	1:E:293:LYS:HZ2	1.68	0.57
1:C:75:THR:HG21	1:C:83:LEU:HD12	1.87	0.57
1:D:10:ILE:HD13	1:D:71:ILE:HG23	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:ALA:HB3	1:E:47:PRO:HD3	1.87	0.57
1:C:65:ASP:O	1:C:92:LYS:NZ	2.38	0.57
1:E:182:MSE:HE2	1:E:216:LEU:HD11	1.87	0.56
1:A:3:LEU:O	1:A:3:LEU:HD22	2.06	0.56
1:E:182:MSE:HE3	1:E:216:LEU:HD21	1.84	0.56
1:E:68:ILE:O	1:E:92:LYS:HE3	2.05	0.56
1:A:137:LYS:O	1:A:141:GLU:HG3	2.04	0.56
1:B:293:LYS:NZ	2:B:360:PGE:H42	2.21	0.56
1:B:179:ILE:HD12	1:B:330:ASN:OD1	2.06	0.56
1:F:155:ILE:HD13	1:F:181:LEU:CD2	2.16	0.56
1:E:3:LEU:HD13	1:E:4:THR:H	1.70	0.56
1:A:102:ASP:OD1	1:A:106:HIS:HD2	1.89	0.56
1:A:75:THR:HB	1:A:76:PRO:CD	2.35	0.56
1:B:256:GLN:O	1:B:260:LEU:HD22	2.05	0.56
1:C:132:ASP:OD1	1:C:238:ARG:HG2	2.05	0.56
1:B:183:ASP:HA	1:B:330:ASN:ND2	2.20	0.56
1:C:34:THR:HG21	3:C:419:HOH:O	2.05	0.56
1:E:6:LYS:HD3	1:E:33:LYS:NZ	2.20	0.56
1:A:179:ILE:HG23	1:A:180:HIS:N	2.20	0.56
1:E:6:LYS:CG	1:E:33:LYS:HZ2	2.19	0.56
1:F:137:LYS:O	1:F:141:GLU:HG3	2.06	0.56
1:B:137:LYS:O	1:B:141:GLU:HG3	2.06	0.56
1:E:168:PRO:HB2	1:E:170:GLU:OE1	2.05	0.56
1:C:155:ILE:HG13	1:C:181:LEU:HD21	1.88	0.55
1:A:137:LYS:HE3	3:A:387:HOH:O	2.06	0.55
1:A:237:PRO:HG3	1:A:251:TYR:CZ	2.41	0.55
1:B:329:THR:O	1:B:333:ILE:HG12	2.06	0.55
1:D:75:THR:CB	1:D:79:THR:HG21	2.37	0.55
1:E:6:LYS:HD3	1:E:33:LYS:HD2	1.88	0.55
1:D:61:GLU:HG3	3:D:534:HOH:O	2.06	0.55
1:A:18:ARG:NH1	1:A:261:LYS:HZ3	2.04	0.55
1:B:350:GLU:HB3	3:B:481:HOH:O	2.06	0.55
1:C:306:TYR:O	1:C:310:VAL:HG23	2.07	0.55
1:C:48:PHE:HB3	1:C:53:VAL:CG1	2.28	0.55
1:D:18:ARG:NH1	1:D:261:LYS:NZ	2.55	0.55
1:F:266:PRO:HA	1:F:271:PHE:CD2	2.41	0.55
1:A:250:LYS:HE3	1:A:278:TYR:O	2.07	0.55
1:C:130:ASP:HB3	1:C:132:ASP:OD2	2.06	0.55
1:D:185:MSE:HG2	1:D:224:VAL:CG1	2.21	0.55
1:D:7:MSE:CE	1:D:30:LEU:HD12	2.36	0.55
1:D:18:ARG:NH1	1:D:261:LYS:HZ3	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:34:THR:OG1	1:F:62:LEU:HD13	2.05	0.55
1:B:264:ILE:N	1:B:264:ILE:HD12	2.22	0.55
1:D:137:LYS:O	1:D:141:GLU:HG3	2.07	0.55
1:F:179:ILE:HG23	1:F:180:HIS:N	2.22	0.54
1:F:40:VAL:O	1:F:41:ASN:CB	2.55	0.54
1:A:133:TYR:CE1	1:A:136:MSE:HE2	2.42	0.54
1:B:7:MSE:HE3	1:B:30:LEU:HB3	1.89	0.54
1:D:21:LEU:O	1:D:25:MSE:HB2	2.08	0.54
1:B:282:VAL:HG12	1:B:284:TYR:HD2	1.72	0.54
1:B:133:TYR:CZ	1:B:184:ARG:HB2	2.43	0.54
1:F:73:ILE:CG2	1:F:75:THR:HG22	2.38	0.54
1:D:40:VAL:HG23	3:D:377:HOH:O	2.08	0.54
1:F:58:ASP:O	1:F:59:LEU:HB3	2.08	0.53
1:B:31:GLU:HA	3:B:643:HOH:O	2.09	0.53
1:C:36:PHE:CE2	1:C:59:LEU:HD13	2.43	0.53
1:E:40:VAL:HG12	3:E:421:HOH:O	2.08	0.53
1:C:277:MSE:HE3	1:C:278:TYR:CE2	2.44	0.53
1:E:132:ASP:OD2	1:E:132:ASP:N	2.40	0.53
1:B:98:LYS:HE3	1:B:180:HIS:CE1	2.43	0.53
1:E:124:TYR:CZ	1:E:126:ASN:HB3	2.43	0.53
1:E:185:MSE:CA	1:E:185:MSE:HE3	2.39	0.53
1:F:9:PHE:HB2	1:F:35:ILE:HD12	1.90	0.53
1:C:185:MSE:HE1	1:C:189:PHE:HE2	1.73	0.53
1:E:88:ILE:HG22	1:E:117:LYS:HD3	1.91	0.53
