WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 19, 2024 – 01:57 PM EDT

PDB ID	:	2D40
Title	:	Crystal Structure of Z3393 from Escherichia coli O157:H7
Authors	:	Adams, M.A.; Jia, Z.; Montreal-Kingston Bacterial Structural Genomics Initiative (BSGI)
Deposited on	:	2005-10-05
Resolution	:	2.41 Å(reported)

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

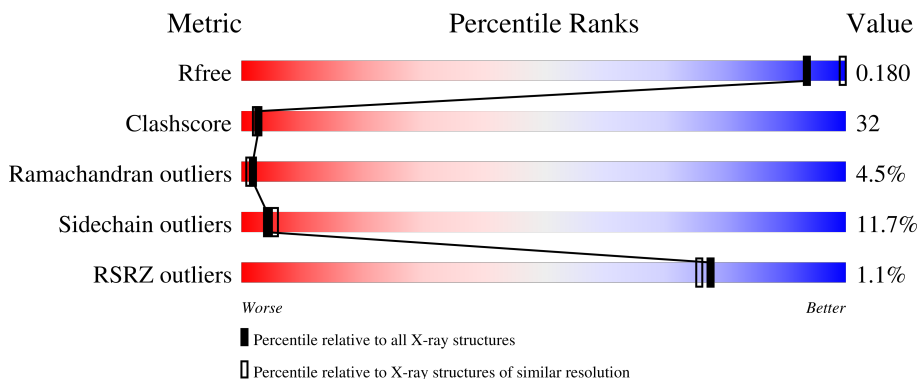|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.41 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		0.180
Clashscore		32
Ramachandran outliers		4.5%
Sidechain outliers		11.7%
RSRZ outliers		1.1%

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$_{free}$	164625	5670 (2.44-2.40)
Clashscore	180529	6299 (2.44-2.40)
Ramachandran outliers	177936	6232 (2.44-2.40)
Sidechain outliers	177891	6233 (2.44-2.40)
RSRZ outliers	164620	5670 (2.44-2.40)

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	354	32% / 33% / 14% / • / 18%
1	B	354	27% / 33% / 15% / 5% / 20%
1	C	354	31% / 34% / 14% / • / 18%
1	D	354	30% / 32% / 13% / 5% / 19%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 9579 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 putative gentisate 1,2-dioxygenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	Se	0	0	0
			2280	1447	399	426	2	6			
1	B	284	Total	C	N	O	S	Se	0	0	0
			2235	1418	392	417	2	6			
1	C	289	Total	C	N	O	S	Se	0	0	0
			2281	1447	399	427	2	6			
1	D	287	Total	C	N	O	S	Se	0	0	0
			2263	1437	396	422	2	6			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MSE	-	expression tag	UNP Q8X655
A	-10	GLY	-	expression tag	UNP Q8X655
A	-9	SER	-	expression tag	UNP Q8X655
A	-8	SER	-	expression tag	UNP Q8X655
A	-7	HIS	-	expression tag	UNP Q8X655
A	-6	HIS	-	expression tag	UNP Q8X655
A	-5	HIS	-	expression tag	UNP Q8X655
A	-4	HIS	-	expression tag	UNP Q8X655
A	-3	HIS	-	expression tag	UNP Q8X655
A	-2	HIS	-	expression tag	UNP Q8X655
A	-1	GLY	-	expression tag	UNP Q8X655
A	0	SER	-	expression tag	UNP Q8X655
A	1	MSE	MET	modified residue	UNP Q8X655
A	96	MSE	MET	modified residue	UNP Q8X655
A	131	MSE	MET	modified residue	UNP Q8X655
A	199	MSE	MET	modified residue	UNP Q8X655
A	241	MSE	MET	modified residue	UNP Q8X655
A	253	MSE	MET	modified residue	UNP Q8X655
A	256	MSE	MET	modified residue	UNP Q8X655
B	-11	MSE	-	expression tag	UNP Q8X655
B	-10	GLY	-	expression tag	UNP Q8X655

