



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 07:09 AM UTC

PDB ID : 7S6B / pdb_00007s6b
Title : Crystal structure of modular polyketide synthase apo-Lsd14 from the Lasalocid biosynthesis pathway, trapped in the transacylation step
Authors : Bagde, S.R.; Mathews, I.I.; Kim, C.-Y.
Deposited on : 2021-09-13
Resolution : 2.35 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

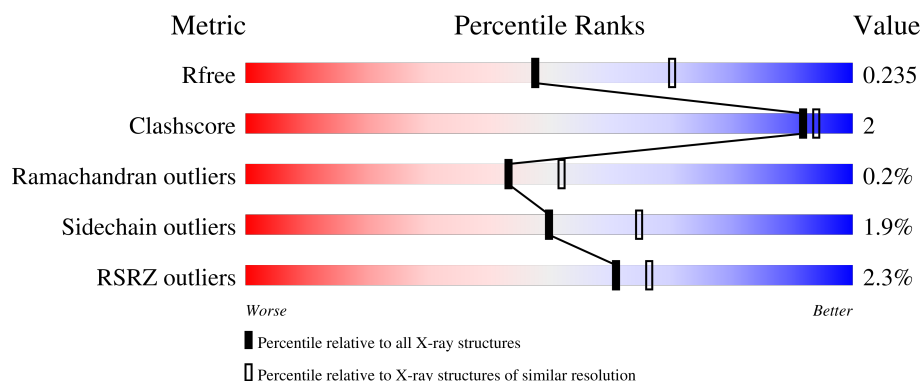
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	944	90% 5%
1	B	944	87% 5% 7%
2	C	544	4% 88% 6% 6%
2	D	544	4% 90% 5% 6%
3	E	179	3% 46% 52%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 42675 atoms, of which 20630 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 Polyketide synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	893	Total	C	H	N	O	S	6437	0	0
			13061	4128	6437	1209	1267	20			
1	B	879	Total	C	H	N	O	S	6313	4	0
			12832	4059	6313	1192	1249	19			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP B6ZK67
A	-18	GLY	-	expression tag	UNP B6ZK67
A	-17	SER	-	expression tag	UNP B6ZK67
A	-16	SER	-	expression tag	UNP B6ZK67
A	-15	HIS	-	expression tag	UNP B6ZK67
A	-14	HIS	-	expression tag	UNP B6ZK67
A	-13	HIS	-	expression tag	UNP B6ZK67
A	-12	HIS	-	expression tag	UNP B6ZK67
A	-11	HIS	-	expression tag	UNP B6ZK67
A	-10	HIS	-	expression tag	UNP B6ZK67
A	-9	SER	-	expression tag	UNP B6ZK67
A	-8	SER	-	expression tag	UNP B6ZK67
A	-7	GLY	-	expression tag	UNP B6ZK67
A	-6	LEU	-	expression tag	UNP B6ZK67
A	-5	VAL	-	expression tag	UNP B6ZK67
A	-4	PRO	-	expression tag	UNP B6ZK67
A	-3	ARG	-	expression tag	UNP B6ZK67
A	-2	GLY	-	expression tag	UNP B6ZK67
A	-1	SER	-	expression tag	UNP B6ZK67
A	0	HIS	-	expression tag	UNP B6ZK67
B	-19	MET	-	initiating methionine	UNP B6ZK67
B	-18	GLY	-	expression tag	UNP B6ZK67
B	-17	SER	-	expression tag	UNP B6ZK67
B	-16	SER	-	expression tag	UNP B6ZK67
B	-15	HIS	-	expression tag	UNP B6ZK67

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP B6ZK67
B	-13	HIS	-	expression tag	UNP B6ZK67
B	-12	HIS	-	expression tag	UNP B6ZK67
B	-11	HIS	-	expression tag	UNP B6ZK67
B	-10	HIS	-	expression tag	UNP B6ZK67
B	-9	SER	-	expression tag	UNP B6ZK67
B	-8	SER	-	expression tag	UNP B6ZK67
B	-7	GLY	-	expression tag	UNP B6ZK67
B	-6	LEU	-	expression tag	UNP B6ZK67
B	-5	VAL	-	expression tag	UNP B6ZK67
B	-4	PRO	-	expression tag	UNP B6ZK67
B	-3	ARG	-	expression tag	UNP B6ZK67
B	-2	GLY	-	expression tag	UNP B6ZK67
B	-1	SER	-	expression tag	UNP B6ZK67
B	0	HIS	-	expression tag	UNP B6ZK67

