



# Full wwPDB X-ray Structure Validation Report ⓘ

May 6, 2025 – 10:12 AM JST

PDB ID : 9J0H / pdb\_00009j0h  
Title : The crystal structure of styrene monooxygenase StyA from *Streptomyces vil-*  
morinianum  
Authors : Wang, L.; Zhou, J.  
Deposited on : 2024-08-02  
Resolution : 2.86 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

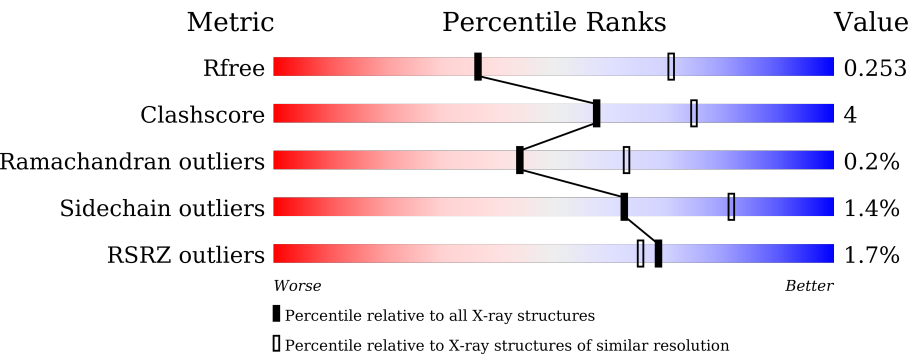
MolProbity : 4-5-2 with Phenix2.0rc1  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.86 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1268 (2.88-2.84)
Clashscore	180529	1351 (2.88-2.84)
Ramachandran outliers	177936	1318 (2.88-2.84)
Sidechain outliers	177891	1319 (2.88-2.84)
RSRZ outliers	164620	1269 (2.88-2.84)

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	446	<div><div></div><div>80%11%9%</div></div>
1	B	446	<div><div>%</div><div>78%11%10%</div></div>
1	C	446	<div><div>%</div><div>82%9%9%</div></div>
1	D	446	<div><div>%</div><div>81%10%9%</div></div>
1	E	446	<div><div>2%</div><div>78%12%10%</div></div>
1	F	446	<div><div>2%</div><div>81%10%9%</div></div>

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Mol	Chain	Length	Quality of chain
1	G	446	<div><div></div><div>3%</div><div>79%</div><div>11%</div><div>10%</div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 21480 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 styrene monooxygenase/indole monooxygenase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	0
			3089	1953	566	562	8			
1	B	401	Total	C	N	O	S	0	0	0
			3047	1931	557	551	8			
1	C	405	Total	C	N	O	S	0	0	0
			3076	1946	564	558	8			
1	D	406	Total	C	N	O	S	0	0	0
			3078	1948	562	560	8			
1	E	402	Total	C	N	O	S	0	0	0
			3044	1930	552	554	8			
1	F	405	Total	C	N	O	S	0	0	0
			3070	1943	561	558	8			
1	G	403	Total	C	N	O	S	0	0	0
			3062	1939	562	554	7			


- Molecule 2 is water.

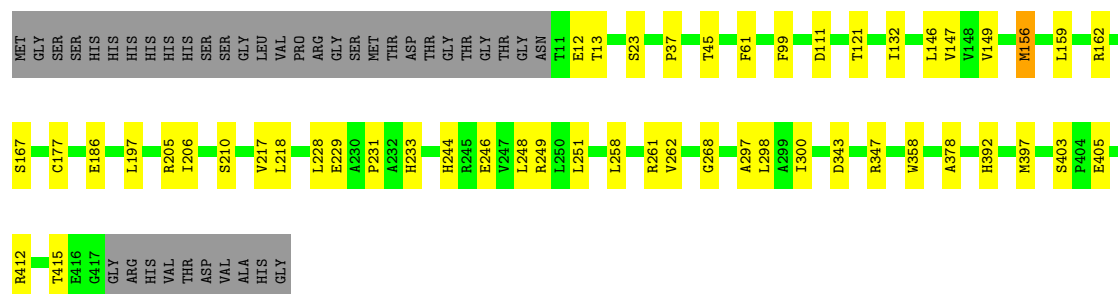
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	O	0	0
			2	2		
2	B	2	Total	O	0	0
			2	2		
2	C	3	Total	O	0	0
			3	3		
2	D	1	Total	O	0	0
			1	1		
2	E	2	Total	O	0	0
			2	2		
2	F	3	Total	O	0	0
			3	3		
2	G	1	Total	O	0	0
			1	1		

