



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 22, 2022 – 06:10 PM JST

PDB ID : 7E6W
Title : Crystal structure of Sesquisabinene B Synthase 1 mutant G418A and F419N
Authors : Singh, S.; Thulasiram, H.V.; Kulkarni, K.A.
Deposited on : 2021-02-24
Resolution : 3.10 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.26
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

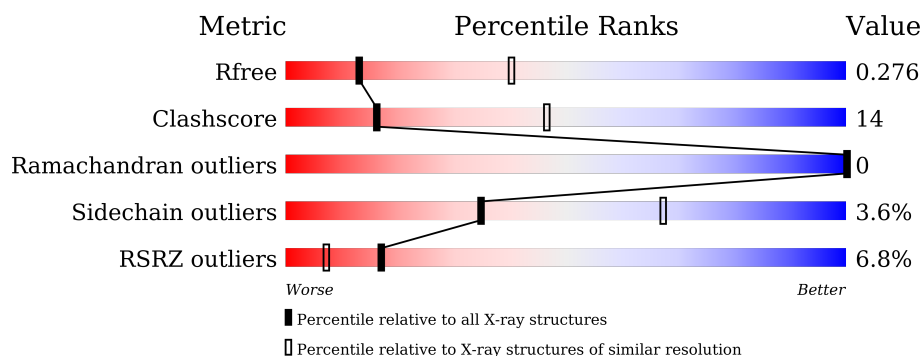
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	555	<div> <div>6%</div> <div> <div></div> <div>65%</div> <div>25%</div> <div>• 9%</div> </div> </div>
1	B	555	<div> <div>6%</div> <div> <div></div> <div>64%</div> <div>26%</div> <div>• 9%</div> </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8165 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 Sesquisabinene B synthase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	506	Total	C	N	O	S	0	0	0
			4098	2647	681	754	16			
1	B	504	Total	C	N	O	S	0	0	0
			4067	2622	678	751	16			

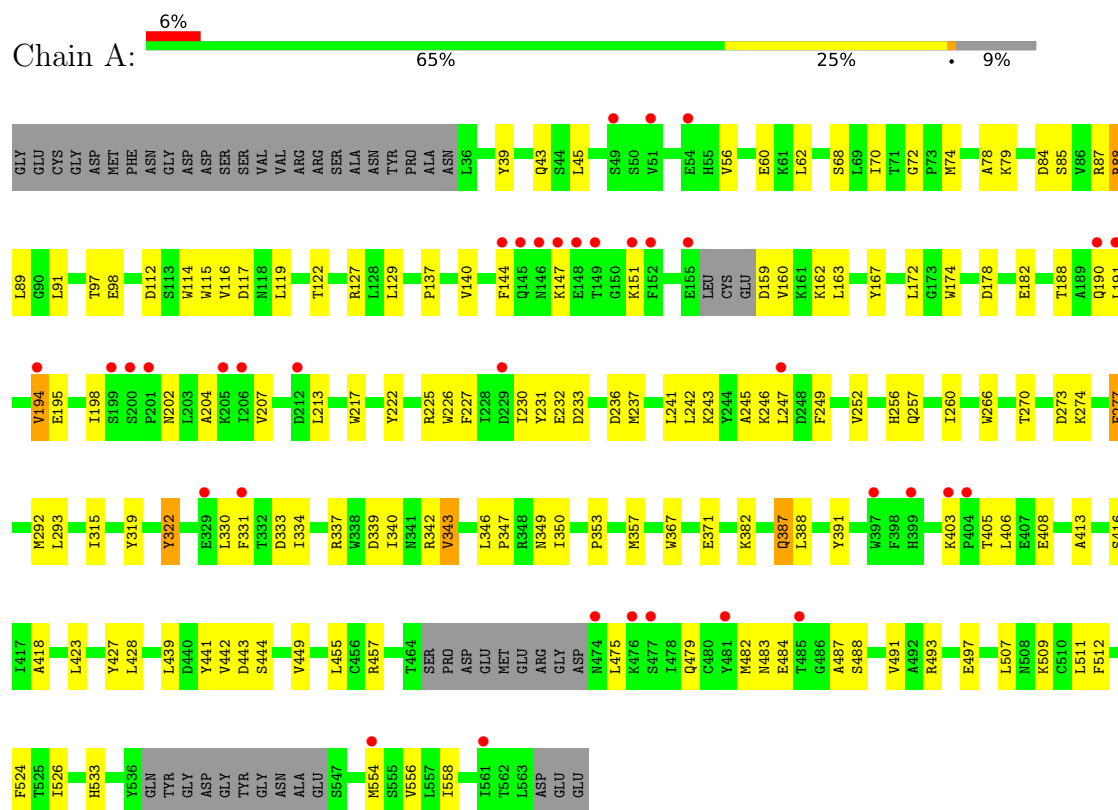
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	GLY	-	expression tag	UNP A0A0A0RDR2
A	13	GLU	-	expression tag	UNP A0A0A0RDR2
A	14	CYS	-	expression tag	UNP A0A0A0RDR2
A	15	GLY	-	expression tag	UNP A0A0A0RDR2
A	16	ASP	-	expression tag	UNP A0A0A0RDR2
A	17	MET	-	expression tag	UNP A0A0A0RDR2
A	162	LYS	GLY	cloning artifact	UNP A0A0A0RDR2
A	196	LYS	GLY	cloning artifact	UNP A0A0A0RDR2
A	418	ALA	GLY	engineered mutation	UNP A0A0A0RDR2
A	419	ASN	PHE	engineered mutation	UNP A0A0A0RDR2
B	12	GLY	-	expression tag	UNP A0A0A0RDR2
B	13	GLU	-	expression tag	UNP A0A0A0RDR2
B	14	CYS	-	expression tag	UNP A0A0A0RDR2
B	15	GLY	-	expression tag	UNP A0A0A0RDR2
B	16	ASP	-	expression tag	UNP A0A0A0RDR2
B	17	MET	-	expression tag	UNP A0A0A0RDR2
B	162	LYS	GLY	cloning artifact	UNP A0A0A0RDR2
B	196	LYS	GLY	cloning artifact	UNP A0A0A0RDR2
B	418	ALA	GLY	engineered mutation	UNP A0A0A0RDR2
B	419	ASN	PHE	engineered mutation	UNP A0A0A0RDR2

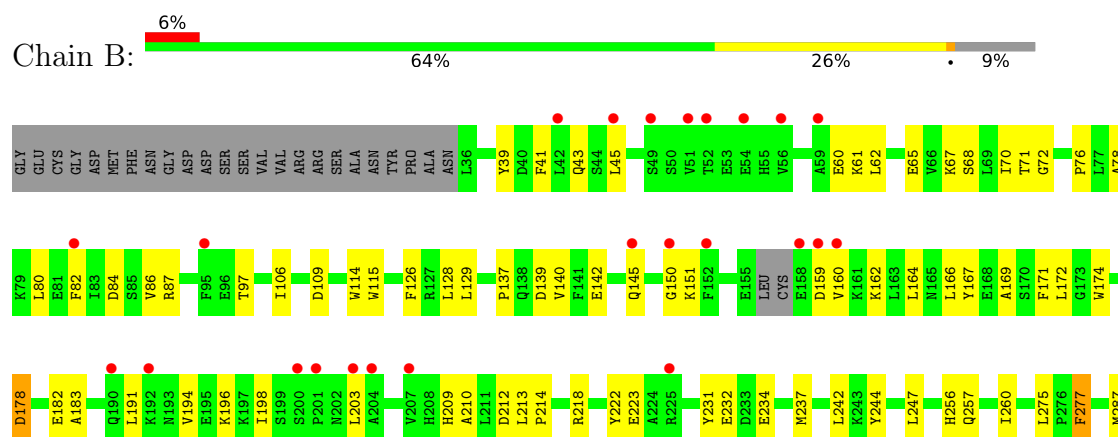
