



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 01:27 AM UTC

PDB ID : 6DX7 / pdb_00006dx7
Title : Crystal structure of chalcone synthase from *Physcomitrella patens*
Authors : Liou, G.; Chiang, Y.C.; Wang, Y.; Weng, J.K.
Deposited on : 2018-06-28
Resolution : 2.61 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

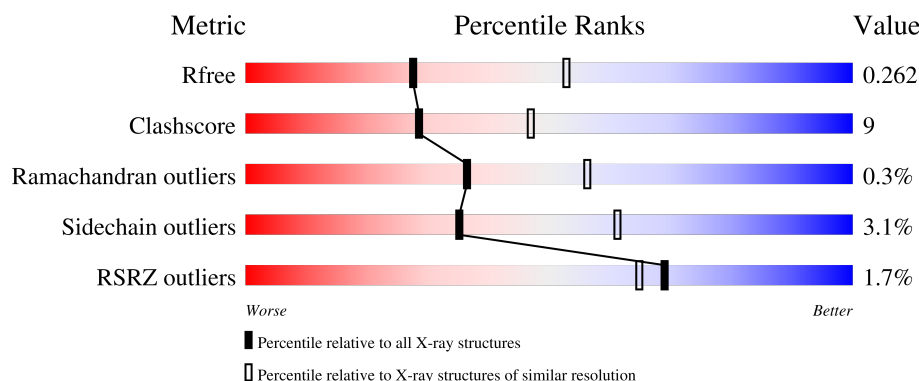
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	397	 2% 79% 17% ..
1	B	397	 % 76% 21% ..
1	C	397	 2% 75% 21% ..
1	D	397	 % 84% 12% ..
1	E	397	 2% 73% 23% ..

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Mol	Chain	Length	Quality of chain
1	F	397	2% 75% 21% ••

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 35469 atoms, of which 17818 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 Chalcone synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	387	Total	C	H	N	O	S	0	0	0
			5902	1871	2970	510	536	15			
1	B	387	Total	C	H	N	O	S	0	0	0
			5902	1871	2970	510	536	15			
1	C	387	Total	C	H	N	O	S	0	0	0
			5902	1871	2970	510	536	15			
1	D	387	Total	C	H	N	O	S	0	0	0
			5902	1871	2970	510	536	15			
1	E	387	Total	C	H	N	O	S	0	0	0
			5902	1871	2970	510	536	15			
1	F	387	Total	C	H	N	O	S	0	0	0
			5900	1871	2968	510	536	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	GLU	ASP	variant	UNP Q2VAZ3
B	44	GLU	ASP	variant	UNP Q2VAZ3
C	44	GLU	ASP	variant	UNP Q2VAZ3
D	44	GLU	ASP	variant	UNP Q2VAZ3
E	44	GLU	ASP	variant	UNP Q2VAZ3
F	44	GLU	ASP	variant	UNP Q2VAZ3

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	14	Total	O	0	0
			14	14		
2	B	8	Total	O	0	0
			8	8		
2	C	13	Total	O	0	0
			13	13		

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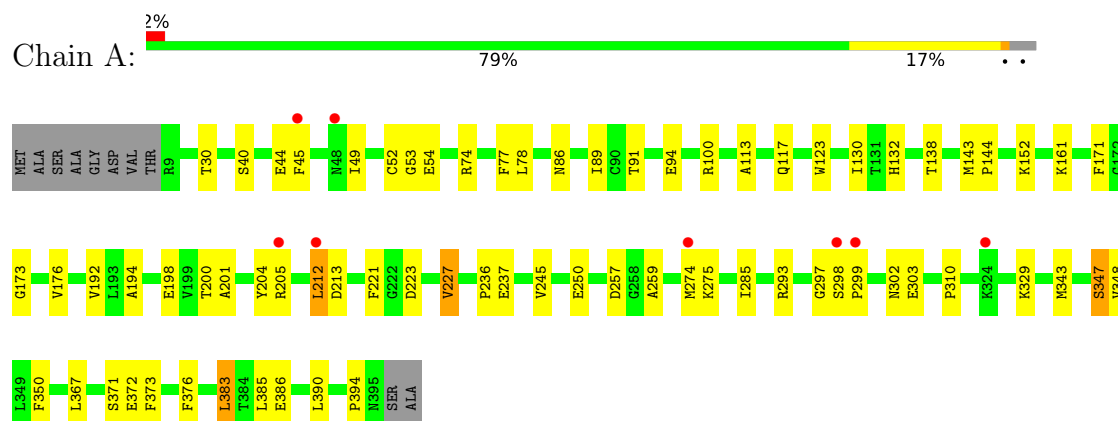
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	7	Total	O	0	0
			7	7		
2	E	6	Total	O	0	0
			6	6		
2	F	11	Total	O	0	0
			11	11		