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	SER	-	expression tag	UNP Q8X655
B	-8	SER	-	expression tag	UNP Q8X655
B	-7	HIS	-	expression tag	UNP Q8X655
B	-6	HIS	-	expression tag	UNP Q8X655
B	-5	HIS	-	expression tag	UNP Q8X655
B	-4	HIS	-	expression tag	UNP Q8X655
B	-3	HIS	-	expression tag	UNP Q8X655
B	-2	HIS	-	expression tag	UNP Q8X655
B	-1	GLY	-	expression tag	UNP Q8X655
B	0	SER	-	expression tag	UNP Q8X655
B	1	MSE	MET	modified residue	UNP Q8X655
B	96	MSE	MET	modified residue	UNP Q8X655
B	131	MSE	MET	modified residue	UNP Q8X655
B	199	MSE	MET	modified residue	UNP Q8X655
B	241	MSE	MET	modified residue	UNP Q8X655
B	253	MSE	MET	modified residue	UNP Q8X655
B	256	MSE	MET	modified residue	UNP Q8X655
C	-11	MSE	-	expression tag	UNP Q8X655
C	-10	GLY	-	expression tag	UNP Q8X655
C	-9	SER	-	expression tag	UNP Q8X655
C	-8	SER	-	expression tag	UNP Q8X655
C	-7	HIS	-	expression tag	UNP Q8X655
C	-6	HIS	-	expression tag	UNP Q8X655
C	-5	HIS	-	expression tag	UNP Q8X655
C	-4	HIS	-	expression tag	UNP Q8X655
C	-3	HIS	-	expression tag	UNP Q8X655
C	-2	HIS	-	expression tag	UNP Q8X655
C	-1	GLY	-	expression tag	UNP Q8X655
C	0	SER	-	expression tag	UNP Q8X655
C	1	MSE	MET	modified residue	UNP Q8X655
C	96	MSE	MET	modified residue	UNP Q8X655
C	131	MSE	MET	modified residue	UNP Q8X655
C	199	MSE	MET	modified residue	UNP Q8X655
C	241	MSE	MET	modified residue	UNP Q8X655
C	253	MSE	MET	modified residue	UNP Q8X655
C	256	MSE	MET	modified residue	UNP Q8X655
D	-11	MSE	-	expression tag	UNP Q8X655
D	-10	GLY	-	expression tag	UNP Q8X655
D	-9	SER	-	expression tag	UNP Q8X655
D	-8	SER	-	expression tag	UNP Q8X655
D	-7	HIS	-	expression tag	UNP Q8X655
D	-6	HIS	-	expression tag	UNP Q8X655

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	HIS	-	expression tag	UNP Q8X655
D	-4	HIS	-	expression tag	UNP Q8X655
D	-3	HIS	-	expression tag	UNP Q8X655
D	-2	HIS	-	expression tag	UNP Q8X655
D	-1	GLY	-	expression tag	UNP Q8X655
D	0	SER	-	expression tag	UNP Q8X655
D	1	MSE	MET	modified residue	UNP Q8X655
D	96	MSE	MET	modified residue	UNP Q8X655
D	131	MSE	MET	modified residue	UNP Q8X655
D	199	MSE	MET	modified residue	UNP Q8X655
D	241	MSE	MET	modified residue	UNP Q8X655
D	253	MSE	MET	modified residue	UNP Q8X655
D	256	MSE	MET	modified residue	UNP Q8X655

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Fe 1	0	0
2	B	1	Total 1	Fe 1	0	0
2	C	1	Total 1	Fe 1	0	0
2	D	1	Total 1	Fe 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	110	Total 110	O 110	0	0
3	B	129	Total 129	O 129	0	0
3	C	130	Total 130	O 130	0	0
3	D	147	Total 147	O 147	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: putative gentisate 1,2-dioxygenase