3 Residue-property plots

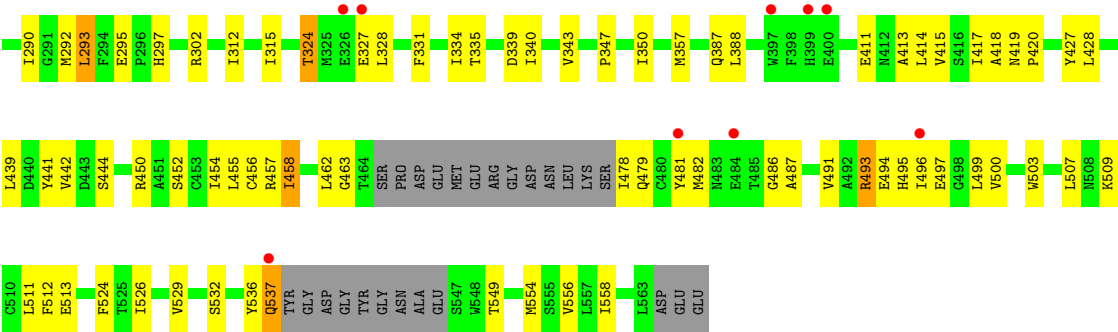
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Sesquisabinene B synthase 1



• Molecule 1: Sesquisabinene B synthase 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.07Å 61.03Å 182.71Å 90.00° 93.04° 90.00°	Depositor
Resolution (Å)	45.61 – 3.10 45.61 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.6 (45.61-3.10) 99.8 (45.61-3.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.238 , 0.275 0.239 , 0.276	Depositor DCC
R_{free} test set	1085 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	90.2	Xtriage
Anisotropy	0.598	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 74.4	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	0.95	EDS
Total number of atoms	8165	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 75.85 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1661e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

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	0.57	0/4197	0.79	0/5690
1	B	0.54	0/4165	0.82	0/5652
All	All	0.55	0/8362	0.80	0/11342

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

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	4098	0	4016	127	0
1	B	4067	0	3955	105	0
All	All	8165	0	7971	232	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 14.

All (232) 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:A:190:GLN:O	1:A:194:VAL:HG12	1.36	1.26
1:B:478:ILE:CD1	1:B:493:ARG:HD3	1.77	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:LEU:HD12	1:A:347:PRO:HD2	1.36	1.07
1:B:478:ILE:HD13	1:B:493:ARG:HD3	1.33	1.07
1:B:493:ARG:HB3	1:B:493:ARG:HH11	1.09	1.06
1:A:198:ILE:HG21	1:A:204:ALA:HB2	1.40	1.03
1:A:387:GLN:HE22	1:A:418:ALA:HA	1.21	1.01
1:B:478:ILE:HD11	1:B:493:ARG:CD	1.96	0.95
1:A:198:ILE:HG21	1:A:204:ALA:CB	1.97	0.94
1:B:487:ALA:HB1	1:B:491:VAL:CG1	1.99	0.92
1:B:478:ILE:CD1	1:B:493:ARG:CD	2.48	0.91
1:A:88:ARG:HG2	1:A:88:ARG:HH11	1.34	0.91
1:B:456:CYS:HG	1:B:532:SER:HG	1.16	0.91
1:A:340:ILE:O	1:A:343:VAL:HG22	1.71	0.90