- Molecule 2 is a protein called Polyketide synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	510	Total	C	H	N	O	S	3578	0	0
			7269	2319	3578	663	706	3			
2	D	514	Total	C	H	N	O	S	3676	0	0
			7426	2355	3676	677	715	3			

- Molecule 3 is a protein called Polyketide synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	86	Total	C	H	N	O	S	626	0	0
			1256	391	626	121	115	3			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	433	Total	O	0	2
			435	435		
4	B	287	Total	O	0	0
			287	287		
4	C	40	Total	O	0	0
			40	40		
4	D	56	Total	O	0	0
			56	56		

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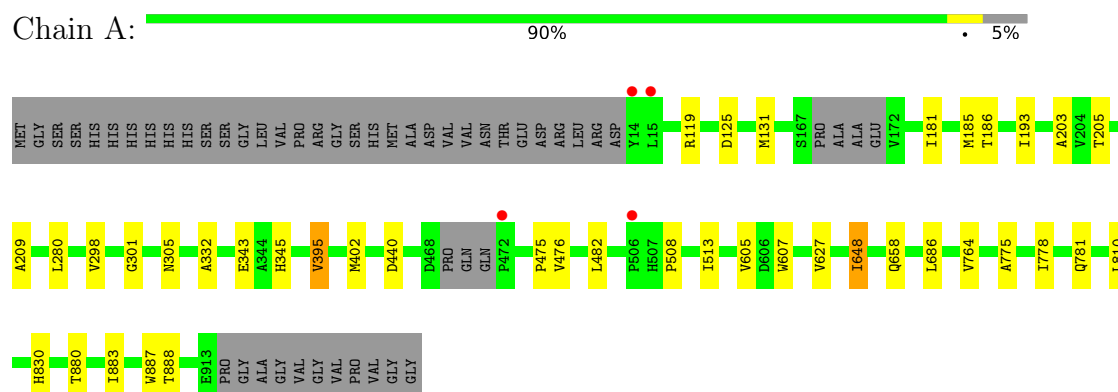
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	13	Total	O	0	0
			13	13		

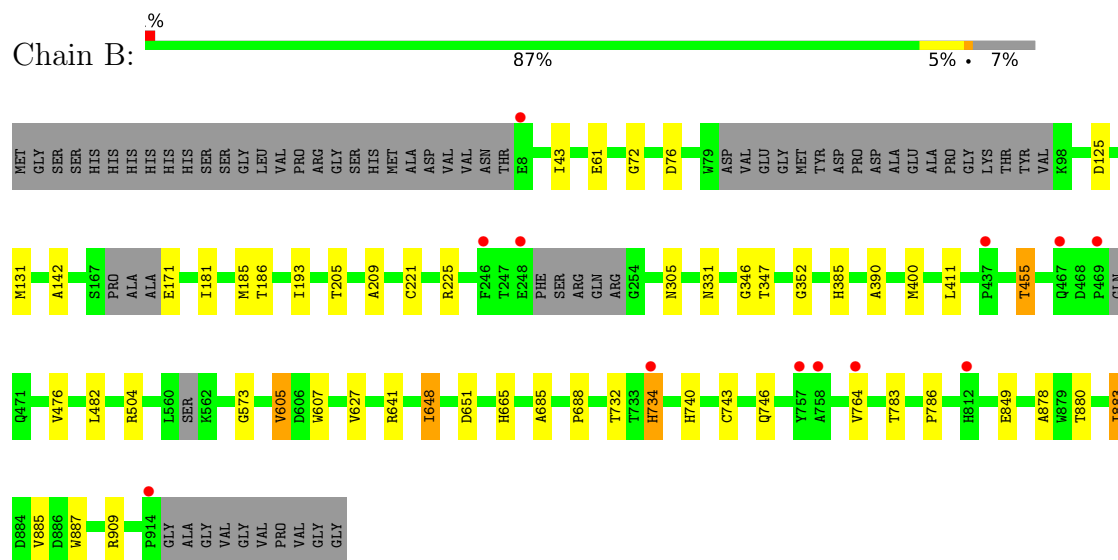
3 Residue-property plots [i](#)

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.