- Molecule 1: putative gentisate 1,2-dioxygenase

GLU GLN GLN P183 V184 T185 R186 K187 E188 G189 D190 Y191 Y195 A196 A197 N198 M199 L200 P201 H204 Q205 T206 G207 N208 S209 F213 N214 Y215 R216 Y217 D218 R219 S220 R221 E222 V223 L224 H225 D226 L227 T228 R229 L230 G231 D232 E235 W236 D237 K240 M241 R242 Y243 V244 N245 P246

V247 T248 G249 G250 Y251 P252 M253 M256 L260 Q261 K265 G266 F267 A268 S269 A272 R273 T274 T275 D276 I279 Y280 H281 V282 V283 E284 G285 S286 G287 Q288 V289 I290 I291 G292 N293 E294 T295 F298 V305 V306 P307 T308 W309 H310 G311 F314 Q315 T316 T317 Q318 D319 S320

V321 L322 F323 S324 F325 S326 D327 R328 P329 V330 Q331 L334 G335 L336 F337 R338 R341 TYR

● Molecule 1: putative gentisate 1,2-dioxygenase

Chain C:

%
31%   34%   14%   ·   18%

MSE GLY SER SER HIS HIS HIS HIS HIS GLY SER MSE THR ASP ASN ASN GLN ASN SER ARG GLU GLN PHE TYR GLN HIS ILE SER GLY GLN ASN LEU THR PRO LEU TRP GLU SER LEU HIS LEU LEU VAL P33 N37 A38 N39 C40 A43 Y44 W45 N46 Y47 Q48 E49 I50 R51