### 3 Residue-property plots [i](#)


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

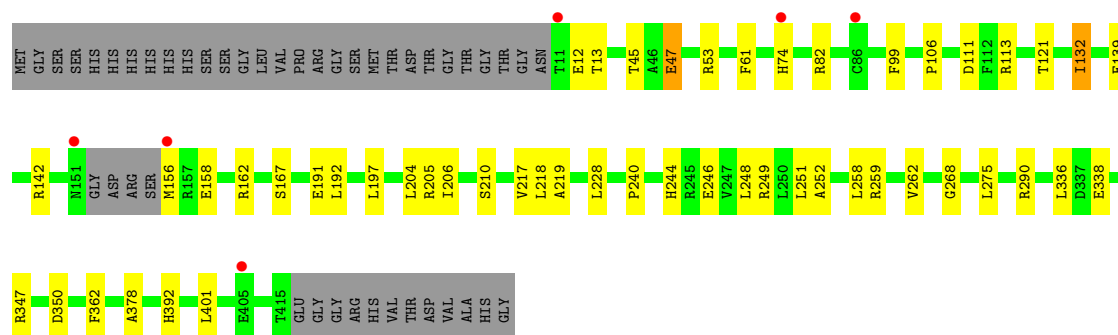
- Molecule 1: styrene monooxygenase/indole monooxygenase family protein

Chain A: 




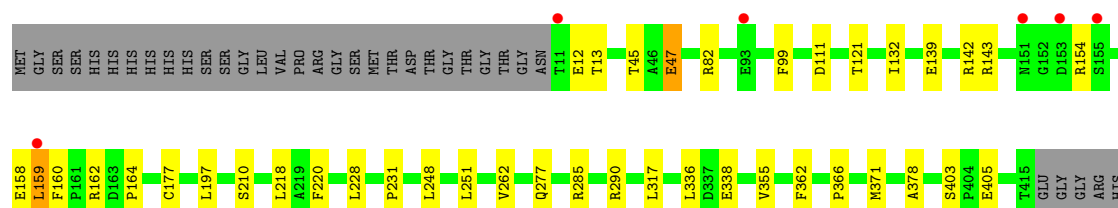
- Molecule 1: styrene monooxygenase/indole monooxygenase family protein

Chain B: 




- Molecule 1: styrene monooxygenase/indole monooxygenase family protein

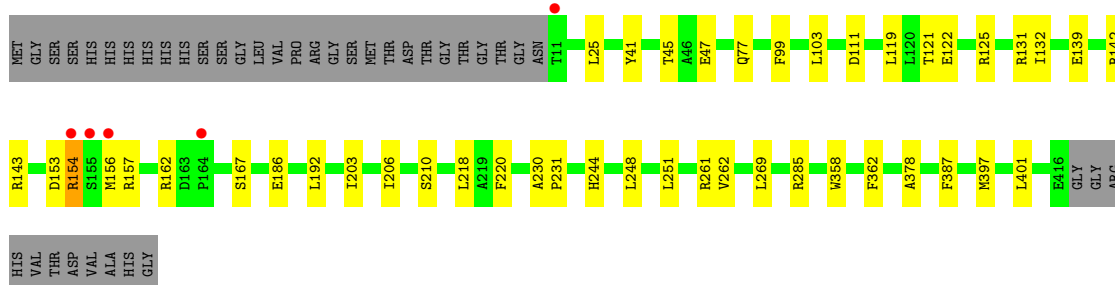
Chain C: 



VAL  
THR  
ASP  
VAL  
ALA  
HIS  
GLY


- Molecule 1: styrene monooxygenase/indole monooxygenase family protein

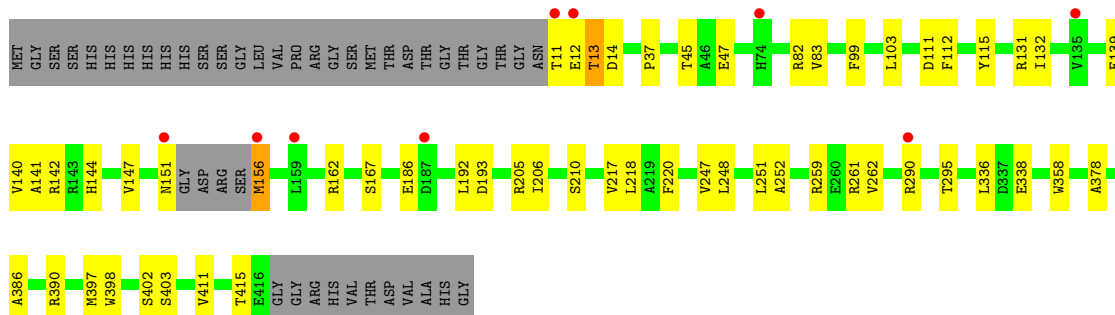
Chain D: 