1:A:160:VAL:HA	1:A:163:LEU:HD12	1.53	0.88
1:A:198:ILE:CG2	1:A:204:ALA:HB2	2.04	0.86
1:A:62:LEU:HD12	1:A:247:LEU:HD12	1.60	0.84
1:A:346:LEU:CD1	1:A:347:PRO:HD2	2.09	0.83
1:A:387:GLN:HE22	1:A:418:ALA:CA	1.90	0.83
1:B:493:ARG:HH11	1:B:493:ARG:CB	1.91	0.83
1:A:322:TYR:HE1	1:A:349:ASN:HD22	1.24	0.82
1:B:478:ILE:HD11	1:B:493:ARG:HD2	1.61	0.82
1:B:493:ARG:HB3	1:B:493:ARG:NH1	1.94	0.79
1:A:191:LEU:HA	1:A:194:VAL:CG1	2.13	0.78
1:A:387:GLN:NE2	1:A:418:ALA:HA	2.00	0.76
1:B:463:GLY:HA3	1:B:536:TYR:HB3	1.66	0.75
1:B:487:ALA:HB1	1:B:491:VAL:HG13	1.67	0.75
1:A:191:LEU:HA	1:A:194:VAL:HG13	1.69	0.74
1:A:413:ALA:HB1	1:A:457:ARG:HG2	1.70	0.72
1:B:78:ALA:O	1:B:82:PHE:HD1	1.72	0.72
1:A:457:ARG:HD3	1:A:457:ARG:O	1.90	0.72
1:A:232:GLU:HG3	1:A:242:LEU:HD21	1.71	0.72
1:B:191:LEU:HA	1:B:194:VAL:HG12	1.75	0.69
1:A:190:GLN:O	1:A:194:VAL:CG1	2.30	0.68
1:B:80:LEU:HD22	1:B:128:LEU:HD22	1.74	0.68
1:A:167:TYR:HE1	1:A:188:THR:HG22	1.59	0.68
1:A:202:ASN:ND2	1:A:233:ASP:HB2	2.09	0.67
1:A:346:LEU:HD12	1:A:347:PRO:CD	2.20	0.67
1:A:147:LYS:O	1:A:147:LYS:HD3	1.94	0.67
1:B:167:TYR:HE2	1:B:210:ALA:HB1	1.58	0.67
1:A:256:HIS:O	1:A:260:ILE:HG13	1.95	0.66
1:A:346:LEU:HD21	1:A:350:ILE:HG22	1.78	0.65
1:A:232:GLU:HG3	1:A:242:LEU:CD2	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:PHE:HE2	1:A:322:TYR:HD1	1.46	0.64
1:B:166:LEU:HD11	1:B:183:ALA:HB1	1.78	0.64
1:B:137:PRO:HG2	1:B:140:VAL:HG23	1.80	0.64
1:B:139:ASP:O	1:B:142:GLU:HG2	1.98	0.63
1:B:487:ALA:HB1	1:B:491:VAL:HG11	1.77	0.63
1:A:119:LEU:HD13	1:A:144:PHE:CG	2.34	0.63
1:A:457:ARG:HD3	1:A:457:ARG:C	2.16	0.62
1:A:387:GLN:HE22	1:A:418:ALA:CB	2.13	0.61
1:B:287:MET:HE1	1:B:549:THR:HB	1.81	0.61
1:A:475:LEU:HD22	1:A:483:ASN:HD21	1.64	0.61
1:A:68:SER:O	1:A:72:GLY:N	2.34	0.60
1:A:119:LEU:HD12	1:A:144:PHE:CD2	2.37	0.60
1:B:70:ILE:HD11	1:B:86:VAL:HG21	1.82	0.59
1:B:334:ILE:HG23	1:B:339:ASP:O	2.02	0.59
1:A:292:MET:HE3	1:A:524:PHE:HB3	1.84	0.59
1:A:243:LYS:O	1:A:247:LEU:HG	2.03	0.59
1:B:324:THR:HG22	1:B:327:GLU:H	1.68	0.59
1:A:511:LEU:HD11	1:A:526:ILE:HG13	1.84	0.59