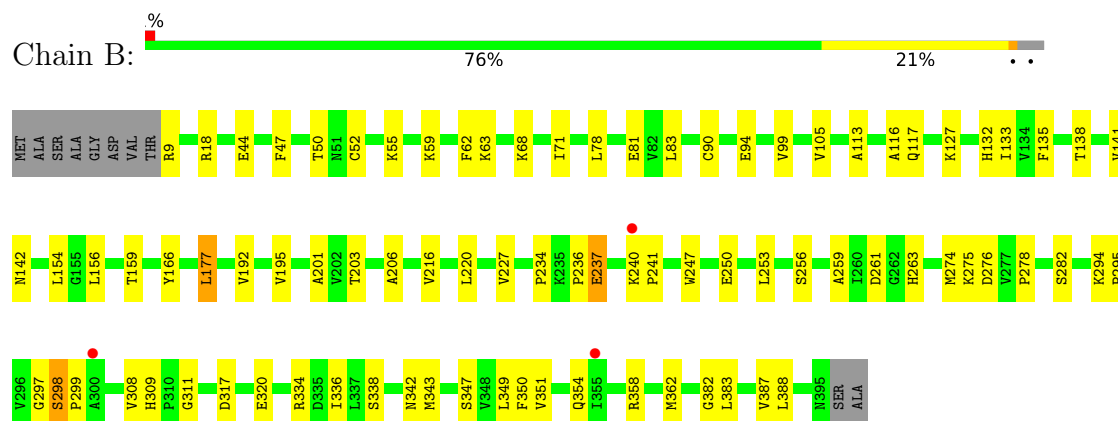
3 Residue-property plots [i](#)

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.