HIS  
VAL  
THR  
ASP  
VAL  
ALA  
HIS  
GLY


- Molecule 1: styrene monooxygenase/indole monooxygenase family protein

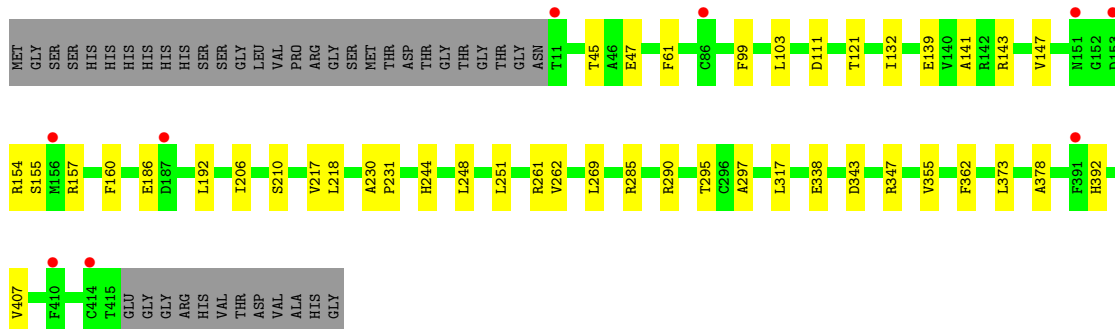
Chain E: 



A386, R390, M397, W398, S402, S403, V411, T415, F416, GLY, ARG, HIS, VAL, THR, ASP, VAL, ALA, HIS, GLY


- Molecule 1: styrene monooxygenase/indole monooxygenase family protein

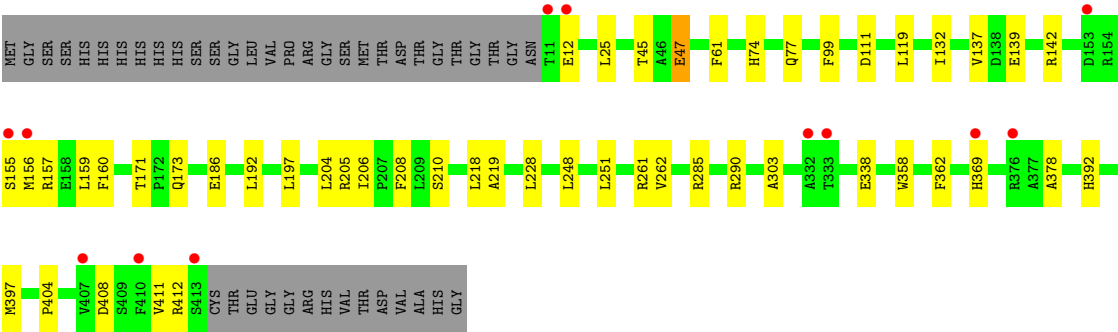
Chain F: 



V407, F410, C414, T415, GLY, GLY, ARG, HIS, VAL, THR, ASP, VAL, ALA, HIS, GLY

- Molecule 1: styrene monooxygenase/indole monooxygenase family protein

Chain G: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.51Å 112.15Å 345.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.25 – 2.86 48.25 – 2.86	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.25-2.86) 99.4 (48.25-2.86)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.32 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.211 , 0.253 0.211 , 0.253	Depositor DCC
$R_{free}$ test set	3964 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.7	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 33.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	21480	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.15	0/3173	0.35	0/4332
1	B	0.17	0/3130	0.39	0/4274
1	C	0.16	0/3160	0.36	0/4315
1	D	0.15	0/3162	0.38	0/4319
1	E	0.14	0/3127	0.36	0/4272
1	F	0.14	0/3154	0.37	0/4308
1	G	0.14	0/3146	0.36	0/4296
All	All	0.15	0/22052	0.37	0/30116

There are no bond length outliers.