1:A:62:LEU:HD12	1:A:247:LEU:CD1	2.32	0.59
1:A:333:ASP:OD2	1:A:337:ARG:NH1	2.33	0.59
1:B:324:THR:O	1:B:328:LEU:HG	2.02	0.59
1:A:403:LYS:HD2	1:A:483:ASN:ND2	2.18	0.59
1:B:256:HIS:O	1:B:260:ILE:HG13	2.04	0.58
1:A:88:ARG:HG2	1:A:88:ARG:NH1	2.12	0.58
1:A:195:GLU:HA	1:A:198:ILE:HG12	1.84	0.58
1:B:222:TYR:HD1	1:B:556:VAL:HG21	1.68	0.58
1:A:488:SER:HB3	1:A:491:VAL:HG12	1.85	0.58
1:A:226:TRP:CH2	1:A:230:ILE:HG13	2.39	0.58
1:B:335:THR:HG21	1:B:388:LEU:HD12	1.87	0.57
1:A:479:GLN:OE1	1:A:479:GLN:N	2.37	0.57
1:B:114:TRP:CE3	1:B:115:TRP:HB3	2.39	0.56
1:B:462:LEU:HD11	1:B:496:ILE:HG22	1.87	0.56
1:B:167:TYR:CE2	1:B:210:ALA:HB1	2.40	0.56
1:A:39:TYR:O	1:A:43:GLN:HG3	2.05	0.56
1:A:159:ASP:O	1:A:163:LEU:HG	2.07	0.56
1:A:88:ARG:HH11	1:A:88:ARG:CG	2.10	0.55
1:B:222:TYR:CD1	1:B:556:VAL:HG21	2.42	0.55
1:A:89:LEU:HD13	1:A:245:ALA:CB	2.37	0.55
1:A:89:LEU:HD13	1:A:245:ALA:HB2	1.87	0.55
1:A:427:TYR:CD2	1:A:442:VAL:HG21	2.41	0.55
1:A:292:MET:CE	1:A:524:PHE:HB3	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:TYR:CE1	1:A:188:THR:HG22	2.41	0.54
1:B:145:GLN:NE2	1:B:150:GLY:O	2.40	0.54
1:A:482:MET:HG2	1:A:487:ALA:O	2.08	0.54
1:A:403:LYS:HB3	1:A:483:ASN:HD22	1.72	0.54
1:B:194:VAL:O	1:B:198:ILE:HG13	2.08	0.54
1:A:89:LEU:HD23	1:A:227:PHE:HD2	1.72	0.54
1:B:496:ILE:HA	1:B:499:LEU:CD1	2.38	0.53
1:A:119:LEU:CD1	1:A:144:PHE:CD2	2.92	0.53
1:A:213:LEU:HD11	1:A:533:HIS:HB3	1.90	0.53
1:B:68:SER:O	1:B:72:GLY:N	2.40	0.53
1:B:198:ILE:HG23	1:B:203:LEU:HD23	1.91	0.53
1:B:428:LEU:HB2	1:B:439:LEU:HD11	1.90	0.53
1:B:231:TYR:HD2	1:B:242:LEU:HD13	1.74	0.53
1:A:112:ASP:O	1:A:116:VAL:HG23	2.09	0.52
1:B:62:LEU:HB3	1:B:244:TYR:HB2	1.91	0.52
1:A:222:TYR:CD1	1:A:556:VAL:HG21	2.45	0.52
1:A:159:ASP:HB3	1:A:162:LYS:HE2	1.92	0.52
1:A:174:TRP:CE3	1:A:509:LYS:HG3	2.45	0.51
1:A:231:TYR:CE2	1:A:237:MET:HG2	2.46	0.51
1:B:213:LEU:HB2	1:B:218:ARG:CZ	2.40	0.51
1:A:347:PRO:HG2	1:A:350:ILE:HD12	1.93	0.51
1:A:406:LEU:N	1:A:484:GLU:OE1	2.30	0.51
1:A:74:MET:HE2	1:A:78:ALA:HB1	1.92	0.51