1:F:124:TYR:CZ	1:F:126:ASN:HB3	2.43	0.53
1:B:294:LYS:CE	1:C:255:GLN:HE21	2.21	0.53
1:C:7:MSE:CE	1:C:30:LEU:HD12	2.35	0.53
1:B:48:PHE:O	1:B:50:GLU:O	2.26	0.53
1:F:133:TYR:CZ	1:F:184:ARG:HB2	2.44	0.53
1:C:198:ASP:O	1:C:212:PHE:HA	2.09	0.52
1:F:133:TYR:CD1	1:F:184:ARG:HD2	2.43	0.52
1:C:34:THR:CG2	1:C:68:ILE:HD11	2.37	0.52
1:B:124:TYR:CZ	1:B:126:ASN:HB3	2.45	0.52
1:B:50:GLU:C	1:B:52:GLY:H	2.13	0.52
1:B:182:MSE:CE	1:B:216:LEU:HD11	2.27	0.52
1:D:92:LYS:N	1:D:92:LYS:HD2	2.24	0.52
1:E:264:ILE:HD12	1:E:264:ILE:N	2.24	0.52
1:E:6:LYS:CB	1:E:33:LYS:HZ2	2.23	0.52
1:A:18:ARG:HH12	1:A:261:LYS:HZ2	1.57	0.52
1:D:48:PHE:HB3	1:D:53:VAL:HG21	1.90	0.52
1:F:237:PRO:HG3	1:F:251:TYR:CZ	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:283:THR:HG23	1:F:293:LYS:HD2	1.91	0.52
1:E:18:ARG:CZ	1:E:261:LYS:HE2	2.39	0.52
1:A:136:MSE:HE3	1:A:137:LYS:N	2.24	0.52
1:B:182:MSE:CE	1:B:333:ILE:HG21	2.39	0.52
1:E:21:LEU:HA	1:E:24:VAL:HG12	1.91	0.51
1:E:151:VAL:HG22	1:E:241:VAL:HG22	1.92	0.51
1:A:196:THR:OG1	1:A:215:ASP:HB2	2.10	0.51
1:D:18:ARG:HH12	1:D:261:LYS:HZ2	1.56	0.51
1:F:2:SER:O	1:F:3:LEU:CB	2.58	0.51
1:F:60:ASN:O	1:F:64:THR:HB	2.10	0.51
1:E:31:GLU:HB3	1:E:33:LYS:NZ	2.13	0.51
1:A:18:ARG:HH12	1:A:261:LYS:NZ	2.07	0.51
1:C:133:TYR:CD1	1:C:184:ARG:HD2	2.46	0.51
1:D:211:TYR:C	1:D:211:TYR:CD2	2.83	0.51
1:E:18:ARG:NH1	1:E:261:LYS:HE2	2.26	0.51
1:E:3:LEU:HB3	1:E:315:LYS:NZ	2.25	0.51
1:F:58:ASP:CB	1:F:61:GLU:HG3	2.41	0.51
1:A:87:ALA:HB3	1:A:94:VAL:HG11	1.93	0.51
1:B:104:LEU:HG	1:B:108:GLU:OE1	2.10	0.51
1:B:183:ASP:HA	1:B:330:ASN:HD21	1.76	0.51
1:E:196:THR:CG2	3:E:599:HOH:O	2.58	0.51
1:E:198:ASP:O	1:E:212:PHE:HA	2.11	0.51
1:B:285:ARG:HA	1:B:290:ASP:O	2.11	0.51
1:B:323:THR:OG1	1:B:326:GLN:HG3	2.11	0.51
1:C:196:THR:O	1:C:214:VAL:HG13	2.11	0.51
1:E:213:ASP:HA	1:E:227:LYS:HG2	1.93	0.51
1:C:98:LYS:HG3	3:C:466:HOH:O	2.11	0.51
1:C:102:ASP:OD2	1:C:106:HIS:HD2	1.94	0.50
1:C:185:MSE:HG3	1:C:224:VAL:CG1	2.41	0.50
1:C:7:MSE:CE	1:C:24:VAL:HG21	2.41	0.50
1:D:201:ASN:HA	1:D:210:ASN:OD1	2.12	0.50
1:B:50:GLU:O	1:B:51:LYS:HB2	2.10	0.50
1:E:155:ILE:HG13	1:E:181:LEU:HD21	1.91	0.50
1:B:25:MSE:HA	1:B:25:MSE:CE	2.40	0.50
1:E:75:THR:CG2	1:E:79:THR:HG23	2.41	0.50
1:C:295:GLN:HG3	1:F:277:MSE:HE2	1.93	0.50
1:A:214:VAL:HB	1:A:226:VAL:CG2	2.41	0.50
1:C:11:GLY:HA3	1:C:74:CYS:O	2.12	0.50
1:C:192:PRO:O	1:C:348:LEU:HG	2.11	0.50
1:C:7:MSE:HE3	1:C:24:VAL:HG21	1.93	0.50
1:A:70:LEU:HD11	1:A:95:ILE:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:LYS:CD	1:C:255:GLN:HE21	2.24	0.49
1:B:48:PHE:HB3	1:B:53:VAL:HG21	1.94	0.49
1:E:306:TYR:O	1:E:310:VAL:HG23	2.12	0.49
2:C:360:PGE:H12	1:D:233:ALA:O	2.12	0.49
1:D:48:PHE:HB3	1:D:53:VAL:CG2	2.42	0.49
1:E:137:LYS:O	1:E:141:GLU:HG3	2.11	0.49
1:A:133:TYR:CE1	1:A:184:ARG:HB2	2.48	0.49
1:E:7:MSE:CE	1:E:30:LEU:HB3	2.36	0.49
1:F:102:ASP:OD1	1:F:106:HIS:HD2	1.94	0.49
1:F:133:TYR:CE1	1:F:184:ARG:HB2	2.46	0.49