There are no bond angle outliers.

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	3089	0	3018	28	0
1	B	3047	0	2983	31	0
1	C	3076	0	3009	23	0
1	D	3078	0	3001	31	0
1	E	3044	0	2967	36	0
1	F	3070	0	2998	23	0
1	G	3062	0	2994	26	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	3	0	0	0	0
2	D	1	0	0	0	0
2	E	2	0	0	0	0
2	F	3	0	0	0	0
2	G	1	0	0	0	0
All	All	21480	0	20970	187	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 4.

All (187) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:GLU:HG2	1:C:143:ARG:HH12	1.29	0.94
1:D:121:THR:HG22	1:D:125:ARG:HE	1.34	0.93
1:D:157:ARG:HH21	1:D:162:ARG:H	1.25	0.85
1:A:218:LEU:HD21	1:A:251:LEU:HD11	1.67	0.76
1:C:139:GLU:HG2	1:C:143:ARG:NH1	2.00	0.76
1:D:157:ARG:HD2	1:D:285:ARG:HE	1.50	0.76
1:F:244:HIS:HE1	1:F:269:LEU:H	1.34	0.76
1:B:13:THR:HG23	1:B:336:LEU:HD11	1.69	0.73
1:A:233:HIS:O	1:C:164:PRO:HB2	1.87	0.73
1:F:99:PHE:HB3	1:F:378:ALA:HA	1.72	0.72
1:B:99:PHE:HB3	1:B:378:ALA:HA	1.74	0.70
1:B:218:LEU:HD21	1:B:251:LEU:HD11	1.72	0.70
1:D:218:LEU:HD21	1:D:251:LEU:HD11	1.73	0.69
1:A:111:ASP:HB2	1:A:210:SER:HA	1.75	0.69
1:A:99:PHE:HB3	1:A:378:ALA:HA	1.76	0.68
1:B:244:HIS:CD2	1:B:268:GLY:HA2	2.28	0.68
1:E:338:GLU:OE2	1:G:412:ARG:HD2	1.93	0.68
1:F:111:ASP:HB2	1:F:210:SER:HA	1.76	0.68
1:D:125:ARG:HD2	1:E:12:GLU:HB2	1.76	0.66
1:G:139:GLU:HG2	1:G:142:ARG:HH21	1.60	0.65
1:B:111:ASP:HB2	1:B:210:SER:HA	1.79	0.65
1:D:153:ASP:OD1	1:D:154:ARG:N	2.29	0.64
1:F:218:LEU:HD21	1:F:251:LEU:HD11	1.79	0.64
1:G:408:ASP:HB3	1:G:412:ARG:NH1	2.13	0.64
1:C:248:LEU:HD21	1:C:262:VAL:HG11	1.79	0.63
1:A:244:HIS:CD2	1:A:268:GLY:HA2	2.34	0.63
1:E:13:THR:HG23	1:E:336:LEU:HD11	1.79	0.63
1:D:121:THR:HG22	1:D:125:ARG:NE	2.08	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:99:PHE:HB3	1:G:378:ALA:HA	1.81	0.63
1:C:111:ASP:HB2	1:C:210:SER:HA	1.79	0.62
1:C:99:PHE:HB3	1:C:378:ALA:HA	1.81	0.62
1:E:99:PHE:HB3	1:E:378:ALA:HA	1.81	0.62
1:D:186:GLU:HA	1:D:261:ARG:HH21	1.64	0.62
1:F:45:THR:HG22	1:F:132:ILE:HG21	1.81	0.62
1:G:111:ASP:HB2	1:G:210:SER:HA	1.83	0.61
1:E:218:LEU:HD21	1:E:251:LEU:HD11	1.84	0.60
1:D:111:ASP:HB2	1:D:210:SER:HA	1.83	0.59
1:G:218:LEU:HD21	1:G:251:LEU:HD11	1.84	0.59
1:C:139:GLU:HG3	1:C:142:ARG:HH21	1.66	0.59
1:A:186:GLU:HA	1:A:261:ARG:HH21	1.66	0.59