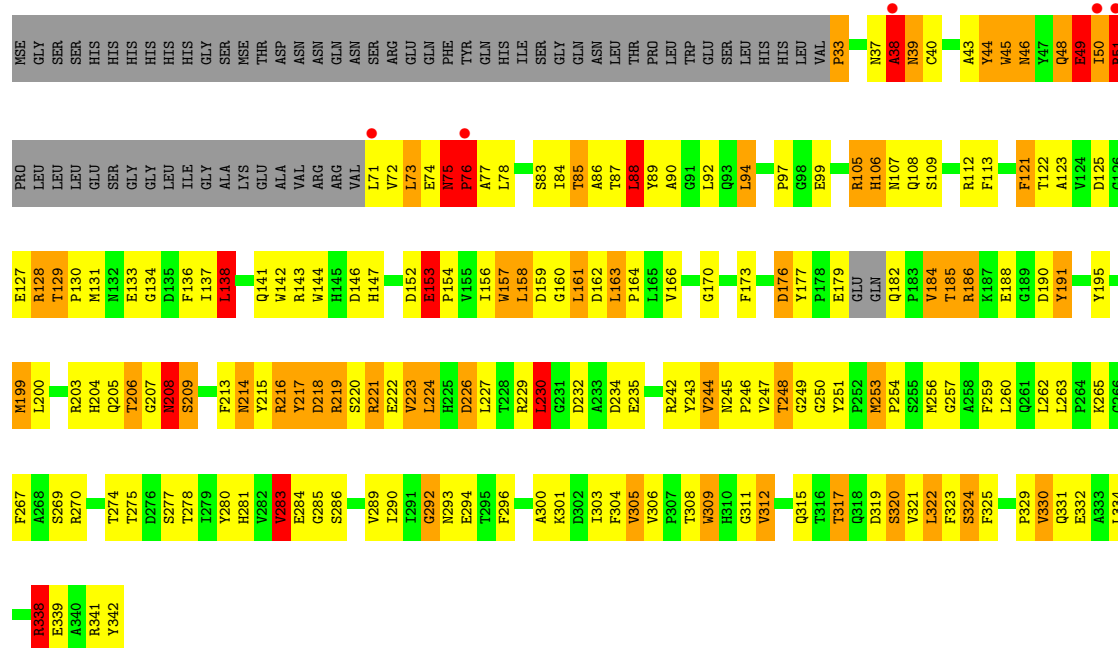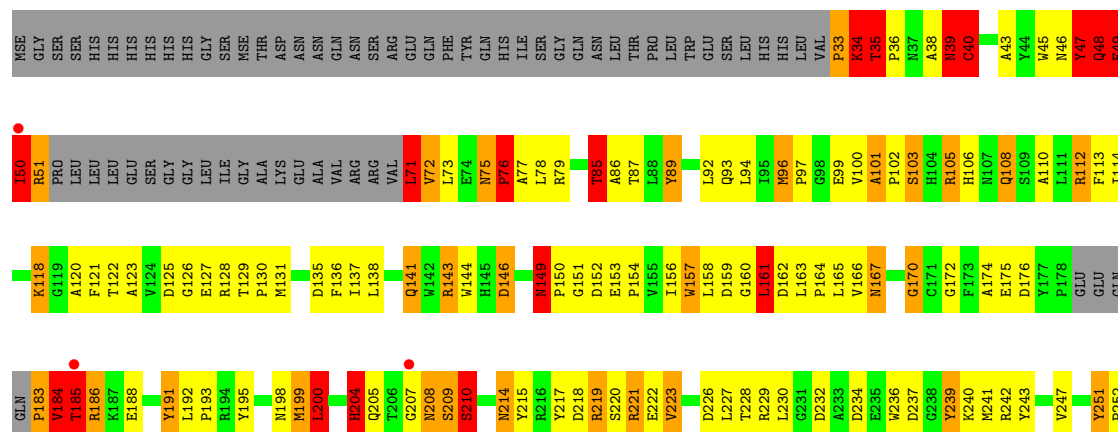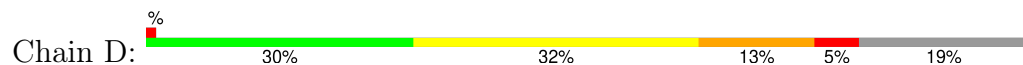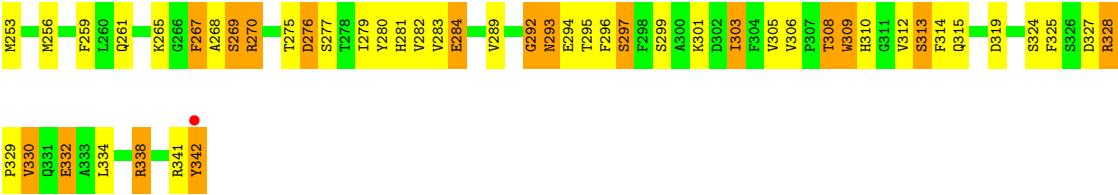
PRO LEU LEU LEU GLU SER GLY GLY LEU ILE GLY ALA LYS GLU ALA VAL ARG ARG VAL L71 V72 L73 E74 N75 P76 A77 L78 S83 I84 T85 A86 T87 L88 Y89 A90 G91 L92 Q93 L94 P97 G98 E99 R105 H106 N107 Q108 S109 R112 F113 F121 T122 A123 V124 D125 G126

E127 R128 T129 P130 M131 N132 E133 G134 D135 F136 I137 L138 Q141 W142 R143 W144 H145 D146 H147 D152 E153 P154 V155 I156 W157 L158 D159 G160 L161 D162 L163 P164 L165 V166 G170 F173 D176 Y177 P178 E179 GLU GLN Q182 P183 V184 T185 R186 K187 E188 G189 D190 Y191 Y195

M199 L200 R203 H204 Q205 T206 G207 N208 S209 F213 N214 Y215 R216 Y217 D218 R219 S220 R221 E222 V223 L224 H225 D226 L227 T228 R229 L230 G231 D232 A233 D234 E235 R242 Y243 V244 N245 P246 V247 T248 G249 G250 Y251 P252 M253 P254 S255 M256 G257 A258 F259 L260 Q261 L262 L263 P264 K265 G266