1:A:265:MSE:HB2	1:A:267:ASP:OD2	2.13	0.49
1:B:198:ASP:O	1:B:212:PHE:HA	2.13	0.49
1:E:182:MSE:HE2	1:E:216:LEU:HD21	1.91	0.49
1:A:198:ASP:O	1:A:212:PHE:HA	2.13	0.49
1:C:282:VAL:HG13	1:C:296:ILE:HD13	1.93	0.49
1:A:211:TYR:CD2	1:A:211:TYR:C	2.86	0.49
1:F:38:LEU:HD22	1:F:38:LEU:H	1.78	0.49
1:E:179:ILE:HG23	1:E:180:HIS:N	2.28	0.48
1:E:347:HIS:HE1	1:E:350:GLU:OE2	1.95	0.48
1:E:185:MSE:HE2	1:E:185:MSE:HA	1.94	0.48
1:E:205:SER:HB3	1:F:220:SER:OG	2.13	0.48
1:F:285:ARG:HH11	1:F:285:ARG:HG3	1.77	0.48
1:A:182:MSE:HG2	1:A:226:VAL:HG11	1.95	0.48
1:A:145:LEU:HD22	1:A:246:GLY:C	2.34	0.48
1:A:9:PHE:HB2	1:A:35:ILE:HD13	1.94	0.48
1:F:155:ILE:HG22	1:F:155:ILE:O	2.14	0.48
2:C:360:PGE:H22	1:E:293:LYS:NZ	2.28	0.48
1:F:347:HIS:HB2	3:F:602:HOH:O	2.12	0.48
1:D:32:VAL:CG1	1:D:35:ILE:HD11	2.44	0.48
1:A:275:SER:HB3	1:D:295:GLN:HB2	1.96	0.48
1:B:75:THR:HB	1:B:76:PRO:HD2	1.94	0.48
1:C:266:PRO:HA	1:C:271:PHE:CD2	2.49	0.48
1:E:179:ILE:C	1:E:179:ILE:HD13	2.34	0.48
1:A:136:MSE:HE3	1:A:137:LYS:HB2	1.95	0.48
1:A:166:GLN:HG2	1:A:206:GLU:HG2	1.96	0.48
1:B:34:THR:HB	1:B:62:LEU:HD13	1.96	0.48
1:E:277:MSE:HE3	1:E:278:TYR:CE2	2.48	0.48
1:B:120:VAL:HG12	1:B:122:MSE:HG3	1.96	0.47
1:C:185:MSE:CE	1:C:189:PHE:HE2	2.27	0.47
1:D:327:ALA:O	1:D:331:ILE:HG12	2.14	0.47
1:F:36:PHE:CE1	1:F:59:LEU:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:46:ALA:HB3	1:F:47:PRO:HD3	1.94	0.47
1:C:242:HIS:CE1	1:D:232:VAL:HG13	2.49	0.47
1:D:132:ASP:OD2	1:D:132:ASP:N	2.48	0.47
1:E:165:GLU:HG2	3:E:554:HOH:O	2.14	0.47
1:E:324:LYS:HG3	1:E:325:GLU:OE2	2.14	0.47
1:F:137:LYS:HG3	1:F:188:LEU:HD11	1.96	0.47
1:B:123:PRO:HD2	1:B:322:VAL:HG11	1.94	0.47
1:B:166:GLN:NE2	3:B:510:HOH:O	2.47	0.47
1:B:211:TYR:CD2	1:B:211:TYR:C	2.88	0.47
1:B:48:PHE:O	1:B:53:VAL:HG22	2.13	0.47
1:C:21:LEU:HA	1:C:24:VAL:CG1	2.45	0.47
1:D:182:MSE:CE	1:D:216:LEU:CD2	2.73	0.47
1:A:65:ASP:OD1	1:A:67:GLU:HB2	2.15	0.47
1:B:292:ILE:N	1:B:292:ILE:HD12	2.30	0.47
1:D:5:VAL:HG23	1:D:311:TYR:HD1	1.80	0.47
1:D:38:LEU:HD23	3:D:776:HOH:O	2.14	0.47
1:B:294:LYS:HD3	1:C:255:GLN:NE2	2.29	0.47
1:A:250:LYS:HD3	1:A:251:TYR:N	2.30	0.47
1:C:279:TYR:OH	1:C:297:LYS:HE3	2.14	0.47
1:E:282:VAL:HG13	1:E:296:ILE:CD1	2.44	0.47
1:E:87:ALA:HB3	1:E:94:VAL:HG11	1.97	0.47
1:B:101:CYS:SG	1:B:110:LEU:HD22	2.55	0.47
1:C:163:ILE:HD12	1:C:210:ASN:HB2	1.97	0.47
1:C:88:ILE:O	1:C:90:ALA:O	2.33	0.47
1:C:232:VAL:HG13	1:D:242:HIS:CE1	2.49	0.47
1:D:32:VAL:HG11	1:D:35:ILE:HD11	1.96	0.47
1:D:198:ASP:O	1:D:212:PHE:HA	2.15	0.47
1:D:350:GLU:HB2	3:D:548:HOH:O	2.14	0.47
1:E:79:THR:OG1	1:E:79:THR:O	2.33	0.47
1:E:10:ILE:HG21	1:E:83:LEU:HD13	1.97	0.47
1:C:234:SER:HB3	1:D:249:ILE:CD1	2.45	0.47
1:F:255:GLN:NE2	1:F:258:ASN:HD22	2.11	0.47
1:A:98:LYS:HD3	1:A:179:ILE:HG21	1.96	0.46
1:A:185:MSE:HG3	1:A:224:VAL:HG11	1.96	0.46
1:D:127:ARG:NH1	1:D:130:ASP:OD2	2.48	0.46
1:E:255:GLN:HE22	1:E:258:ASN:ND2	2.07	0.46
