



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:19 AM UTC

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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

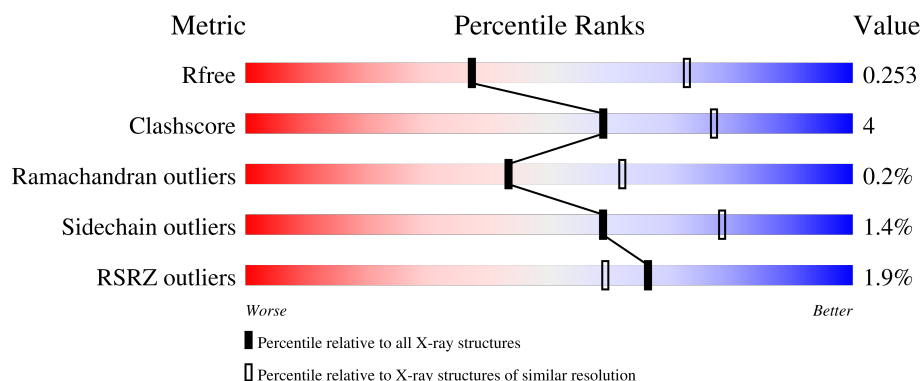
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.86 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.



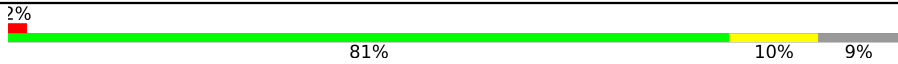
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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 $\leq 5\%$. 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	
1	B	446	
1	C	446	
1	D	446	
1	E	446	

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Mol	Chain	Length	Quality of chain
1	F	446	 2% 81% 10% 9%
1	G	446	 4% 79% 11% 10%

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			

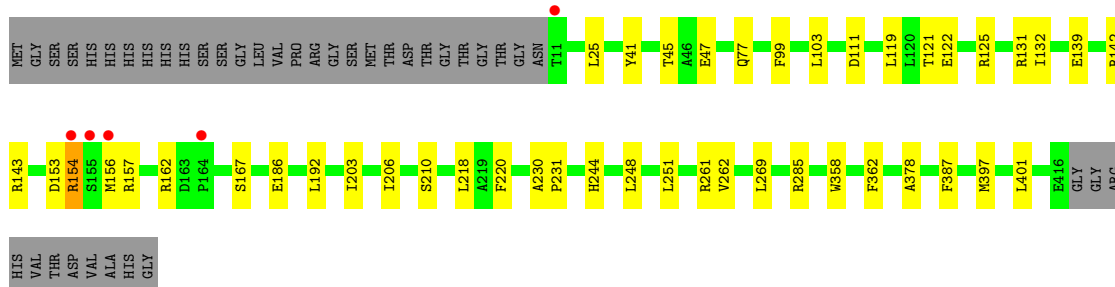
- Molecule 2 is water.

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		

VAL
THR
ASP
VAL
ALA
HIS
GLY

- Molecule 1: styrene monooxygenase/indole monooxygenase family protein

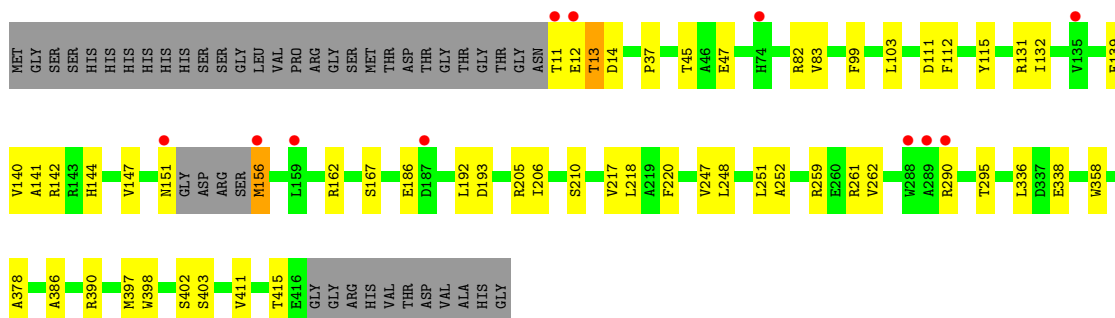
Chain D: 



HIS
VAL
THR
ASP
VAL
ALA
HIS
GLY

- Molecule 1: styrene monooxygenase/indole monooxygenase family protein

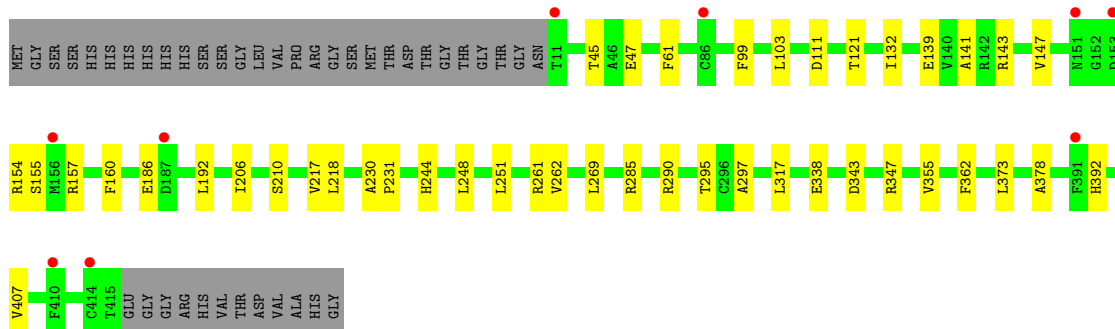
Chain E: 



A378, A386, R390, R397, W398, S402, S403, V411, T415, E416, GLY, GLY, ARG, HIS, VAL, THR, ASP, THR, VAL, ALA, HIS, GLY.