1:A:114:TRP:CZ3	1:A:115:TRP:HB3	2.46	0.51
1:A:367:TRP:CE2	1:A:371:GLU:HG3	2.45	0.51
1:A:315:ILE:HD11	1:A:357:MET:HB2	1.93	0.51
1:B:166:LEU:HD11	1:B:183:ALA:CB	2.40	0.51
1:A:151:LYS:HG2	1:A:182:GLU:OE2	2.11	0.50
1:B:312:ILE:HD13	1:B:418:ALA:HB1	1.93	0.50
1:A:413:ALA:CB	1:A:457:ARG:HG2	2.39	0.50
1:A:88:ARG:HB3	1:A:227:PHE:CD2	2.47	0.50
1:B:126:PHE:HD2	1:B:169:ALA:HB1	1.76	0.50
1:B:411:GLU:HG3	1:B:450:ARG:HH21	1.77	0.50
1:B:174:TRP:HZ2	1:B:512:PHE:CD1	2.31	0.49
1:A:198:ILE:HG21	1:A:204:ALA:CA	2.41	0.49
1:B:482:MET:HG2	1:B:487:ALA:O	2.12	0.49
1:B:234:GLU:HB2	1:B:237:MET:HB2	1.93	0.49
1:A:236:ASP:OD1	1:A:236:ASP:N	2.46	0.49
1:B:415:VAL:HA	1:B:420:PRO:HG3	1.94	0.49
1:A:330:LEU:HD11	1:A:342:ARG:HE	1.76	0.49
1:A:88:ARG:NH1	1:A:88:ARG:CG	2.72	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:PRO:HG2	1:A:140:VAL:HG23	1.94	0.49
1:B:67:LYS:O	1:B:71:THR:OG1	2.24	0.49
1:B:41:PHE:HE2	1:B:558:ILE:HD13	1.77	0.49
1:A:277:PHE:HE2	1:A:322:TYR:CD1	2.29	0.48
1:A:266:TRP:O	1:A:270:THR:HG23	2.12	0.48
1:B:167:TYR:CE1	1:B:171:PHE:HE2	2.30	0.48
1:B:427:TYR:CD2	1:B:442:VAL:HG21	2.47	0.48
1:A:114:TRP:CE3	1:A:115:TRP:HB3	2.48	0.48
1:A:334:ILE:HG23	1:A:339:ASP:O	2.12	0.48
1:B:209:HIS:O	1:B:218:ARG:NH1	2.47	0.48
1:B:554:MET:SD	1:B:558:ILE:HD12	2.54	0.48
1:A:554:MET:HA	1:A:558:ILE:HD13	1.95	0.48
1:B:292:MET:HE3	1:B:524:PHE:HB3	1.96	0.48
1:B:482:MET:O	1:B:486:GLY:N	2.45	0.48
1:B:159:ASP:HB3	1:B:162:LYS:HD2	1.96	0.48
1:A:277:PHE:HZ	1:A:349:ASN:O	1.97	0.47
1:B:347:PRO:HG2	1:B:350:ILE:HD12	1.96	0.47
1:A:174:TRP:CD1	1:A:174:TRP:N	2.80	0.47
1:A:226:TRP:CZ2	1:A:230:ILE:HG13	2.50	0.47
1:A:427:TYR:CE2	1:A:442:VAL:HG21	2.49	0.47
1:B:214:PRO:O	1:B:218:ARG:HG3	2.15	0.47
1:A:493:ARG:O	1:A:497:GLU:HG3	2.14	0.47
1:B:166:LEU:CD1	1:B:183:ALA:HB1	2.43	0.47
1:A:322:TYR:HD2	1:A:322:TYR:O	1.97	0.47
1:B:387:GLN:NE2	1:B:418:ALA:HB2	2.30	0.47
1:A:330:LEU:CD1	1:A:342:ARG:HE	2.28	0.46
1:B:76:PRO:HB2	1:B:114:TRP:CE3	2.50	0.46
1:A:117:ASP:O	1:A:144:PHE:HE1	1.97	0.46
1:A:405:THR:OG1	1:A:408:GLU:HB2	2.15	0.46