1:E:62:LEU:HD21	1:E:71:ILE:HD12	1.97	0.46
1:A:350:GLU:CG	1:A:350:GLU:O	2.58	0.46
1:F:250:LYS:NZ	1:F:274:ASP:OD2	2.48	0.46
1:A:242:HIS:CE1	1:B:232:VAL:HG13	2.50	0.46
1:D:169:LYS:HG2	3:D:576:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:122:MSE:SE	1:E:320:GLN:HB2	2.65	0.46
1:F:40:VAL:O	1:F:41:ASN:HB3	2.16	0.46
1:F:73:ILE:HG23	1:F:75:THR:HG22	1.97	0.46
1:B:22:PRO:HG3	1:B:265:MSE:HE1	1.97	0.46
1:D:325:GLU:HG2	3:D:388:HOH:O	2.16	0.46
1:B:191:ARG:HB2	3:B:418:HOH:O	2.16	0.46
1:D:323:THR:OG1	1:D:326:GLN:HG3	2.15	0.46
1:B:264:ILE:H	1:B:264:ILE:HD12	1.81	0.46
1:C:211:TYR:C	1:C:211:TYR:CD2	2.88	0.46
1:D:79:THR:HG23	1:D:83:LEU:HD12	1.97	0.46
1:C:26:ILE:HD12	1:C:267:ASP:OD2	2.15	0.46
1:A:212:PHE:CE1	1:A:228:THR:HB	2.50	0.46
1:B:127:ARG:HD2	1:B:130:ASP:OD2	2.16	0.46
1:B:152:GLU:OE2	1:B:154:HIS:CE1	2.69	0.46
1:C:210:ASN:O	1:C:230:HIS:HD2	1.99	0.46
1:C:5:VAL:HG23	1:C:311:TYR:CD1	2.51	0.46
1:D:14:LYS:H	1:D:14:LYS:HZ2	1.63	0.46
1:E:7:MSE:CE	1:E:24:VAL:HG21	2.46	0.46
1:B:214:VAL:HB	1:B:226:VAL:CG2	2.45	0.46
1:B:64:THR:O	1:B:66:PRO:HD3	2.16	0.46
1:D:151:VAL:HB	1:D:224:VAL:HG22	1.98	0.45
1:E:166:GLN:HG3	3:E:684:HOH:O	2.15	0.45
1:E:76:PRO:O	1:E:79:THR:CG2	2.64	0.45
1:C:21:LEU:HA	1:C:24:VAL:HG12	1.97	0.45
1:F:255:GLN:HE22	1:F:258:ASN:HD22	1.64	0.45
1:B:142:GLN:NE2	1:C:264:ILE:HD12	2.31	0.45
1:B:195:VAL:HG22	1:B:216:LEU:HD22	1.97	0.45
1:C:45:ALA:O	1:C:49:LYS:HD3	2.16	0.45
1:D:123:PRO:CG	1:D:125:GLN:HE21	2.29	0.45
1:D:77:ALA:C	1:D:79:THR:H	2.19	0.45
1:E:282:VAL:HG13	1:E:296:ILE:HD13	1.98	0.45
1:C:154:HIS:HD2	1:C:156:ASP:OD2	1.98	0.45
1:C:151:VAL:HG22	1:C:241:VAL:HG13	1.99	0.45
1:A:151:VAL:HG11	1:A:185:MSE:CE	2.46	0.45
1:A:232:VAL:HG13	1:B:242:HIS:CE1	2.52	0.45
1:E:14:LYS:NZ	1:E:18:ARG:NH1	2.65	0.45
1:F:58:ASP:HB3	1:F:61:GLU:HG3	1.98	0.45
1:A:286:ASN:ND2	1:A:290:ASP:HB2	2.31	0.45
1:E:165:GLU:O	1:E:165:GLU:HG3	2.16	0.45
1:F:27:ARG:NH2	3:F:698:HOH:O	2.49	0.45
1:E:3:LEU:HD13	1:E:4:THR:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:285:ARG:HD2	1:D:291:TRP:CZ2	2.51	0.45
1:D:2:SER:HA	1:D:315:LYS:CE	2.47	0.45
1:F:323:THR:OG1	1:F:326:GLN:HG3	2.16	0.45
1:F:211:TYR:CD2	1:F:211:TYR:C	2.90	0.45
1:B:187:ALA:HA	1:B:326:GLN:NE2	2.32	0.45
1:D:212:PHE:CE1	1:D:228:THR:HB	2.52	0.45
1:F:185:MSE:HG3	1:F:224:VAL:HG11	1.98	0.45
1:C:133:TYR:CE1	1:C:184:ARG:HB2	2.52	0.44
1:F:22:PRO:HG3	1:F:265:MSE:HE1	1.98	0.44
1:A:132:ASP:HA	1:A:250:LYS:HZ2	1.83	0.44
1:E:179:ILE:HD13	1:E:179:ILE:O	2.18	0.44
1:E:27:ARG:NH2	1:E:304:GLY:HA3	2.32	0.44
1:E:195:VAL:HG23	1:E:348:LEU:HD21	1.99	0.44
1:F:101:CYS:SG	1:F:110:LEU:HD12	2.56	0.44
1:A:101:CYS:SG	1:A:107:ALA:HA	2.57	0.44
1:D:124:TYR:CZ	1:D:126:ASN:HB3	2.52	0.44
1:F:133:TYR:CD1	1:F:136:MSE:CE	3.00	0.44
1:A:155:ILE:HG13	1:A:181:LEU:HD21	1.99	0.44
1:A:18:ARG:NH1	1:A:261:LYS:HZ2	2.12	0.44
1:B:349:LYS:HG2	1:B:350:GLU:HG3	2.00	0.44
1:F:65:ASP:HA	1:F:66:PRO:HD3	1.73	0.44