F267 A268 S269 R270 T274 T275 D276 S277 T278 I279 Y280 H281 V282 V283 E284 G285 S286 V289 I290 I291 G292 N293 E294 T295 F296 A300 K301 D302 I303 F304 V305 V306 P307 T308 W309 H310 G311 V312 Q315 T316 T317 Q318 D319 S320 V321 L322 F323 S324 F325 P329 V330 Q331 E332 A333 L334

R338 E339 A340 R341 Y342

● Molecule 1: putative gentisate 1,2-dioxygenase

Chain D:

%
30%   32%   13%   5%   19%

MSE GLY SER SER HIS HIS HIS HIS HIS GLY SER MSE THR ASP ASN ASN GLN ASN SER ARG GLU GLN PHE TYR GLN HIS ILE SER GLY GLN ASN LEU THR PRO LEU TRP GLU SER LEU HIS LEU LEU VAL P33 K34 T35 P36 N37 A38 N39 C40 A43 Y44 W45 N46 Y47 Q48 E49

I50 R51 PRO LEU LEU LEU GLU SER GLY GLY LEU ILE GLY ALA LYS GLU ALA VAL ARG ARG VAL L71 V72 L73 E74 N75 P76 A77 L78 R79 T85 A86 T87 L88 Y89 L92 Q93 L94 I95 M96 P97 G98 E99 V100 A101 P102 S103 H104 R105 H106 N107 Q108 S109 A110 L111 R112 F113 I114

K118 G119 A120 F121 T122 A123 V124 D125 G126 E127 R128 T129 P130 M131 N132 D135 F136 I137 L138 Q141 W142 R143 W144 H145 D146 N149 P150 G151 D152 E153 P154 V155 I156 W157 L158 D159 G160 L161 D162 L163 P164 L165 V166 N167 G170 C171 G172 F173 A174 E175 D176 Y177 P178 GLU GLN

GLN P183 V184 T185 R186 K187 E188 Y191 L192 P193 R194 Y195 M198 M199 L200 H204 Q205 T206 G207 N208 S209 S210 N214 Y215 R216 Y217 D218 R219 S220 R221 E222 V223 D226 L227 T228 R229 L230 G231 D232 A233 D234 E235 W236 D237 G238 Y239 K240 M241 R242 Y243 V247 Y251 P252

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M253 M256 F259 L260 Q261 K265 G266 F267 A268 S269 R270 T275 D276 S277 T278 I279 Y280 H281 V282 V283 E284 V289 G292 N293 E294 T295 F296 S297 F298 S299 A300 K301 D302 I303 F304 V305 V306 P307 T308 W309 H310 G311 V312 S313 F314 Q315 D319 S324 F325 S326 D327 R328

P329 V330 Q331 E332 A333 L334 R338 R341 Y342

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	54.13Å 76.08Å 85.46Å 114.08° 94.93° 108.11°	Depositor
Resolution (Å)	34.50 – 2.41 34.50 – 2.41	Depositor EDS
% Data completeness (in resolution range)	100.0 (34.50-2.41) 93.6 (34.50-2.41)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	6.71 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.173 , 0.249 0.188 , 0.180	Depositor DCC
R_{free} test set	2048 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	27.0	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 48.8	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	0.94	EDS
Total number of atoms	9579	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.47% 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 ⓘ

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

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	2.32	88/2340 (3.8%)	1.67	39/3182 (1.2%)
1	B	2.31	92/2294 (4.0%)	1.63	41/3118 (1.3%)
1	C	2.31	90/2341 (3.8%)	1.77	49/3181 (1.5%)
1	D	2.38	100/2323 (4.3%)	1.73	55/3156 (1.7%)
All	All	2.33	370/9298 (4.0%)	1.70	184/12637 (1.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	D	0	2
All	All	0	5

The worst 5 of 370 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	77	ALA	CA-CB	-14.93	1.21	1.52
1	D	50	ILE	CA-CB	12.29	1.83	1.54
1	B	289	VAL	CB-CG2	-11.71	1.28	1.52
1	D	267	PHE	CD2-CE2	-10.95	1.17	1.39
1	D	76	PRO	CA-CB	10.78	1.75	1.53