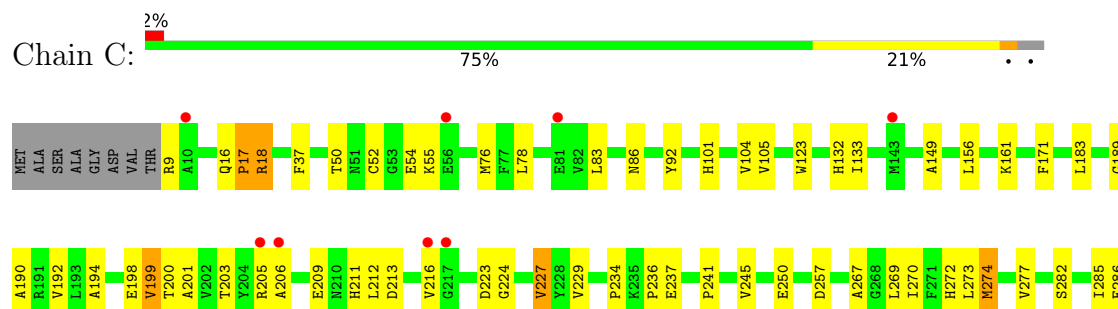
• Molecule 1: Chalcone synthase



• Molecule 1: Chalcone synthase

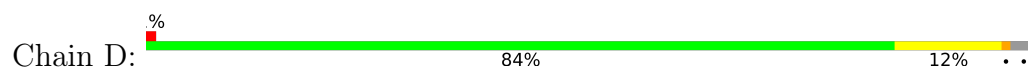


• Molecule 1: Chalcone synthase

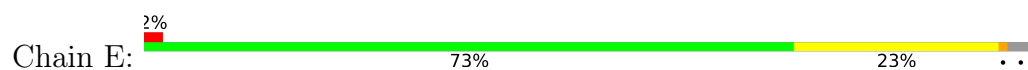




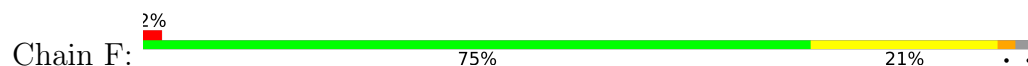
• Molecule 1: Chalcone synthase



• Molecule 1: Chalcone synthase



• Molecule 1: Chalcone synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.60Å 192.83Å 195.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.01 – 2.61 37.01 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.0 (37.01-2.61) 98.9 (37.01-2.61)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.181 , 0.263 0.197 , 0.262	Depositor DCC
R_{free} test set	1967 reflections (2.36%)	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.717	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	35469	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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	0.70	0/2996	0.77	2/4053 (0.0%)
1	B	0.64	0/2996	0.75	0/4053
1	C	0.64	0/2996	0.74	0/4053
1	D	0.62	1/2996 (0.0%)	0.72	0/4053
1	E	0.56	0/2996	0.70	0/4053
1	F	0.62	0/2996	0.73	2/4053 (0.0%)
All	All	0.63	1/17976 (0.0%)	0.73	4/24318 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	E	0	1
1	F	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	18	ARG	NE-CZ	6.15	1.39	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	PRO	CA-C-N	5.69	131.95	121.70
1	A	394	PRO	C-N-CA	5.69	131.95	121.70
1	F	299	PRO	CA-C-N	5.46	131.53	121.70
1	F	299	PRO	C-N-CA	5.46	131.53	121.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	382	GLY	Peptide
1	E	382	GLY	Peptide
1	F	382	GLY	Peptide

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	2932	2970	2970	46	0
1	B	2932	2970	2970	51	0
1	C	2932	2970	2970	61	1
1	D	2932	2970	2970	28	1
1	E	2932	2970	2970	69	0
1	F	2932	2968	2970	74	0
2	A	14	0	0	2	0
2	B	8	0	0	0	0
2	C	13	0	0	5	0
2	D	7	0	0	0	0
2	E	6	0	0	0	0
2	F	11	0	0	0	0
All	All	17651	17818	17820	313	1

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 9.