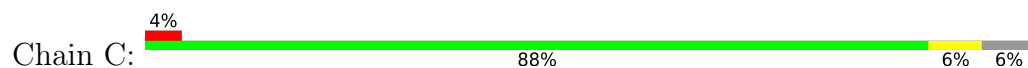
- Molecule 1: Polyketide synthase

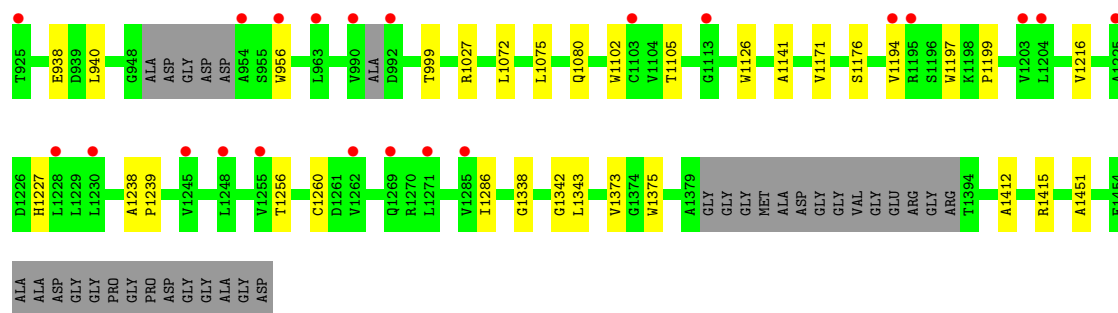


- Molecule 1: Polyketide synthase

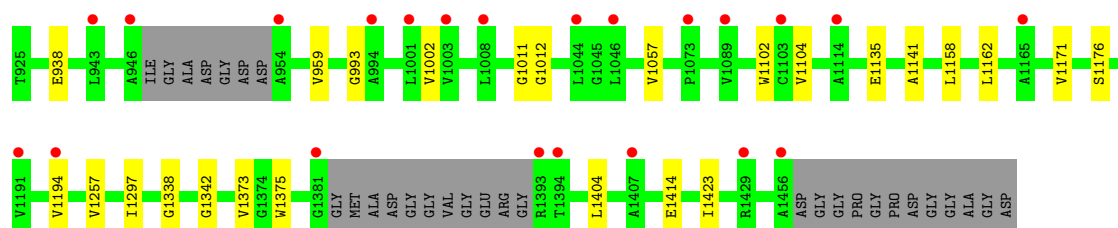
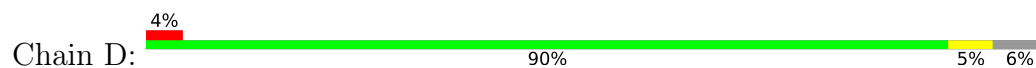


- Molecule 2: Polyketide synthase

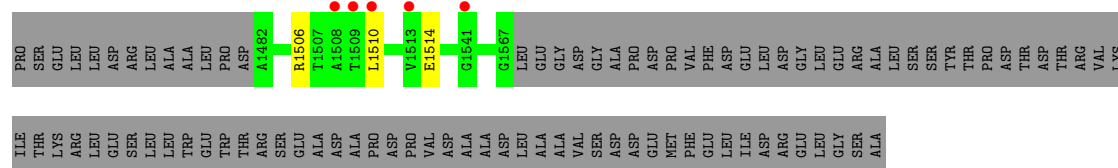




• Molecule 2: Polyketide synthase



• Molecule 3: Polyketide synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	87.74Å 92.85Å 107.45Å 99.63° 94.93° 106.07°	Depositor
Resolution (Å)	39.20 – 2.35 39.20 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.1 (39.20-2.35) 98.0 (39.20-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.34Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.206 , 0.241 0.200 , 0.235	Depositor DCC
R_{free} test set	6501 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	49.2	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	42675	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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	0.77	2/6775 (0.0%)	1.01	4/9260 (0.0%)
1	B	0.74	1/6681 (0.0%)	1.01	6/9135 (0.1%)
2	C	0.68	0/3769	0.93	0/5162
2	D	0.68	0/3829	0.94	1/5242 (0.0%)
3	E	0.72	0/639	1.07	0/868
All	All	0.73	3/21693 (0.0%)	0.99	11/29667 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	209	ALA	CA-C	9.74	1.62	1.52
1	B	209	ALA	CA-C	5.91	1.60	1.53
1	A	402	MET	SD-CE	-5.12	1.66	1.79