1:A:132:ASP:N	1:A:132:ASP:OD1	2.50	0.44
1:C:166:GLN:N	1:C:166:GLN:OE1	2.50	0.44
1:D:155:ILE:CG2	1:D:177:LEU:HD13	2.48	0.44
1:F:151:VAL:HG11	1:F:185:MSE:HE2	1.99	0.44
1:B:29:THR:C	1:B:30:LEU:HD12	2.38	0.44
1:B:333:ILE:HD11	1:B:348:LEU:HD11	2.00	0.44
1:A:286:ASN:HD21	1:A:290:ASP:HB2	1.83	0.44
1:D:255:GLN:NE2	1:D:258:ASN:HD22	2.16	0.44
1:F:132:ASP:OD2	1:F:132:ASP:N	2.51	0.44
1:D:75:THR:OG1	1:D:79:THR:HG21	2.18	0.43
1:E:136:MSE:HE3	1:E:136:MSE:HB3	1.80	0.43
1:E:285:ARG:HA	1:E:290:ASP:O	2.18	0.43
1:E:3:LEU:HB3	1:E:315:LYS:HZ3	1.83	0.43
1:D:155:ILE:HD13	1:D:181:LEU:CD2	2.37	0.43
1:D:270:GLY:HA2	1:D:273:GLU:OE2	2.18	0.43
1:F:324:LYS:HG3	1:F:325:GLU:N	2.33	0.43
1:A:102:ASP:OD1	1:A:102:ASP:N	2.51	0.43
1:D:191:ARG:NE	1:D:350:GLU:OE1	2.49	0.43
1:E:14:LYS:HZ3	1:E:18:ARG:NH1	2.16	0.43
1:E:14:LYS:NZ	1:E:18:ARG:HH12	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:GLN:HE21	1:C:264:ILE:HD12	1.83	0.43
1:F:7:MSE:CE	1:F:30:LEU:HB3	2.38	0.43
1:A:133:TYR:CZ	1:A:184:ARG:HB2	2.53	0.43
1:B:196:THR:HG22	1:B:345:VAL:HG22	2.01	0.43
1:B:8:GLY:HA3	1:B:62:LEU:HD11	2.01	0.43
1:D:155:ILE:HG21	1:D:177:LEU:HD13	2.01	0.43
1:A:169:LYS:HG2	3:A:700:HOH:O	2.18	0.43
1:A:221:LYS:HD3	3:B:644:HOH:O	2.18	0.43
1:A:293:LYS:NZ	2:F:360:PGE:H4	2.33	0.43
1:A:46:ALA:N	1:A:47:PRO:HD2	2.33	0.43
1:B:140:VAL:HG22	1:B:148:ILE:CD1	2.48	0.43
1:B:241:VAL:HB	1:B:248:PHE:HB3	1.99	0.43
1:D:151:VAL:HA	1:D:240:ILE:O	2.19	0.43
1:E:75:THR:HG21	1:E:83:LEU:CD1	2.42	0.43
1:B:25:MSE:HE1	3:B:643:HOH:O	2.19	0.43
1:C:21:LEU:HB3	3:C:470:HOH:O	2.17	0.43
1:C:90:ALA:O	1:C:92:LYS:N	2.47	0.43
1:E:5:VAL:HG21	1:E:314:LEU:HD11	2.01	0.43
1:F:166:GLN:HA	1:F:207:ALA:HA	2.00	0.43
1:A:124:TYR:CZ	1:A:126:ASN:HB3	2.54	0.43
1:C:227:LYS:HG2	3:C:387:HOH:O	2.19	0.43
1:C:75:THR:HG23	1:C:79:THR:HG21	1.98	0.43
1:D:64:THR:O	1:D:66:PRO:HD3	2.19	0.43
1:E:323:THR:OG1	1:E:326:GLN:HG3	2.19	0.43
1:F:237:PRO:HG2	1:F:240:ILE:CD1	2.42	0.43
1:F:34:THR:HA	1:F:54:ASN:O	2.19	0.43
1:A:58:ASP:OD2	1:A:61:GLU:HB3	2.18	0.43
1:B:27:ARG:NH2	1:B:304:GLY:HA3	2.33	0.43
1:C:48:PHE:C	1:C:53:VAL:HG12	2.39	0.43
1:D:14:LYS:H	1:D:14:LYS:HZ1	1.64	0.43
1:D:257:GLU:O	1:D:261:LYS:HG2	2.19	0.43
1:F:198:ASP:O	1:F:212:PHE:HA	2.19	0.43
1:B:30:LEU:CD2	1:B:307:TYR:HB3	2.46	0.42
1:A:62:LEU:HD12	1:A:68:ILE:HD12	2.01	0.42
1:C:123:PRO:HG2	1:C:322:VAL:HG11	2.01	0.42
1:C:82:ASP:O	1:C:86:GLN:HG3	2.19	0.42
1:E:182:MSE:HE1	1:E:216:LEU:HD21	1.94	0.42
1:B:122:MSE:SE	1:B:320:GLN:HB2	2.69	0.42
1:F:285:ARG:HA	1:F:290:ASP:O	2.20	0.42
1:F:174:PHE:CE2	1:F:334:LEU:HD12	2.53	0.42
1:F:75:THR:CG2	1:F:79:THR:OG1	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:LEU:O	1:B:63:LEU:HD13	2.20	0.42
3:A:413:HOH:O	1:D:297:LYS:HG3	2.19	0.42
1:E:133:TYR:CD1	1:E:136:MSE:CE	3.03	0.42
3:E:431:HOH:O	1:F:221:LYS:HG3	2.19	0.42
1:E:76:PRO:O	1:E:79:THR:HG22	2.20	0.42
1:C:120:VAL:HG12	1:C:122:MSE:HG3	2.02	0.42
1:D:130:ASP:HB3	1:D:132:ASP:OD2	2.20	0.42