All (313) 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:F:293:ARG:NE	1:F:299:PRO:O	1.93	1.00
1:C:205:ARG:NH2	1:C:267:ALA:O	2.05	0.90
1:A:77:PHE:O	2:A:401:HOH:O	1.91	0.86
1:A:212:LEU:HD12	1:A:213:ASP:H	1.45	0.81
1:A:293:ARG:HB3	1:A:298:SER:HA	1.64	0.80
1:C:277:VAL:HG13	1:C:383:LEU:HD11	1.64	0.79
1:F:299:PRO:HB3	1:F:300:ALA:HB3	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:395:ASN:OD1	2:C:402:HOH:O	2.05	0.74
1:A:200:THR:HG23	1:A:223:ASP:OD1	1.89	0.73
1:A:205:ARG:CZ	1:A:205:ARG:HB3	2.19	0.71
1:D:293:ARG:HB3	1:D:298:SER:HA	1.74	0.70
1:C:9:ARG:NE	2:C:401:HOH:O	1.97	0.70
1:C:245:VAL:HG12	1:C:390:LEU:HD22	1.76	0.68
1:C:213:ASP:O	1:C:216:VAL:HG12	1.93	0.68
1:F:205:ARG:HB3	1:F:205:ARG:CZ	2.23	0.68
1:F:72:ARG:NH1	1:F:339:GLU:OE2	2.28	0.67
1:A:45:PHE:O	1:A:49:ILE:HD12	1.95	0.67
1:B:253:LEU:HD12	1:B:383:LEU:HD12	1.77	0.66
1:A:257:ASP:OD2	2:A:402:HOH:O	2.14	0.66
1:E:316:LEU:HG	1:E:330:MET:HE2	1.77	0.65
1:B:216:VAL:O	1:B:220:LEU:HD12	1.95	0.65
1:C:50:THR:HG21	1:C:206:ALA:HA	1.79	0.65
1:E:111:LEU:HD22	1:E:225:ALA:HB3	1.80	0.64
1:E:113:ALA:O	1:E:117:GLN:HG2	1.98	0.64
1:E:311:GLY:HA2	1:E:342:ASN:HD22	1.62	0.62
1:F:293:ARG:NH2	1:F:300:ALA:H	1.96	0.62
1:F:104:VAL:HG12	1:F:199:VAL:HG22	1.81	0.62
1:C:92:TYR:O	1:C:205:ARG:NH1	2.31	0.62
1:B:259:ALA:HB3	1:B:383:LEU:HD23	1.82	0.62
1:E:320:GLU:OE1	1:E:334:ARG:NH2	2.30	0.62
1:E:330:MET:HE3	1:E:330:MET:HA	1.81	0.61
1:E:253:LEU:HD12	1:E:383:LEU:HD12	1.83	0.60
1:E:297:GLY:O	1:E:299:PRO:HD3	2.01	0.60
1:C:367:LEU:HD22	1:C:393:ALA:HB3	1.83	0.60
1:E:73:LYS:NZ	1:E:75:HIS:NE2	2.49	0.59
1:F:299:PRO:CB	1:F:300:ALA:HB3	2.31	0.59
1:D:198:GLU:HG3	1:D:343:MET:O	2.01	0.59
1:B:259:ALA:HA	1:B:275:LYS:HG3	1.83	0.59
1:C:203:THR:HG22	1:C:269:LEU:HD23	1.84	0.58
1:A:30:THR:HB	1:A:350:PHE:CZ	2.38	0.58
1:C:101:HIS:O	1:C:105:VAL:HG12	2.03	0.58
1:B:236:PRO:O	1:B:237:GLU:HB2	2.03	0.58
1:E:71:ILE:HA	1:E:338:SER:HA	1.86	0.58
1:E:11:ALA:HA	1:F:391:ARG:HH12	1.68	0.57
1:B:132:HIS:HB2	1:B:192:VAL:HG22	1.86	0.57
1:A:161:LYS:HA	1:B:250:GLU:OE2	2.03	0.57
1:F:203:THR:HG22	1:F:269:LEU:HD23	1.86	0.57
1:E:92:TYR:CZ	1:E:93:MET:HE2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:ILE:HD12	1:B:350:PHE:HB3	1.86	0.57
1:E:321:ALA:O	1:E:324:LYS:HE3	2.04	0.57
1:A:132:HIS:HB2	1:A:192:VAL:HG22	1.86	0.57
1:A:52:CYS:C	1:A:54:GLU:H	2.12	0.56
1:D:73:LYS:NZ	1:D:75:HIS:NE2	2.54	0.56
1:F:236:PRO:O	1:F:237:GLU:HB2	2.05	0.55