1:B:39:TYR:O	1:B:43:GLN:HG3	2.15	0.46
1:B:511:LEU:HD11	1:B:526:ILE:HG13	1.98	0.46
1:A:387:GLN:NE2	1:A:418:ALA:CB	2.78	0.46
1:B:479:GLN:OE1	1:B:479:GLN:N	2.44	0.46
1:A:222:TYR:HD1	1:A:556:VAL:HG21	1.80	0.45
1:B:496:ILE:HA	1:B:499:LEU:HD12	1.98	0.45
1:B:151:LYS:HG3	1:B:182:GLU:OE2	2.16	0.45
1:B:164:LEU:HD23	1:B:191:LEU:HD13	1.98	0.45
1:A:119:LEU:HD13	1:A:144:PHE:CB	2.46	0.45
1:B:212:ASP:HB3	1:B:537:GLN:OE1	2.15	0.45
1:B:275:LEU:HD13	1:B:277:PHE:CE1	2.52	0.45
1:B:295:GLU:HB3	1:B:297:HIS:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:LEU:HD22	1:A:257:GLN:HG2	1.99	0.45
1:A:441:TYR:O	1:A:444:SER:OG	2.27	0.44
1:A:475:LEU:CD2	1:A:483:ASN:HD21	2.30	0.44
1:A:315:ILE:HG21	1:A:388:LEU:HD21	1.98	0.44
1:B:419:ASN:N	1:B:420:PRO:HD2	2.32	0.44
1:A:382:LYS:HE2	1:A:443:ASP:OD2	2.17	0.44
1:B:509:LYS:O	1:B:513:GLU:HG2	2.17	0.44
1:B:455:LEU:HG	1:B:503:TRP:HB3	1.99	0.44
1:B:452:SER:OG	1:B:529:VAL:HG23	2.18	0.43
1:B:178:ASP:OD1	1:B:178:ASP:N	2.51	0.43
1:B:413:ALA:HB1	1:B:457:ARG:NE	2.33	0.43
1:A:428:LEU:HB2	1:A:439:LEU:HD11	2.01	0.43
1:B:450:ARG:O	1:B:454:ILE:HG13	2.18	0.43
1:A:174:TRP:HZ2	1:A:512:PHE:CD1	2.37	0.43
1:A:507:LEU:HG	1:A:526:ILE:CD1	2.49	0.43
1:B:497:GLU:O	1:B:500:VAL:HB	2.19	0.43
1:B:507:LEU:HD12	1:B:507:LEU:HA	1.76	0.43
1:A:198:ILE:HD11	1:A:207:VAL:HG21	2.00	0.43
1:A:147:LYS:HD3	1:A:147:LYS:C	2.39	0.42
1:B:293:LEU:HD13	1:B:302:ARG:HB2	2.00	0.42
1:A:172:LEU:HD13	1:A:172:LEU:HA	1.84	0.42
1:A:350:ILE:O	1:A:353:PRO:HD2	2.18	0.42
1:B:511:LEU:HD23	1:B:511:LEU:HA	1.88	0.42
1:A:242:LEU:O	1:A:246:LYS:HG3	2.19	0.42
1:A:252:VAL:HG12	1:A:256:HIS:CE1	2.54	0.42
1:A:277:PHE:CE2	1:A:322:TYR:HD1	2.30	0.42
1:B:196:LYS:HE3	1:B:196:LYS:HB2	1.85	0.42
1:A:350:ILE:C	1:A:353:PRO:HD2	2.39	0.42
1:B:507:LEU:HG	1:B:526:ILE:CD1	2.49	0.42
1:A:122:THR:CG2	1:A:140:VAL:HG12	2.49	0.42
1:B:45:LEU:HD22	1:B:257:GLN:HG2	2.01	0.42
1:B:106:ILE:O	1:B:109:ASP:HB2	2.20	0.42
1:B:160:VAL:HG11	1:B:203:LEU:HD21	2.02	0.42
1:A:319:TYR:CE1	1:A:388:LEU:HD22	2.55	0.42
1:B:114:TRP:CZ3	1:B:115:TRP:HB3	2.54	0.42