1:F:310:VAL:HG23	3:F:386:HOH:O	2.20	0.42
1:A:293:LYS:NZ	2:F:360:PGE:H62	2.34	0.42
1:A:136:MSE:O	1:A:140:VAL:HG23	2.18	0.42
1:A:295:GLN:HG3	1:E:277:MSE:CE	2.48	0.42
1:A:211:TYR:CD2	1:A:212:PHE:N	2.88	0.42
1:B:10:ILE:CG2	1:B:83:LEU:HD13	2.46	0.42
1:C:87:ALA:O	1:C:90:ALA:O	2.38	0.42
1:E:89:LEU:HD12	1:E:89:LEU:HA	1.90	0.42
1:D:75:THR:HB	1:D:76:PRO:HD2	2.02	0.42
1:A:179:ILE:CG2	1:A:180:HIS:N	2.83	0.42
1:A:266:PRO:HA	1:A:271:PHE:CD2	2.55	0.42
1:A:292:ILE:HD12	1:A:292:ILE:N	2.35	0.42
1:B:248:PHE:HD1	1:B:282:VAL:HG22	1.83	0.42
1:C:25:MSE:HE1	1:C:32:VAL:HB	2.02	0.42
1:D:286:ASN:HD21	1:D:290:ASP:HB2	1.83	0.42
1:D:308:ASP:HA	3:D:400:HOH:O	2.20	0.42
1:E:101:CYS:SG	1:E:110:LEU:HD12	2.59	0.42
1:E:133:TYR:CE1	1:E:136:MSE:HE1	2.54	0.42
1:E:75:THR:OG1	1:E:76:PRO:HD2	2.20	0.42
1:C:124:TYR:CZ	1:C:126:ASN:HB3	2.54	0.41
1:C:13:GLY:HA3	1:C:14:LYS:HE2	2.02	0.41
1:E:185:MSE:CA	1:E:185:MSE:CE	2.92	0.41
1:B:214:VAL:HB	1:B:226:VAL:HG23	2.03	0.41
1:E:294:LYS:HG2	1:E:295:GLN:N	2.35	0.41
1:E:315:LYS:HA	1:E:315:LYS:HD2	1.79	0.41
1:E:10:ILE:HD12	1:E:73:ILE:CD1	2.51	0.41
1:C:269:PRO:HD2	3:C:404:HOH:O	2.18	0.41
1:D:234:SER:HA	1:D:235:PRO:HD2	1.92	0.41
1:E:242:HIS:CE1	1:F:232:VAL:HG13	2.55	0.41
1:A:221:LYS:CD	3:B:644:HOH:O	2.67	0.41
1:B:44:ALA:O	1:B:47:PRO:HD2	2.20	0.41
1:B:294:LYS:HE2	1:C:255:GLN:HE21	1.85	0.41
1:A:234:SER:HA	1:A:235:PRO:HD3	1.82	0.41
1:A:33:LYS:HE2	1:A:67:GLU:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:MSE:CE	1:B:189:PHE:HE2	2.34	0.41
1:C:75:THR:CG2	1:C:79:THR:HG23	2.50	0.41
1:F:38:LEU:HD22	1:F:38:LEU:N	2.35	0.41
1:A:163:ILE:HD13	3:A:404:HOH:O	2.19	0.41
1:C:46:ALA:O	1:C:49:LYS:HB2	2.21	0.41
1:D:133:TYR:CZ	1:D:184:ARG:HB2	2.55	0.41
1:F:47:PRO:O	1:F:51:LYS:HE3	2.20	0.41
1:F:34:THR:HG23	1:F:68:ILE:HD11	2.03	0.41
1:B:95:ILE:HD11	1:B:310:VAL:HG21	2.02	0.41
1:C:132:ASP:OD2	1:C:132:ASP:N	2.54	0.41
1:C:14:LYS:HE3	3:C:415:HOH:O	2.21	0.41
1:E:133:TYR:HE1	1:E:185:MSE:HE1	1.84	0.41
1:E:163:ILE:HD12	1:E:210:ASN:CB	2.48	0.41
1:F:185:MSE:CE	1:F:189:PHE:CE2	3.01	0.41
1:A:276:PRO:HA	1:A:279:TYR:CE1	2.56	0.41
1:C:234:SER:HA	1:C:235:PRO:HD3	1.80	0.41
1:C:34:THR:HA	1:C:54:ASN:O	2.21	0.41
1:E:116:GLU:HG3	1:E:117:LYS:N	2.35	0.41
1:B:140:VAL:HG22	1:B:148:ILE:HD13	2.02	0.41
1:C:285:ARG:HA	1:C:290:ASP:O	2.21	0.41
2:C:360:PGE:H42	2:C:360:PGE:H6	1.89	0.41
1:A:255:GLN:HG3	1:D:294:LYS:CD	2.50	0.41
1:D:38:LEU:CD2	3:D:776:HOH:O	2.67	0.41
1:E:247:SER:OG	1:F:233:ALA:HB3	2.21	0.41
1:E:6:LYS:CD	1:E:33:LYS:NZ	2.83	0.41
1:E:6:LYS:HD3	1:E:33:LYS:HZ2	1.86	0.41
1:F:27:ARG:HD3	1:F:308:ASP:OD1	2.20	0.41
1:B:333:ILE:CD1	1:B:348:LEU:HD11	2.51	0.41
1:D:330:ASN:HA	1:D:330:ASN:HD22	1.68	0.41
1:D:55:PHE:N	1:D:55:PHE:CD2	2.89	0.41
1:F:58:ASP:O	1:F:59:LEU:CB	2.69	0.41
1:A:122:MSE:HE1	1:A:310:VAL:HG22	2.02	0.41
1:C:206:GLU:H	1:C:206:GLU:CD	2.24	0.41
1:E:195:VAL:HG22	1:E:216:LEU:CD2	2.51	0.41