1:A:162:ARG:NH2	1:A:167:SER:O	2.36	0.59
1:C:13:THR:HG23	1:C:336:LEU:HD11	1.84	0.59
1:D:99:PHE:HB3	1:D:378:ALA:HA	1.84	0.58
1:E:162:ARG:NH2	1:E:167:SER:O	2.37	0.58
1:E:111:ASP:HB2	1:E:210:SER:HA	1.85	0.57
1:E:192:LEU:HD13	1:E:206:ILE:HG23	1.87	0.57
1:A:403:SER:OG	1:B:350:ASP:OD1	2.23	0.57
1:G:137:VAL:HG11	1:G:159:LEU:HD11	1.86	0.57
1:F:139:GLU:HG2	1:F:143:ARG:NH1	2.20	0.56
1:B:204:LEU:HB2	1:B:219:ALA:HB3	1.87	0.56
1:B:205:ARG:HB2	1:B:258:LEU:HD21	1.87	0.56
1:G:290:ARG:NH1	1:G:338:GLU:OE1	2.39	0.56
1:B:240:PRO:O	1:B:244:HIS:ND1	2.30	0.55
1:D:162:ARG:NH2	1:D:167:SER:O	2.40	0.54
1:C:220:PHE:HD2	1:C:228:LEU:HD22	1.71	0.53
1:G:192:LEU:HD12	1:G:206:ILE:HG23	1.89	0.53
1:D:157:ARG:CD	1:D:285:ARG:HE	2.19	0.53
1:B:206:ILE:HB	1:B:217:VAL:HB	1.90	0.53
1:G:248:LEU:HD21	1:G:262:VAL:HG11	1.91	0.52
1:D:125:ARG:NH1	1:E:13:THR:H	2.06	0.52
1:C:231:PRO:O	1:C:277:GLN:NE2	2.42	0.52
1:D:244:HIS:HE1	1:D:269:LEU:H	1.58	0.52
1:E:358:TRP:CZ2	1:E:397:MET:HG2	2.45	0.52
1:F:248:LEU:HD21	1:F:262:VAL:HG11	1.90	0.52
1:D:41:TYR:OH	1:D:131:ARG:NH1	2.42	0.52
1:A:177:CYS:SG	1:A:231:PRO:HB2	2.50	0.51
1:C:403:SER:HB2	1:C:405:GLU:OE1	2.10	0.51
1:D:248:LEU:HD21	1:D:262:VAL:HG11	1.93	0.51
1:E:386:ALA:O	1:E:390:ARG:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:186:GLU:HA	1:F:261:ARG:HH21	1.75	0.50
1:A:149:VAL:HG11	1:A:156:MET:HG2	1.94	0.50
1:A:405:GLU:HG2	1:B:347:ARG:NH1	2.27	0.50
1:F:206:ILE:HB	1:F:217:VAL:HB	1.94	0.50
1:B:45:THR:HA	1:B:132:ILE:HD12	1.94	0.49
1:B:111:ASP:OD2	1:B:113:ARG:NH2	2.41	0.49
1:D:125:ARG:HH11	1:E:13:THR:H	1.59	0.49
1:G:61:PHE:HB3	1:G:392:HIS:ND1	2.27	0.49
1:B:45:THR:HG22	1:B:132:ILE:HG21	1.95	0.49
1:G:186:GLU:HA	1:G:261:ARG:HH21	1.78	0.49
1:B:192:LEU:CD1	1:B:206:ILE:HG12	2.42	0.49
1:E:83:VAL:HG12	1:E:103:LEU:HD12	1.94	0.49
1:F:373:LEU:HB2	1:F:407:VAL:HG13	1.94	0.48
1:A:248:LEU:HD21	1:A:262:VAL:HG11	1.96	0.48
1:B:61:PHE:HB3	1:B:392:HIS:ND1	2.28	0.48
1:B:252:ALA:HB2	1:B:259:ARG:HG2	1.95	0.48
1:F:160:PHE:O	1:F:285:ARG:HD3	2.13	0.48
1:A:156:MET:HG3	1:A:159:LEU:HD12	1.95	0.48
1:C:366:PRO:HB2	1:C:371:MET:HG2	1.97	0.47
1:A:61:PHE:HB3	1:A:392:HIS:ND1	2.30	0.47
1:F:192:LEU:HD13	1:F:206:ILE:HG23	1.96	0.47
1:A:412:ARG:HA	1:A:415:THR:HG22	1.96	0.47
1:C:160:PHE:O	1:C:285:ARG:HD3	2.14	0.47
1:D:125:ARG:HH11	1:E:13:THR:N	2.12	0.47