1:E:290:ASN:HA	1:E:293:ARG:HD2	1.88	0.55
1:C:236:PRO:O	1:C:237:GLU:HB2	2.06	0.55
1:C:234:PRO:HG2	1:C:241:PRO:HG3	1.88	0.55
1:A:212:LEU:HD13	1:A:213:ASP:CG	2.31	0.55
1:E:236:PRO:O	1:E:237:GLU:HB2	2.07	0.55
1:E:78:LEU:HD11	1:E:201:ALA:HA	1.89	0.54
1:C:92:TYR:HA	1:C:206:ALA:HB3	1.89	0.54
1:E:27:GLY:HA2	1:E:122:GLU:HG2	1.89	0.54
1:F:278:PRO:HG3	1:F:315:ILE:HG13	1.89	0.54
1:F:293:ARG:CZ	1:F:299:PRO:O	2.55	0.54
1:C:205:ARG:CB	1:C:205:ARG:CZ	2.86	0.54
1:F:299:PRO:HA	1:F:300:ALA:CB	2.38	0.53
1:C:37:PHE:CE1	1:C:76:MET:HB2	2.43	0.53
1:E:249:GLY:HA2	1:F:161:LYS:HE3	1.89	0.53
1:E:293:ARG:NH2	1:E:299:PRO:O	2.41	0.53
1:C:200:THR:HG23	1:C:223:ASP:OD1	2.09	0.53
1:E:238:VAL:HG22	1:E:238:VAL:O	2.08	0.53
1:E:381:PRO:HG2	1:F:143:MET:HE2	1.89	0.53
1:C:372:GLU:HG2	1:C:373:PHE:CD2	2.44	0.53
1:A:250:GLU:HB3	1:A:386:GLU:HG2	1.91	0.52
1:D:132:HIS:HA	1:D:161:LYS:O	2.09	0.52
1:B:216:VAL:HG12	1:B:220:LEU:HD13	1.91	0.52
1:F:293:ARG:CD	1:F:299:PRO:O	2.56	0.52
1:B:81:GLU:H	1:B:81:GLU:CD	2.18	0.52
1:F:92:TYR:CE1	1:F:93:MET:HE2	2.45	0.52
1:C:293:ARG:HB3	1:C:298:SER:HA	1.92	0.52
1:C:361:LYS:NZ	1:E:213:ASP:OD1	2.37	0.52
1:F:200:THR:HG23	1:F:223:ASP:OD1	2.08	0.52
1:A:52:CYS:O	1:A:54:GLU:N	2.41	0.52
1:D:78:LEU:HD11	1:D:201:ALA:HA	1.91	0.52
1:F:126:ARG:NH1	1:F:129:ASP:OD2	2.43	0.52
1:C:205:ARG:CZ	1:C:205:ARG:HB3	2.39	0.52
1:A:45:PHE:CD1	1:A:49:ILE:HD13	2.45	0.51
1:B:47:PHE:CZ	1:B:59:LYS:HA	2.45	0.51
1:F:259:ALA:HA	1:F:274:MET:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:ILE:HD11	1:B:156:LEU:HD12	1.92	0.51
1:E:311:GLY:HA2	1:E:342:ASN:ND2	2.25	0.51
1:A:236:PRO:O	1:A:237:GLU:HB2	2.11	0.51
1:C:205:ARG:NH1	1:C:205:ARG:HB2	2.25	0.51
1:E:354:GLN:O	1:E:358:ARG:HG3	2.11	0.51
1:F:276:ASP:O	1:F:280:LEU:HG	2.10	0.51
1:D:320:GLU:OE2	1:D:334:ARG:NH2	2.44	0.51
1:C:315:ILE:HG21	1:C:379:PHE:CZ	2.46	0.51
1:D:38:LEU:HD23	1:D:72:ARG:O	2.11	0.51
1:F:265:THR:HG21	1:F:270:ILE:HD13	1.93	0.51
1:F:315:ILE:HG21	1:F:379:PHE:CZ	2.44	0.51
1:D:132:HIS:HB2	1:D:192:VAL:HG22	1.92	0.51
1:F:299:PRO:CA	1:F:300:ALA:HB3	2.41	0.51
1:E:92:TYR:CE2	1:E:93:MET:HE2	2.46	0.51
1:E:199:VAL:HG23	1:E:223:ASP:OD2	2.10	0.51
1:E:310:PRO:HD2	1:E:347:SER:HB3	1.92	0.50
1:F:91:THR:OG1	1:F:94:GLU:HB2	2.11	0.50
1:F:68:LYS:O	1:F:313:PRO:HG3	2.12	0.50
1:B:78:LEU:HD11	1:B:201:ALA:HA	1.91	0.50
1:C:203:THR:CG2	1:C:269:LEU:HD23	2.42	0.50
1:F:30:THR:HB	1:F:350:PHE:CZ	2.46	0.50