The worst 5 of 184 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	128	ARG	NE-CZ-NH1	-16.78	111.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	ARG	NE-CZ-NH1	15.39	128.00	120.30
1	C	128	ARG	NE-CZ-NH2	15.21	127.91	120.30
1	A	341	ARG	NE-CZ-NH2	-12.57	114.02	120.30
1	D	237	ASP	CB-CG-OD1	-12.19	107.33	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	37	ASN	Peptide
1	B	39	ASN	Peptide
1	B	76	PRO	Peptide
1	D	149	ASN	Mainchain
1	D	47	TYR	Peptide

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	2280	0	2134	129	0
1	B	2235	0	2093	180	0
1	C	2281	0	2135	137	0
1	D	2263	0	2122	144	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	110	0	0	9	0
3	B	129	0	0	26	0
3	C	130	0	0	21	0
3	D	147	0	0	25	2
All	All	9579	0	8484	565	2

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 32.

The worst 5 of 565 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:PRO:CB	1:D:76:PRO:CA	1.75	1.61
1:B:227:LEU:CG	1:B:227:LEU:CD2	1.74	1.59
1:C:50:ILE:CB	1:C:50:ILE:CG2	1.76	1.59
1:D:50:ILE:CA	1:D:50:ILE:CB	1.83	1.56
1:C:33:PRO:CG	1:C:33:PRO:CB	1.78	1.53

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:THR:N	3:D:1122:HOH:O[1_455]	1.91	0.29
1:D:33:PRO:CB	3:D:1136:HOH:O[1_455]	1.98	0.22

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	283/354 (80%)	257 (91%)	13 (5%)	13 (5%)	2	1
1	B	278/354 (78%)	248 (89%)	15 (5%)	15 (5%)	1	1
1	C	283/354 (80%)	251 (89%)	25 (9%)	7 (2%)	4	4
1	D	281/354 (79%)	249 (89%)	16 (6%)	16 (6%)	1	0
All	All	1125/1416 (79%)	1005 (89%)	69 (6%)	51 (4%)	2	1

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	ALA
1	A	50	ILE
1	A	77	ALA
1	A	141	GLN
1	A	182	GLN

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	232/293 (79%)	210 (90%)	22 (10%)	7	10
1	B	227/293 (78%)	196 (86%)	31 (14%)	3	3
1	C	232/293 (79%)	204 (88%)	28 (12%)	4	5
1	D	230/293 (78%)	203 (88%)	27 (12%)	4	5
All	All	921/1172 (79%)	813 (88%)	108 (12%)	4	5

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	75	ASN
1	C	208	ASN
1	D	214	ASN
1	C	92	LEU
1	C	158	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	205	GLN
1	D	75	ASN
1	C	208	ASN
1	C	310	HIS
1	D	149	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 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, 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	283/354 (79%)	-0.53	0	100	100	13, 26, 47, 55	0
1	B	278/354 (78%)	-0.44	3 (1%)	77	76	15, 27, 51, 64	0
1	C	283/354 (79%)	-0.38	5 (1%)	67	64	17, 28, 50, 66	0
1	D	281/354 (79%)	-0.46	4 (1%)	73	71	14, 26, 49, 65	0
All	All	1125/1416 (79%)	-0.45	12 (1%)	77	76	13, 27, 49, 66	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	50	ILE	4.4
1	C	50	ILE	3.8
1	B	208	ASN	3.1
1	D	342	TYR	3.1
1	D	207	GLY	2.7

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 ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FE	B	1002	1/1	0.99	0.08	26,26,26,26	0
2	FE	D	1004	1/1	0.99	0.05	31,31,31,31	0
2	FE	C	1003	1/1	1.00	0.05	31,31,31,31	0
2	FE	A	1001	1/1	1.00	0.03	27,27,27,27	0

6.5 Other polymers (i)

There are no such residues in this entry.