1:G:45:THR:HG22	1:G:132:ILE:HG21	1.97	0.47
1:F:343:ASP:O	1:F:347:ARG:HG3	2.15	0.47
1:A:197:LEU:HD12	1:A:228:LEU:HD11	1.97	0.46
1:A:147:VAL:O	1:A:297:ALA:HA	2.15	0.46
1:F:192:LEU:CD1	1:F:206:ILE:HG12	2.45	0.46
1:A:23:SER:HB2	1:A:300:ILE:HD12	1.96	0.46
1:G:160:PHE:O	1:G:285:ARG:HD3	2.15	0.46
1:B:162:ARG:NH2	1:B:167:SER:O	2.49	0.46
1:E:140:VAL:HG12	1:E:147:VAL:HG22	1.97	0.46
1:F:61:PHE:HB3	1:F:392:HIS:ND1	2.30	0.46
1:F:244:HIS:CE1	1:F:269:LEU:H	2.22	0.46
1:F:155:SER:O	1:F:157:ARG:N	2.49	0.45
1:B:82:ARG:HB3	1:B:106:PRO:HB2	1.98	0.45
1:D:131:ARG:HH12	1:D:143:ARG:HD3	1.82	0.45
1:F:290:ARG:NH1	1:F:338:GLU:OE1	2.48	0.45
1:G:197:LEU:HD12	1:G:228:LEU:HD11	1.98	0.45
1:B:156:MET:C	1:B:158:GLU:N	2.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:GLU:OE1	1:E:11:THR:HB	2.17	0.45
1:E:192:LEU:CD1	1:E:206:ILE:HG12	2.47	0.45
1:E:186:GLU:HA	1:E:261:ARG:HH21	1.81	0.45
1:B:139:GLU:HG2	1:B:142:ARG:HH21	1.81	0.45
1:D:203:ILE:HG12	1:D:220:PHE:CD1	2.51	0.45
1:G:25:LEU:HD13	1:G:119:LEU:HB2	1.98	0.45
1:C:177:CYS:SG	1:C:231:PRO:HB2	2.58	0.44
1:D:203:ILE:HG12	1:D:220:PHE:HD1	1.82	0.44
1:A:358:TRP:CZ2	1:A:397:MET:HG2	2.52	0.44
1:C:162:ARG:O	1:C:164:PRO:HD3	2.18	0.44
1:D:45:THR:HG22	1:D:132:ILE:HG21	1.99	0.44
1:B:362:PHE:HE1	1:B:401:LEU:HD13	1.83	0.44
1:A:13:THR:O	1:A:37:PRO:HD2	2.18	0.44
1:E:206:ILE:HB	1:E:217:VAL:HB	1.99	0.44
1:G:358:TRP:CZ2	1:G:397:MET:HG2	2.53	0.44
1:D:125:ARG:NH1	1:E:13:THR:OG1	2.50	0.44
1:B:244:HIS:HD2	1:B:268:GLY:HA2	1.79	0.43
1:B:246:GLU:OE2	1:B:249:ARG:NH2	2.51	0.43
1:E:112:PHE:HA	1:E:115:TYR:HB3	2.00	0.43
1:E:205:ARG:HA	1:E:217:VAL:O	2.19	0.43
1:E:139:GLU:HG2	1:E:142:ARG:HH21	1.84	0.43
1:A:246:GLU:OE2	1:A:249:ARG:NH2	2.41	0.43
1:G:155:SER:HB3	1:G:303:ALA:HA	2.01	0.43
1:B:47:GLU:H	1:B:47:GLU:CD	2.25	0.43
1:B:290:ARG:NH1	1:B:338:GLU:OE1	2.51	0.43
1:A:146:LEU:HD21	1:A:298:LEU:HD12	2.00	0.43
1:G:369:HIS:CD2	1:G:404:PRO:HG3	2.54	0.43
1:E:151:ASN:HD21	1:E:156:MET:HG2	1.84	0.43
1:G:74:HIS:CE1	1:G:77:GLN:HE21	2.37	0.43
1:C:158:GLU:HG3	1:C:159:LEU:HD22	2.01	0.43
1:C:197:LEU:HD12	1:C:228:LEU:HD11	2.01	0.43
1:E:141:ALA:HB1	1:E:295:THR:HB	2.01	0.43
1:G:47:GLU:CD	1:G:47:GLU:H	2.27	0.43
1:B:197:LEU:HD12	1:B:228:LEU:HD11	2.01	0.42
1:E:248:LEU:HD21	1:E:262:VAL:HG11	2.01	0.42