- Molecule 1: styrene monooxygenase/indole monooxygenase family protein

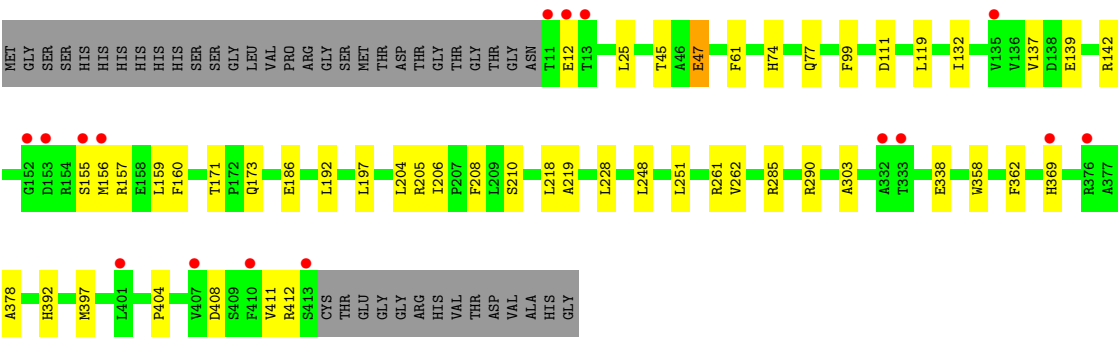
Chain F: 



V407, F410, C414, T415, GLY, 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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	3939 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	56.7	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 33.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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%)	43	62
1	D	404/446 (91%)	396 (98%)	6 (2%)	2 (0%)	24	42
1	E	398/446 (89%)	390 (98%)	7 (2%)	1 (0%)	36	54
1	F	403/446 (90%)	394 (98%)	8 (2%)	1 (0%)	43	62
1	G	401/446 (90%)	393 (98%)	6 (2%)	2 (0%)	24	42
All	All	2811/3122 (90%)	2754 (98%)	50 (2%)	7 (0%)	43	62

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%)	55	76
1	B	310/344 (90%)	305 (98%)	5 (2%)	55	76
1	C	313/344 (91%)	307 (98%)	6 (2%)	50	72
1	D	312/344 (91%)	309 (99%)	3 (1%)	68	83
1	E	309/344 (90%)	305 (99%)	4 (1%)	61	79
1	F	312/344 (91%)	309 (99%)	3 (1%)	68	83
1	G	310/344 (90%)	305 (98%)	5 (2%)	55	76
All	All	2180/2408 (90%)	2149 (99%)	31 (1%)	59	78

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	407/446 (91%)	-0.18	1 (0%) 91 91	27, 41, 65, 87	0
1	B	401/446 (89%)	0.10	6 (1%) 72 65	27, 50, 74, 104	0
1	C	405/446 (90%)	0.04	7 (1%) 69 63	29, 49, 83, 108	0
1	D	406/446 (91%)	0.21	5 (1%) 76 71	33, 57, 83, 112	0
1	E	402/446 (90%)	0.37	11 (2%) 56 47	36, 63, 92, 110	0
1	F	405/446 (90%)	0.19	9 (2%) 62 53	30, 59, 99, 120	0
1	G	403/446 (90%)	0.33	16 (3%) 42 33	35, 60, 104, 119	0
All	All	2829/3122 (90%)	0.15	55 (1%) 66 59	27, 54, 90, 120	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	11	THR	4.0
1	G	413	SER	4.0
1	D	156	MET	3.4
1	G	156	MET	3.2
1	B	405	GLU	3.1
1	C	153	ASP	3.0
1	G	333	THR	3.0
1	G	155	SER	2.9
1	E	74	HIS	2.9
1	C	11	THR	2.9
1	E	151	ASN	2.8
1	F	187	ASP	2.8
1	B	74	HIS	2.7
1	B	156	MET	2.7
1	C	155	SER	2.7
1	D	154	ARG	2.7
1	D	164	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	11	THR	2.7
1	C	151	ASN	2.6
1	E	156	MET	2.6
1	C	159	LEU	2.6
1	G	153	ASP	2.6
1	E	135	VAL	2.5
1	B	11	THR	2.4
1	G	407	VAL	2.4
1	G	11	THR	2.4
1	D	155	SER	2.4
1	G	410	PHE	2.4
1	G	332	ALA	2.4
1	B	151	ASN	2.4
1	E	187	ASP	2.4
1	F	391	PHE	2.4
1	E	12	GLU	2.3
1	D	11	THR	2.3
1	F	151	ASN	2.3
1	E	290	ARG	2.3
1	F	156	MET	2.3
1	B	86	CYS	2.3
1	F	414	CYS	2.2
1	F	153	ASP	2.2
1	G	376	ARG	2.2
1	F	86	CYS	2.2
1	F	410	PHE	2.2
1	E	159	LEU	2.2
1	C	93	GLU	2.2
1	G	369	HIS	2.1
1	G	401	LEU	2.1
1	G	12	GLU	2.1
1	G	13	THR	2.1
1	E	288	TRP	2.1
1	A	417	GLY	2.0
1	G	152	GLY	2.0
1	C	415	THR	2.0
1	E	289	ALA	2.0
1	G	135	VAL	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 [i](#)

There are no oligosaccharides 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.