1:E:294:LYS:HB2	1:E:295:PRO:HD3	1.93	0.50
1:C:194:ALA:O	1:C:227:VAL:HA	2.11	0.50
1:C:211:HIS:CE1	1:C:270:ILE:HG23	2.47	0.50
1:C:290:ASN:OD1	1:C:293:ARG:NH2	2.44	0.50
1:D:349:LEU:CD2	1:D:376:PHE:HZ	2.25	0.50
1:A:45:PHE:O	1:A:49:ILE:CD1	2.59	0.49
1:E:259:ALA:HB3	1:E:383:LEU:HD23	1.93	0.49
1:F:259:ALA:HB3	1:F:383:LEU:HD23	1.94	0.49
1:B:336:ILE:HG13	1:B:351:VAL:HA	1.94	0.49
1:A:194:ALA:O	1:A:227:VAL:HA	2.12	0.49
1:C:52:CYS:C	1:C:54:GLU:H	2.19	0.49
1:C:189:GLY:O	1:C:190:ALA:C	2.54	0.49
1:E:132:HIS:CD2	1:E:183:LEU:HD23	2.48	0.49
1:A:78:LEU:HD11	1:A:201:ALA:HA	1.95	0.49
1:D:127:LYS:HD2	1:D:154:LEU:O	2.12	0.49
1:E:327:LYS:N	1:E:327:LYS:HD2	2.27	0.49
1:E:52:CYS:SG	1:E:55:LYS:HE3	2.52	0.49
1:F:285:ILE:HG23	1:F:286:GLU:N	2.27	0.49
1:A:171:PHE:CD1	1:A:171:PHE:C	2.91	0.49
1:F:105:VAL:HG22	1:F:142:ASN:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:299:PRO:CA	1:F:300:ALA:CB	2.91	0.49
1:A:259:ALA:HB3	1:A:383:LEU:HD23	1.94	0.49
1:E:98:ASN:CG	1:F:266:GLU:HG3	2.37	0.49
1:C:331:GLN:HG2	1:C:358:ARG:NH2	2.27	0.48
1:E:382:GLY:H	1:F:144:PRO:HG3	1.78	0.48
1:F:74:ARG:NH1	1:F:221:PHE:O	2.46	0.48
1:F:310:PRO:HD2	1:F:347:SER:HB3	1.94	0.48
1:D:349:LEU:HD23	1:D:376:PHE:HZ	1.78	0.48
1:E:296:VAL:C	1:E:297:GLY:O	2.49	0.48
1:E:314:ALA:O	1:E:318:GLN:HG3	2.14	0.48
1:E:111:LEU:HD22	1:E:225:ALA:CB	2.42	0.48
1:B:68:LYS:C	1:B:68:LYS:HD2	2.39	0.48
1:D:89:ILE:O	1:D:89:ILE:HG22	2.13	0.48
1:E:37:PHE:CE1	1:E:76:MET:HB2	2.48	0.48
1:C:344:SER:OG	1:C:345:SER:N	2.46	0.48
1:E:293:ARG:HG3	1:E:298:SER:HA	1.95	0.48
1:E:348:VAL:HG13	1:E:376:PHE:CZ	2.49	0.48
1:A:198:GLU:HG3	1:A:343:MET:O	2.14	0.47
1:F:12:LEU:HD13	1:F:13:PRO:HD2	1.96	0.47
1:A:212:LEU:CD1	1:A:213:ASP:H	2.23	0.47
1:E:248:ALA:HB2	1:E:388:LEU:HD23	1.97	0.47
1:F:304:MET:HA	1:F:373:PHE:O	2.13	0.47
1:D:236:PRO:O	1:D:237:GLU:HB2	2.14	0.47
1:E:98:ASN:OD1	1:F:266:GLU:HG3	2.14	0.47
1:E:330:MET:CE	1:E:333:SER:HB2	2.45	0.47
1:E:33:PRO:HD3	1:E:111:LEU:HD11	1.97	0.47
1:F:276:ASP:OD1	1:F:279:GLY:N	2.41	0.46
1:A:274:MET:O	1:A:275:LYS:HG3	2.15	0.46
1:B:127:LYS:HD2	1:B:154:LEU:O	2.16	0.46
1:D:281:ILE:HG21	1:D:315:ILE:HD11	1.97	0.46
1:E:100:ARG:NH1	1:E:201:ALA:O	2.49	0.46
1:E:391:ARG:NH1	1:F:12:LEU:HD23	2.31	0.46
1:C:78:LEU:HD11	1:C:201:ALA:HA	1.98	0.46
1:A:86:ASN:HB3	1:A:89:ILE:HD12	1.98	0.46
1:B:113:ALA:O	1:B:117:GLN:HG2	2.15	0.46
1:C:285:ILE:HG23	1:C:286:GLU:N	2.31	0.46
1:C:9:ARG:NH2	2:C:401:HOH:O	2.48	0.46