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	305	ASN	CA-CB-CG	5.75	118.35	112.60
1	A	125	ASP	CA-CB-CG	5.68	118.28	112.60
2	D	1012	GLY	N-CA-C	5.66	115.36	110.21
1	B	390	ALA	N-CA-C	5.41	117.17	111.28
1	B	305	ASN	CA-CB-CG	5.36	117.96	112.60
1	B	411	LEU	N-CA-C	5.36	117.61	110.53
1	A	345	HIS	N-CA-C	-5.26	105.44	111.07
1	B	573	GLY	N-CA-C	5.24	120.98	114.37
1	B	352	GLY	N-CA-C	5.22	118.81	112.49
1	B	125	ASP	CA-CB-CG	5.17	117.77	112.60
1	A	343	GLU	N-CA-C	-5.13	98.97	107.99

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6624	6437	6433	19	0
1	B	6519	6313	6288	25	0
2	C	3691	3578	3576	16	0
2	D	3750	3676	3673	11	0
3	E	630	626	625	0	0
4	A	435	0	0	1	0
4	B	287	0	0	1	0
4	C	40	0	0	0	0
4	D	56	0	0	1	0
4	E	13	0	0	0	0
All	All	22045	20630	20595	68	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 2.

All (68) 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)
2:C:1105:THR:HG21	2:C:1126:TRP:HE1	1.51	0.74
1:B:186:THR:HG22	1:B:205:THR:HG21	1.75	0.69
1:B:181:ILE:O	1:B:185:MET:HG3	1.95	0.66
2:C:1105:THR:HG21	2:C:1126:TRP:NE1	2.14	0.63
1:A:830:HIS:CG	1:A:883:ILE:HD11	2.36	0.61
1:B:400:MET:HA	1:B:400:MET:HE2	1.81	0.61
1:B:878:ALA:HB1	1:B:883:ILE:HG12	1.83	0.60
2:C:1227:HIS:NE2	2:C:1256:THR:OG1	2.31	0.58
1:B:648:ILE:N	1:B:648:ILE:HD13	2.20	0.56
1:A:508:PRO:HB2	1:A:513:ILE:HD11	1.88	0.54
1:A:203:ALA:O	1:B:455:THR:HG21	2.07	0.53
2:C:1238:ALA:HB1	2:C:1239:PRO:CD	2.37	0.53
2:D:1194:VAL:O	2:D:1414:GLU:O	2.27	0.53
1:A:482:LEU:HD11	1:A:887:TRP:CE2	2.45	0.52
1:A:119:ARG:NH2	2:C:1451:ALA:O	2.43	0.51
1:B:732:THR:OG1	1:B:734:HIS:CE1	2.65	0.50
1:B:743:CYS:O	1:B:746:GLN:O	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:648:ILE:HD13	1:A:648:ILE:N	2.27	0.50
2:D:1102:TRP:CE2	2:D:1141:ALA:HB1	2.46	0.50
1:B:482:LEU:HD11	1:B:887:TRP:CE2	2.48	0.49
2:D:1102:TRP:NE1	2:D:1141:ALA:HB1	2.29	0.47
1:A:605:VAL:HG11	1:A:607:TRP:CE2	2.49	0.47
2:C:1072:LEU:HD23	2:C:1075:LEU:HD12	1.96	0.47
2:C:1412:ALA:O	2:C:1415:ARG:O	2.32	0.47
1:A:605:VAL:HG11	1:A:607:TRP:CD2	2.50	0.46
1:B:732:THR:HG1	1:B:734:HIS:CE1	2.33	0.46
1:A:475:PRO:HB3	4:A:1881:HOH:O	2.15	0.46
1:B:648:ILE:HD11	1:B:885:VAL:HG22	1.98	0.46
1:B:131:MET:HB3	1:B:193:ILE:HD11	1.98	0.46
1:B:641:ARG:NH2	1:B:665:HIS:HE1	2.13	0.46
1:A:607:TRP:CE2	1:A:627:VAL:HG23	2.50	0.45
1:A:686:LEU:HD21	1:A:810:LEU:HD11	1.98	0.45
2:C:956:TRP:CE2	2:D:959:VAL:HG13	2.51	0.45
2:D:1423:ILE:HG13	4:D:1720:HOH:O	2.17	0.45
1:B:685:ALA:O	1:B:688:PRO:HD2	2.17	0.44
1:A:605:VAL:CG1	1:A:607:TRP:CE2	2.99	0.44
1:A:605:VAL:CG1	1:A:607:TRP:CD2	3.00	0.44