1:B:290:ILE:HG23	1:B:290:ILE:HD12	1.68	0.42
1:B:167:TYR:CE1	1:B:171:PHE:CE2	3.08	0.42
1:B:172:LEU:HD13	1:B:172:LEU:HA	1.80	0.42
1:B:454:ILE:HG22	1:B:458:ILE:HD13	2.01	0.42
1:A:84:ASP:CG	1:A:127:ARG:HH22	2.23	0.42
1:A:117:ASP:O	1:A:144:PHE:CE1	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ASP:OD2	1:A:274:LYS:HD3	2.20	0.42
1:A:475:LEU:HD12	1:A:475:LEU:H	1.82	0.42
1:A:507:LEU:HA	1:A:507:LEU:HD12	1.78	0.42
1:A:347:PRO:CG	1:A:350:ILE:HD12	2.49	0.41
1:A:423:LEU:HD13	1:A:449:VAL:HG13	2.02	0.41
1:A:217:TRP:N	1:A:217:TRP:CD1	2.88	0.41
1:A:91:LEU:HD12	1:A:241:LEU:HD11	2.01	0.41
1:B:62:LEU:HD12	1:B:247:LEU:HD12	2.01	0.41
1:A:122:THR:HG22	1:A:140:VAL:HG12	2.02	0.41
1:A:391:TYR:CE1	1:A:416:SER:HB2	2.56	0.41
1:B:218:ARG:HH11	1:B:218:ARG:HD2	1.73	0.41
1:A:225:ARG:HD3	1:A:249:PHE:CZ	2.55	0.41
1:B:61:LYS:NZ	1:B:65:GLU:OE2	2.36	0.41
1:B:481:TYR:CE1	1:B:495:HIS:CE1	3.09	0.41
1:A:85:SER:O	1:A:89:LEU:HG	2.21	0.41
1:B:191:LEU:HA	1:B:191:LEU:HD23	1.83	0.41
1:B:231:TYR:O	1:B:237:MET:HG3	2.20	0.41
1:B:232:GLU:HG3	1:B:242:LEU:CD2	2.51	0.40
1:B:315:ILE:HD11	1:B:357:MET:HB2	2.03	0.40
1:B:292:MET:CE	1:B:524:PHE:HB3	2.51	0.40
1:A:70:ILE:O	1:A:79:LYS:HE2	2.21	0.40
1:B:340:ILE:O	1:B:343:VAL:HG22	2.20	0.40
1:B:414:LEU:O	1:B:417:ILE:HG22	2.21	0.40
1:B:441:TYR:O	1:B:444:SER:OG	2.34	0.40
1:A:511:LEU:HA	1:A:511:LEU:HD23	1.80	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	498/555 (90%)	486 (98%)	12 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	496/555 (89%)	492 (99%)	4 (1%)	0	100	100
All	All	994/1110 (90%)	978 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	438/489 (90%)	422 (96%)	16 (4%)	34	66
1	B	432/489 (88%)	417 (96%)	15 (4%)	36	68
All	All	870/978 (89%)	839 (96%)	31 (4%)	35	67

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

Mol	Chain	Res	Type
1	A	56	VAL
1	A	60	GLU
1	A	87	ARG
1	A	88	ARG
1	A	97	THR
1	A	98	GLU
1	A	129	LEU
1	A	178	ASP
1	A	194	VAL
1	A	277	PHE
1	A	293	LEU
1	A	322	TYR
1	A	331	PHE
1	A	343	VAL
1	A	387	GLN
1	A	455	LEU
1	B	60	GLU
1	B	84	ASP