1:E:262:GLY:HA3	1:F:143:MET:HB2	1.97	0.46
1:B:294:LYS:HB2	1:B:295:PRO:HD3	1.98	0.45
1:C:250:GLU:HB3	1:C:386:GLU:HG2	1.97	0.45
1:E:28:ILE:HG21	1:E:353:ASP:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:285:ILE:HG12	1:F:289:LEU:HD11	1.97	0.45
1:C:149:ALA:O	2:C:403:HOH:O	2.21	0.45
1:F:141:VAL:HA	1:F:166:TYR:CE1	2.52	0.45
1:A:212:LEU:HD12	1:A:213:ASP:N	2.21	0.45
1:A:372:GLU:HG2	1:A:373:PHE:CD2	2.51	0.45
1:F:297:GLY:C	1:F:299:PRO:HD3	2.41	0.45
1:B:83:LEU:HB3	1:B:90:CYS:SG	2.57	0.45
1:B:261:ASP:OD1	1:B:263:HIS:CE1	2.70	0.45
1:C:133:ILE:HD11	1:C:156:LEU:HD12	1.98	0.45
1:A:113:ALA:O	1:A:117:GLN:HG2	2.17	0.45
1:A:205:ARG:CZ	1:A:205:ARG:CB	2.93	0.45
1:B:116:ALA:HA	1:B:227:VAL:HG11	1.98	0.45
1:E:245:VAL:HG22	1:E:390:LEU:HD22	1.97	0.45
1:C:132:HIS:HB2	1:C:192:VAL:HG22	1.99	0.45
1:C:320:GLU:HA	1:C:325:LEU:HD12	1.98	0.45
1:D:101:HIS:HA	1:D:104:VAL:HG22	1.98	0.45
1:B:50:THR:HG21	1:B:206:ALA:HA	1.99	0.45
1:B:276:ASP:OD1	1:B:278:PRO:HD2	2.17	0.45
1:C:104:VAL:HG12	1:C:199:VAL:CG2	2.47	0.45
1:C:372:GLU:HG2	1:C:373:PHE:CE2	2.51	0.45
1:B:116:ALA:CA	1:B:227:VAL:HG11	2.47	0.44
1:B:308:VAL:O	1:B:309:HIS:C	2.58	0.44
1:F:23:ALA:O	1:F:245:VAL:HG12	2.17	0.44
1:F:275:LYS:HD3	1:F:276:ASP:H	1.82	0.44
1:A:74:ARG:HD2	1:A:221:PHE:O	2.17	0.44
1:B:320:GLU:CD	1:B:334:ARG:HH22	2.25	0.44
1:A:310:PRO:HD2	1:A:347:SER:HB2	1.99	0.44
1:C:315:ILE:HD12	1:C:315:ILE:H	1.83	0.44
1:D:259:ALA:O	1:D:273:LEU:HA	2.18	0.44
1:D:224:GLY:HA3	1:D:343:MET:SD	2.58	0.44
1:F:181:LYS:NZ	1:F:185:GLU:OE1	2.49	0.44
1:F:265:THR:CG2	1:F:270:ILE:HD13	2.47	0.44
1:A:100:ARG:NH1	1:A:204:TYR:O	2.48	0.44
1:F:78:LEU:HD11	1:F:201:ALA:HA	2.00	0.44
1:A:143:MET:HA	1:A:144:PRO:C	2.42	0.44
1:B:47:PHE:HE1	1:B:62:PHE:CD2	2.36	0.44
1:F:293:ARG:NH2	1:F:301:TRP:CD2	2.86	0.44
1:A:86:ASN:CB	1:A:89:ILE:HD12	2.48	0.44
1:C:123:TRP:CG	1:C:229:VAL:HG11	2.53	0.44
1:E:320:GLU:CD	1:E:334:ARG:NH2	2.76	0.44
1:A:348:VAL:HG13	1:A:376:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:278:PRO:HB3	1:F:315:ILE:HA	2.00	0.43
1:F:300:ALA:O	1:F:301:TRP:C	2.60	0.43
1:E:224:GLY:HA3	1:E:343:MET:SD	2.59	0.43
1:E:198:GLU:HG3	1:E:343:MET:O	2.18	0.43
1:F:247:TRP:HB3	1:F:389:VAL:HB	1.99	0.43
1:D:310:PRO:HD3	1:D:351:VAL:HG21	2.00	0.43
1:C:132:HIS:HA	1:C:161:LYS:O	2.18	0.43
1:E:16:GLN:OE1	1:F:247:TRP:HA	2.19	0.43
1:B:343:MET:N	1:B:347:SER:OG	2.48	0.43
1:D:290:ASN:OD1	1:D:293:ARG:NH2	2.52	0.43