1:B:605:VAL:CG1	1:B:607:TRP:CE2	3.00	0.44
2:C:1197:TRP:O	2:C:1199:PRO:HD3	2.17	0.44
2:C:1338:GLY:O	2:C:1342:GLY:HA2	2.18	0.44
1:A:186:THR:HG22	1:A:205:THR:HG21	2.00	0.44
1:B:605:VAL:HG13	1:B:607:TRP:CE2	2.53	0.44
1:A:280:LEU:HD11	1:A:395:VAL:HG21	2.00	0.44
2:D:1002:VAL:HG23	2:D:1002:VAL:O	2.18	0.43
1:A:131:MET:HB3	1:A:193:ILE:HD11	1.99	0.43
1:B:651:ASP:O	1:B:786:PRO:HD2	2.18	0.43
2:C:1194:VAL:HG12	2:C:1194:VAL:O	2.18	0.43
1:A:301:GLY:HA3	1:A:332:ALA:HB2	2.00	0.43
2:D:1102:TRP:CG	2:D:1162:LEU:HD22	2.54	0.43
1:A:775:ALA:O	1:A:778:ILE:HG12	2.19	0.43
1:B:43:ILE:O	1:B:142:ALA:HA	2.19	0.42
1:B:76:ASP:O	1:B:909:ARG:NH2	2.53	0.42
1:B:605:VAL:CG1	1:B:607:TRP:CD2	3.02	0.42
1:B:783:THR:HG21	4:B:1715:HOH:O	2.19	0.42
2:C:1102:TRP:CE2	2:C:1141:ALA:HB1	2.55	0.42
2:D:1373:VAL:HG11	2:D:1375:TRP:CE2	2.55	0.42
1:B:225:ARG:NH2	1:B:331:ASN:HD21	2.18	0.42
2:D:1338:GLY:O	2:D:1342:GLY:HA2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:VAL:HG13	1:B:607:TRP:CD1	2.55	0.41
1:B:221:CYS:O	1:B:225:ARG:HG3	2.21	0.41
2:C:1373:VAL:HG11	2:C:1375:TRP:CE2	2.55	0.41
2:D:1135:GLU:OE1	2:D:1297:ILE:HG12	2.20	0.41
1:A:181:ILE:O	1:A:185:MET:HG3	2.21	0.41
2:D:1158:LEU:O	2:D:1162:LEU:HG	2.21	0.41
1:B:347:THR:HG22	1:B:385:HIS:CD2	2.56	0.41
2:C:1216:VAL:HG11	2:C:1286:ILE:HG21	2.02	0.41
2:C:1102:TRP:NE1	2:C:1141:ALA:HB1	2.37	0.40
2:C:999:THR:HG22	2:C:1027:ARG:HD3	2.04	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	887/944 (94%)	864 (97%)	22 (2%)	1 (0%)	48	59
1	B	871/944 (92%)	848 (97%)	21 (2%)	2 (0%)	43	52
2	C	502/544 (92%)	470 (94%)	32 (6%)	0	100	100
2	D	508/544 (93%)	488 (96%)	18 (4%)	2 (0%)	30	34
3	E	84/179 (47%)	81 (96%)	3 (4%)	0	100	100
All	All	2852/3155 (90%)	2751 (96%)	96 (3%)	5 (0%)	43	52

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	993	GLY
2	D	1011	GLY
1	A	440	ASP
1	B	346	GLY

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Mol	Chain	Res	Type
1	B	72	GLY

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	671/724 (93%)	662 (99%)	9 (1%)	61	76
1	B	661/724 (91%)	647 (98%)	14 (2%)	47	61
2	C	356/388 (92%)	349 (98%)	7 (2%)	48	63
2	D	366/388 (94%)	359 (98%)	7 (2%)	50	65
3	E	61/144 (42%)	58 (95%)	3 (5%)	22	28
All	All	2115/2368 (89%)	2075 (98%)	40 (2%)	50	65

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	298	VAL
1	A	395	VAL
1	A	476	VAL
1	A	648	ILE
1	A	658	GLN
1	A	764	VAL
1	A	781	GLN
1	A	880	THR
1	A	888	THR
1	B	61	GLU
1	B	171	GLU
1	B	455	THR
1	B	476	VAL
1	B	504	ARG
1	B	605	VAL
1	B	627	VAL
1	B	648	ILE
1	B	734	HIS