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Mol	Chain	Res	Type
1	B	87	ARG
1	B	97	THR
1	B	129	LEU
1	B	178	ASP
1	B	223	GLU
1	B	277	PHE
1	B	293	LEU
1	B	324	THR
1	B	331	PHE
1	B	458	ILE
1	B	493	ARG
1	B	494	GLU
1	B	537	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	GLN
1	A	297	HIS
1	A	387	GLN
1	A	399	HIS
1	A	483	ASN
1	B	284	GLN
1	B	297	HIS
1	B	495	HIS
1	B	537	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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(Å ²)	Q<0.9
1	A	506/555 (91%)	0.46	36 (7%)	16 6	57, 103, 165, 220	0
1	B	504/555 (90%)	0.43	33 (6%)	18 8	62, 109, 160, 209	0
All	All	1010/1110 (90%)	0.44	69 (6%)	17 7	57, 106, 162, 220	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	399	HIS	4.7
1	B	496	ILE	4.4
1	B	159	ASP	4.3
1	B	399	HIS	4.2
1	A	152	PHE	4.0
1	B	160	VAL	4.0
1	B	203	LEU	3.8
1	A	155	GLU	3.8
1	B	201	PRO	3.7
1	A	247	LEU	3.7
1	A	149	THR	3.7
1	A	146	ASN	3.7
1	B	400	GLU	3.6
1	B	145	GLN	3.6
1	A	474	ASN	3.6
1	A	481	TYR	3.6
1	A	485	THR	3.5
1	B	537	GLN	3.4
1	A	206	ILE	3.4
1	B	481	TYR	3.4
1	A	49	SER	3.3
1	A	200	SER	3.3
1	B	326	GLU	3.2
1	A	191	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	51	VAL	3.2
1	A	477	SER	3.2
1	B	150	GLY	3.0
1	A	54	GLU	3.0
1	B	45	LEU	3.0
1	A	151	LYS	3.0
1	A	51	VAL	3.0
1	A	199	SER	2.9
1	A	403	LYS	2.9
1	B	207	VAL	2.9
1	B	152	PHE	2.9
1	A	561	ILE	2.8
1	B	56	VAL	2.8
1	A	201	PRO	2.7
1	B	192	LYS	2.7
1	A	194	VAL	2.6
1	B	484	GLU	2.6
1	B	158	GLU	2.6
1	B	397	TRP	2.6
1	A	397	TRP	2.6
1	B	95	PHE	2.6
1	B	49	SER	2.6
1	A	229	ASP	2.5
1	A	476	LYS	2.5
1	A	190	GLN	2.5
1	B	190	GLN	2.5
1	A	331	PHE	2.5
1	A	205	LYS	2.5
1	B	54	GLU	2.4
1	B	59	ALA	2.4
1	B	200	SER	2.4
1	B	327	GLU	2.4
1	A	147	LYS	2.4
1	B	225	ARG	2.4
1	B	42	LEU	2.4
1	A	144	PHE	2.3
1	B	52	THR	2.3
1	B	82	PHE	2.2
1	A	145	GLN	2.2
1	A	148	GLU	2.2
1	A	554	MET	2.2
1	A	404	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	204	ALA	2.0
1	A	329	GLU	2.0
1	A	212	ASP	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 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.