1:A:205:ARG:HB2	1:A:258:LEU:HD21	2.01	0.42
1:C:290:ARG:NH1	1:C:338:GLU:OE1	2.52	0.42
1:D:192:LEU:HD12	1:D:206:ILE:HG23	2.00	0.42
1:F:141:ALA:HB1	1:F:295:THR:HB	2.01	0.42
1:B:248:LEU:HD21	1:B:262:VAL:HG11	2.00	0.42
1:C:317:LEU:HD13	1:C:355:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:358:TRP:CZ2	1:D:397:MET:HG2	2.54	0.42
1:C:45:THR:OG1	1:C:47:GLU:HG2	2.19	0.42
1:C:218:LEU:HD21	1:C:251:LEU:HD11	2.01	0.42
1:A:205:ARG:HA	1:A:217:VAL:O	2.19	0.42
1:D:103:LEU:HD23	1:D:103:LEU:HA	1.85	0.42
1:E:45:THR:HG22	1:E:132:ILE:HG21	2.01	0.42
1:D:25:LEU:HD13	1:D:119:LEU:HB2	2.02	0.42
1:D:387:PHE:HE1	1:D:401:LEU:HD21	1.85	0.42
1:E:14:ASP:O	1:E:144:HIS:HB3	2.19	0.42
1:G:205:ARG:NH2	1:G:261:ARG:HH22	2.17	0.42
1:D:139:GLU:HG2	1:D:142:ARG:HH21	1.84	0.42
1:F:230:ALA:HB3	1:F:231:PRO:HD3	2.02	0.42
1:G:408:ASP:HB3	1:G:412:ARG:HH12	1.84	0.42
1:B:191:GLU:O	1:B:205:ARG:NH2	2.54	0.41
1:A:205:ARG:NH2	1:A:261:ARG:HH22	2.18	0.41
1:A:218:LEU:HD12	1:A:218:LEU:HA	1.90	0.41
1:A:343:ASP:O	1:A:347:ARG:HG3	2.20	0.41
1:B:192:LEU:HD13	1:B:206:ILE:HG23	2.02	0.41
1:E:13:THR:O	1:E:37:PRO:HD2	2.20	0.41
1:E:411:VAL:O	1:E:415:THR:HG22	2.21	0.41
1:C:220:PHE:CD2	1:C:228:LEU:HD22	2.53	0.41
1:B:53:ARG:NH2	1:B:275:LEU:O	2.53	0.41
1:E:131:ARG:HD3	1:E:131:ARG:HA	1.95	0.41
1:F:103:LEU:HD23	1:F:103:LEU:HA	1.90	0.41
1:G:171:THR:O	1:G:173:GLN:NE2	2.48	0.41
1:D:230:ALA:HB3	1:D:231:PRO:HD3	2.02	0.41
1:C:45:THR:HG22	1:C:132:ILE:HG21	2.02	0.40
1:F:317:LEU:HD13	1:F:355:VAL:HG21	2.02	0.40
1:A:45:THR:HG22	1:A:132:ILE:HG21	2.04	0.40
1:E:193:ASP:OD2	1:E:205:ARG:NH2	2.41	0.40
1:E:252:ALA:HB2	1:E:259:ARG:HG2	2.03	0.40
1:E:398:TRP:O	1:E:402:SER:OG	2.38	0.40
1:F:147:VAL:O	1:F:297:ALA:HA	2.21	0.40
1:G:204:LEU:HB2	1:G:219:ALA:HB3	2.02	0.40
1:E:220:PHE:CE2	1:E:247:VAL:HG13	2.57	0.40
1:E:290:ARG:NH2	1:G:412:ARG:HD3	2.35	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	405/446 (91%)	397 (98%)	8 (2%)	0	100	100
1	B	397/446 (89%)	390 (98%)	7 (2%)	0	100	100
1	C	403/446 (90%)	394 (98%)	8 (2%)	1 (0%)	44	63
1	D	404/446 (91%)	396 (98%)	6 (2%)	2 (0%)	25	43
1	E	398/446 (89%)	390 (98%)	7 (2%)	1 (0%)	37	55
1	F	403/446 (90%)	394 (98%)	8 (2%)	1 (0%)	44	63
1	G	401/446 (90%)	393 (98%)	6 (2%)	2 (0%)	25	43
All	All	2811/3122 (90%)	2754 (98%)	50 (2%)	7 (0%)	44	63