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Mol	Chain	Res	Type
1	B	740	HIS
1	B	764	VAL
1	B	849	GLU
1	B	880	THR
1	B	883	ILE
2	C	938	GLU
2	C	940	LEU
2	C	1080	GLN
2	C	1171	VAL
2	C	1176	SER
2	C	1260	CYS
2	C	1343	LEU
2	D	938	GLU
2	D	1057	VAL
2	D	1104	VAL
2	D	1171	VAL
2	D	1176	SER
2	D	1257	VAL
2	D	1404	LEU
3	E	1506	ARG
3	E	1510	LEU
3	E	1514	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	GLN
1	A	404	HIS
1	A	515	HIS
1	A	779	ASN
1	A	781	GLN
1	A	881	HIS
1	A	906	GLN
1	B	226	GLN
1	B	331	ASN
1	B	524	HIS
1	B	645	HIS
1	B	646	HIS
1	B	665	HIS
1	B	830	HIS
1	B	906	GLN
2	C	973	GLN

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Mol	Chain	Res	Type
2	C	1080	GLN
2	C	1138	HIS
2	D	970	GLN
2	D	1136	HIS
2	D	1269	GLN
2	D	1307	GLN
2	D	1435	HIS
2	D	1450	GLN
3	E	1495	ASN
3	E	1561	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	893/944 (94%)	-0.09	4 (0%) 88 91	16, 27, 46, 90	0
1	B	879/944 (93%)	0.14	12 (1%) 73 78	18, 35, 63, 131	2 (0%)
2	C	510/544 (93%)	0.72	22 (4%) 40 45	32, 54, 92, 120	0
2	D	514/544 (94%)	0.55	22 (4%) 40 45	22, 48, 76, 101	0
3	E	86/179 (48%)	0.49	5 (5%) 29 33	24, 44, 79, 95	0
All	All	2882/3155 (91%)	0.25	65 (2%) 61 66	16, 38, 74, 131	2 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	1228	LEU	4.3
3	E	1509	THR	4.2
3	E	1508	ALA	4.1
1	B	248	GLU	3.9
1	A	14	TYR	3.8
1	B	246	PHE	3.8
3	E	1510	LEU	3.8
1	B	812[A]	HIS	3.7
2	C	1194	VAL	3.7
3	E	1513	VAL	3.6
2	D	954	ALA	3.6
2	C	954	ALA	3.2
2	D	943	LEU	3.0
1	A	506	PRO	3.0
1	B	757	TYR	2.9
2	C	1285	VAL	2.9
1	B	914	PRO	2.8
2	D	1394	THR	2.8
2	C	956	TRP	2.8
2	C	1245	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
2	C	1195	ARG	2.7
2	D	946	ALA	2.7
2	D	1003	VAL	2.7
2	D	1381	GLY	2.7
1	A	472	PRO	2.7
2	D	1393	ARG	2.7
2	C	990	VAL	2.6
2	C	1271	LEU	2.6
2	D	1073	PRO	2.6
2	C	1203	VAL	2.5
2	C	1230	LEU	2.5
2	C	992	ASP	2.5
1	B	758	ALA	2.5
2	D	994	ALA	2.5
2	C	1269	GLN	2.5
2	D	1114	ALA	2.4
2	C	1262	VAL	2.4
2	D	1046	LEU	2.4
1	B	437	PRO	2.3
1	B	469	PRO	2.3
2	D	1407	ALA	2.3
1	B	734	HIS	2.3
2	C	963	LEU	2.3
2	D	1165	ALA	2.3
2	C	925	THR	2.3
1	B	764	VAL	2.3
1	B	8	GLU	2.2
2	C	1255	VAL	2.2
2	C	1248	LEU	2.2
2	C	1113	GLY	2.2
2	D	1103	CYS	2.2
2	C	1204	LEU	2.1
2	D	1089	VAL	2.1
2	D	1191	VAL	2.1
2	C	1225	ALA	2.1
2	D	1008	LEU	2.1
2	D	1194	VAL	2.1
2	D	1429	ARG	2.1
2	D	1456	ALA	2.1
1	B	467	GLN	2.1
2	D	1044	LEU	2.1
3	E	1541	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	1103	CYS	2.0
2	D	1001	LEU	2.0
1	A	15	LEU	2.0

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

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.