1:E:256:GLN:O	1:E:260:LEU:HD22	2.21	0.41
1:E:48:PHE:O	1:E:49:LYS:C	2.59	0.41
1:F:248:PHE:CD1	1:F:282:VAL:HG22	2.56	0.41
1:F:274:ASP:HB3	1:F:298:THR:HB	2.03	0.41
1:B:14:LYS:HE3	1:B:14:LYS:HB2	1.83	0.40
1:C:65:ASP:HA	1:C:66:PRO:HD3	1.89	0.40
1:E:211:TYR:CD2	1:E:211:TYR:C	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:44:ALA:HB1	3:F:765:HOH:O	2.21	0.40
1:C:25:MSE:SE	3:C:470:HOH:O	2.89	0.40
1:E:133:TYR:CE1	1:E:185:MSE:HE1	2.56	0.40
1:E:62:LEU:HD11	1:E:71:ILE:HD11	2.03	0.40
1:F:59:LEU:HD13	1:F:63:LEU:HD22	2.01	0.40
1:B:282:VAL:HG12	1:B:284:TYR:CD2	2.55	0.40
1:E:3:LEU:CD1	1:E:315:LYS:HZ1	2.34	0.40
1:F:122:MSE:SE	1:F:320:GLN:HB2	2.72	0.40
1:F:332:GLU:OE2	1:F:348:LEU:HD13	2.21	0.40
1:A:34:THR:HA	1:A:54:ASN:O	2.21	0.40
1:C:15:SER:HB3	1:C:97:GLU:OE2	2.21	0.40
1:E:28:GLU:HG2	3:E:495:HOH:O	2.22	0.40
1:F:185:MSE:HE3	1:F:189:PHE:CE2	2.56	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	346/359 (96%)	329 (95%)	16 (5%)	1 (0%)	44	55
1	B	346/359 (96%)	326 (94%)	19 (6%)	1 (0%)	44	55
1	C	345/359 (96%)	327 (95%)	13 (4%)	5 (1%)	13	12
1	D	347/359 (97%)	329 (95%)	17 (5%)	1 (0%)	44	55
1	E	347/359 (97%)	328 (94%)	17 (5%)	2 (1%)	28	34
1	F	347/359 (97%)	326 (94%)	18 (5%)	3 (1%)	20	23
All	All	2078/2154 (96%)	1965 (95%)	100 (5%)	13 (1%)	28	34

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	75	THR
1	F	41	ASN
1	A	155	ILE
1	B	155	ILE
1	E	51	LYS
1	F	42	GLU
1	D	78	HIS
1	F	3	LEU
1	C	37	ASP
1	C	91	GLY
1	C	155	ILE
1	E	78	HIS
1	C	76	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	297/298 (100%)	286 (96%)	11 (4%)	39	53
1	B	297/298 (100%)	282 (95%)	15 (5%)	28	37
1	C	296/298 (99%)	282 (95%)	14 (5%)	30	41
1	D	298/298 (100%)	278 (93%)	20 (7%)	19	24
1	E	298/298 (100%)	276 (93%)	22 (7%)	16	20
1	F	298/298 (100%)	283 (95%)	15 (5%)	28	38
All	All	1784/1788 (100%)	1687 (95%)	97 (5%)	26	35

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	14	LYS
1	A	27	ARG
1	A	42	GLU
1	A	60	ASN
1	A	132	ASP

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Mol	Chain	Res	Type
1	A	136	MSE
1	A	165	GLU
1	A	193	ASP
1	A	277	MSE
1	A	350	GLU
1	B	3	LEU
1	B	25	MSE
1	B	27	ARG
1	B	42	GLU
1	B	43	LYS
1	B	50	GLU
1	B	68	ILE
1	B	108	GLU
1	B	110	LEU
1	B	193	ASP
1	B	260	LEU
1	B	285	ARG
1	B	330	ASN
1	B	334	LEU
1	B	335	GLU
1	C	14	LYS
1	C	25	MSE
1	C	33	LYS
1	C	34	THR
1	C	38	LEU
1	C	50	GLU
1	C	62	LEU
1	C	74	CYS
1	C	165	GLU
1	C	166	GLN
1	C	193	ASP
1	C	196	THR
1	C	260	LEU
1	C	335	GLU
1	D	3	LEU
1	D	14	LYS
1	D	18	ARG
1	D	60	ASN
1	D	61	GLU
1	D	62	LEU
1	D	69	GLU
1	D	79	THR

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Mol	Chain	Res	Type
1	D	82	ASP
1	D	92	LYS
1	D	136	MSE
1	D	185	MSE
1	D	193	ASP
1	D	260	LEU
1	D	261	LYS
1	D	297	LYS
1	D	305	ARG
1	D	316	ASN
1	D	330	ASN
1	D	348	LEU
1	E	3	LEU
1	E	24	VAL
1	E	27	ARG
1	E	33	LYS
1	E	53	VAL
1	E	69	GLU
1	E	89	LEU
1	E	98	LYS
1	E	116	GLU
1	E	117	LYS
1	E	153	THR
1	E	179	ILE
1	E	185	MSE