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	154	ARG
1	D	156	MET
1	E	403	SER
1	G	157	ARG
1	F	154	ARG
1	G	156	MET
1	C	154	ARG

### 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	314/344 (91%)	309 (98%)	5 (2%)	58	79
1	B	310/344 (90%)	305 (98%)	5 (2%)	58	79
1	C	313/344 (91%)	307 (98%)	6 (2%)	52	74
1	D	312/344 (91%)	309 (99%)	3 (1%)	73	87
1	E	309/344 (90%)	305 (99%)	4 (1%)	65	83
1	F	312/344 (91%)	309 (99%)	3 (1%)	73	87
1	G	310/344 (90%)	305 (98%)	5 (2%)	58	79
All	All	2180/2408 (90%)	2149 (99%)	31 (1%)	62	82

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLU
1	A	121	THR
1	A	156	MET
1	A	206	ILE
1	A	229	GLU
1	B	12	GLU
1	B	47	GLU
1	B	74	HIS
1	B	121	THR
1	B	132	ILE
1	C	12	GLU
1	C	47	GLU
1	C	82	ARG
1	C	121	THR
1	C	159	LEU
1	C	362	PHE
1	D	47	GLU
1	D	77	GLN
1	D	362	PHE
1	E	13	THR
1	E	47	GLU
1	E	82	ARG
1	E	156	MET
1	F	47	GLU
1	F	121	THR
1	F	362	PHE
1	G	12	GLU
1	G	47	GLU
1	G	208	PHE

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Mol	Chain	Res	Type
1	G	362	PHE
1	G	411	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	173	GLN
1	B	360	ASN
1	C	307	ASN
1	D	244	HIS
1	D	360	ASN
1	E	65	GLN
1	E	118	HIS
1	F	118	HIS
1	F	244	HIS
1	G	32	GLN
1	G	77	GLN
1	G	118	HIS
1	G	307	ASN
1	G	369	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	407/446 (91%)	-0.33	0 100 100	27, 41, 65, 87	0
1	B	401/446 (89%)	-0.05	6 (1%) 71 68	27, 50, 74, 104	0
1	C	405/446 (90%)	-0.10	6 (1%) 71 68	29, 49, 83, 108	0
1	D	406/446 (91%)	0.06	5 (1%) 76 74	33, 57, 83, 112	0
1	E	402/446 (90%)	0.23	9 (2%) 62 59	36, 63, 92, 110	0
1	F	405/446 (90%)	0.05	9 (2%) 62 59	30, 59, 99, 120	0
1	G	403/446 (90%)	0.19	12 (2%) 52 49	35, 60, 104, 119	0
All	All	2829/3122 (90%)	0.01	47 (1%) 69 65	27, 54, 90, 120	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	11	THR	3.9
1	G	413	SER	3.9
1	D	156	MET	3.3
1	B	405	GLU	3.1
1	G	156	MET	3.0
1	C	153	ASP	2.9
1	G	333	THR	2.9
1	G	155	SER	2.8
1	C	11	THR	2.8
1	E	74	HIS	2.8
1	E	151	ASN	2.7
1	F	187	ASP	2.7
1	D	154	ARG	2.6
1	B	74	HIS	2.6
1	C	155	SER	2.6
1	B	156	MET	2.6
1	F	11	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	151	ASN	2.5
1	D	164	PRO	2.5
1	E	156	MET	2.5
1	C	159	LEU	2.5
1	G	153	ASP	2.4
1	E	135	VAL	2.4
1	B	11	THR	2.3
1	G	407	VAL	2.3
1	G	11	THR	2.3
1	D	155	SER	2.3
1	G	332	ALA	2.3
1	B	151	ASN	2.3
1	E	12	GLU	2.3
1	E	187	ASP	2.3
1	G	410	PHE	2.2
1	D	11	THR	2.2
1	E	290	ARG	2.2
1	F	391	PHE	2.2
1	F	151	ASN	2.2
1	G	376	ARG	2.1
1	F	156	MET	2.1
1	B	86	CYS	2.1
1	F	153	ASP	2.1
1	F	414	CYS	2.1
1	C	93	GLU	2.1
1	F	86	CYS	2.1
1	E	159	LEU	2.0
1	G	369	HIS	2.0
1	G	12	GLU	2.0
1	F	410	PHE	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 [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.