1	E	193	ASP
1	E	196	THR
1	E	206	GLU
1	E	253	GLU
1	E	260	LEU
1	E	313	THR
1	E	324	LYS
1	E	339	LEU
1	E	351	ASN
1	F	3	LEU
1	F	27	ARG
1	F	34	THR
1	F	42	GLU
1	F	51	LYS
1	F	53	VAL
1	F	98	LYS
1	F	188	LEU

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Mol	Chain	Res	Type
1	F	196	THR
1	F	221	LYS
1	F	260	LEU
1	F	324	LYS
1	F	325	GLU
1	F	330	ASN
1	F	350	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	HIS
1	A	180	HIS
1	A	194	GLN
1	A	255	GLN
1	A	258	ASN
1	A	316	ASN
1	A	330	ASN
1	B	60	ASN
1	B	86	GLN
1	B	125	GLN
1	B	142	GLN
1	B	154	HIS
1	B	166	GLN
1	B	230	HIS
1	B	255	GLN
1	B	288	ASN
1	B	330	ASN
1	C	106	HIS
1	C	154	HIS
1	C	171	ASN
1	C	194	GLN
1	C	217	HIS
1	C	230	HIS
1	C	255	GLN
1	C	258	ASN
1	C	288	ASN
1	C	316	ASN
1	D	115	GLN
1	D	125	GLN
1	D	180	HIS
1	D	194	GLN

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Mol	Chain	Res	Type
1	D	255	GLN
1	D	330	ASN
1	E	115	GLN
1	E	125	GLN
1	E	154	HIS
1	E	180	HIS
1	E	255	GLN
1	E	316	ASN
1	E	347	HIS
1	F	106	HIS
1	F	125	GLN
1	F	194	GLN
1	F	230	HIS
1	F	255	GLN
1	F	288	ASN
1	F	316	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	PGE	B	360	-	9,9,9	0.64	0	8,8,8	1.41	2 (25%)
2	PGE	C	360	-	9,9,9	0.65	0	8,8,8	1.46	2 (25%)
2	PGE	F	360	-	9,9,9	0.75	0	8,8,8	1.45	2 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PGE	B	360	-	-	0/7/7/7	0/0/0/0
2	PGE	C	360	-	-	0/7/7/7	0/0/0/0
2	PGE	F	360	-	-	0/7/7/7	0/0/0/0

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	360	PGE	C3-O2-C2	2.33	123.42	113.30
2	C	360	PGE	C3-O2-C2	2.43	123.84	113.30
2	F	360	PGE	C5-O3-C4	2.44	123.86	113.30
2	B	360	PGE	C5-O3-C4	2.52	124.21	113.30
2	C	360	PGE	C5-O3-C4	2.55	124.36	113.30
2	F	360	PGE	C3-O2-C2	2.63	124.69	113.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	360	PGE	1	0
2	C	360	PGE	5	0
2	F	360	PGE	2	0

5.7 Other polymers (i)

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, 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(Å²)	Q<0.9
1	A	340/359 (94%)	-0.30	1 (0%)	93	95	12, 25, 46, 57	0
1	B	340/359 (94%)	-0.31	1 (0%)	93	95	10, 22, 40, 58	0
1	C	339/359 (94%)	-0.06	5 (1%)	74	72	12, 27, 47, 61	0
1	D	341/359 (94%)	-0.30	0	100	100	11, 22, 40, 57	0
1	E	341/359 (94%)	-0.29	4 (1%)	79	78	9, 22, 40, 64	0
1	F	341/359 (94%)	-0.37	1 (0%)	93	95	11, 19, 36, 65	0
All	All	2042/2154 (94%)	-0.27	12 (0%)	89	90	9, 22, 43, 65	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	52	GLY	4.1
1	E	41	ASN	3.2
1	C	51	LYS	3.2
1	B	43	LYS	3.1
1	E	43	LYS	2.9
1	A	350	GLU	2.8
1	C	53	VAL	2.7
1	E	40	VAL	2.7
1	F	42	GLU	2.6
1	C	91	GLY	2.3
1	E	78	HIS	2.2
1	C	76	PRO	2.1

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 (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	PGE	F	360	10/10	0.84	0.22	3.65	30,31,37,39	0
2	PGE	B	360	10/10	0.91	0.18	1.41	31,32,35,36	0
2	PGE	C	360	10/10	0.91	0.18	0.91	31,34,35,37	0

6.5 Other polymers (i)

There are no such residues in this entry.