1:D:297:GLY:C	1:D:299:PRO:HD3	2.43	0.43
1:F:275:LYS:O	1:F:277:VAL:N	2.51	0.43
1:F:367:LEU:CD1	1:F:395:ASN:HB2	2.49	0.43
1:E:362:MET:HE2	1:E:362:MET:HB3	1.92	0.43
1:B:247:TRP:O	1:B:388:LEU:HA	2.19	0.43
1:E:123:TRP:CD2	1:E:229:VAL:HG11	2.54	0.43
1:C:292:ALA:O	1:C:295:PRO:HD2	2.19	0.43
1:F:132:HIS:HA	1:F:161:LYS:O	2.19	0.43
1:A:302:ASN:HA	1:A:329:LYS:HE3	2.01	0.42
1:A:303:GLU:O	1:A:371:SER:HB3	2.19	0.42
1:C:16:GLN:O	1:C:17:PRO:C	2.61	0.42
1:D:104:VAL:HG11	1:D:202:VAL:HG23	2.00	0.42
1:D:141:VAL:HG12	1:D:166:TYR:CG	2.53	0.42
1:D:177:LEU:HD23	1:D:177:LEU:HA	1.92	0.42
1:E:104:VAL:HG12	1:E:199:VAL:HG13	2.01	0.42
1:E:330:MET:HE3	1:E:330:MET:CA	2.47	0.42
1:F:191:ARG:NH2	1:F:239:GLU:OE1	2.47	0.42
1:C:198:GLU:HG3	1:C:343:MET:O	2.19	0.42
1:B:274:MET:O	1:B:275:LYS:HG2	2.19	0.42
1:C:104:VAL:CG1	1:C:201:ALA:HB3	2.49	0.42
1:C:171:PHE:CD1	1:C:171:PHE:C	2.97	0.42
1:D:36:GLU:HG2	1:D:75:HIS:CE1	2.54	0.42
1:D:293:ARG:HD2	1:D:299:PRO:O	2.20	0.42
1:D:343:MET:HE1	1:D:350:PHE:CD2	2.55	0.42
1:E:151:ALA:HA	1:E:156:LEU:HD12	2.00	0.42
1:C:104:VAL:HG12	1:C:199:VAL:HG23	2.01	0.42
1:A:245:VAL:HG22	1:A:390:LEU:HD22	2.02	0.42
1:B:116:ALA:N	1:B:227:VAL:HG11	2.34	0.42
1:B:317:ASP:OD1	1:B:334:ARG:NH1	2.53	0.42
1:B:358:ARG:O	1:B:362:MET:HG2	2.20	0.42
1:E:9:ARG:NH1	1:E:10:ALA:H	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:253:LEU:CD1	1:E:383:LEU:HD12	2.48	0.42
1:B:234:PRO:HG2	1:B:241:PRO:HG3	2.00	0.42
1:C:9:ARG:CZ	2:C:401:HOH:O	2.55	0.42
1:D:97:LEU:HA	1:D:100:ARG:HD2	2.01	0.42
1:F:132:HIS:HB2	1:F:192:VAL:HG22	2.01	0.42
1:B:71:ILE:HA	1:B:338:SER:HA	2.01	0.42
1:B:274:MET:C	1:B:275:LYS:HG2	2.45	0.42
1:E:191:ARG:HD3	1:E:191:ARG:HA	1.81	0.42
1:B:177:LEU:HD23	1:B:177:LEU:HA	1.92	0.41
1:B:256:SER:OG	1:B:383:LEU:HB2	2.20	0.41
1:C:78:LEU:HB3	1:C:83:LEU:HD21	2.02	0.41
1:C:274:MET:HE2	1:C:274:MET:HA	2.02	0.41
1:E:248:ALA:H	1:F:16:GLN:HE22	1.68	0.41
1:B:297:GLY:O	1:B:299:PRO:HD3	2.20	0.41
1:F:104:VAL:HG13	1:F:201:ALA:HB3	2.02	0.41
1:A:297:GLY:C	1:A:299:PRO:HD3	2.45	0.41
1:B:105:VAL:HG22	1:B:142:ASN:HB2	2.02	0.41
1:F:83:LEU:HD23	1:F:83:LEU:HA	1.95	0.41
1:F:177:LEU:HD23	1:F:177:LEU:HA	1.82	0.41
1:F:383:LEU:HD13	1:F:383:LEU:HA	1.82	0.41
1:A:91:THR:OG1	1:A:94:GLU:HG2	2.21	0.41
1:C:132:HIS:CD2	1:C:183:LEU:HD23	2.56	0.41
1:E:31:ALA:C	1:E:111:LEU:HD21	2.46	0.41
1:E:31:ALA:O	1:E:111:LEU:HD21	2.21	0.41
1:F:354:GLN:O	1:F:358:ARG:HG3	2.21	0.41
1:B:274:MET:HG3	1:F:339:GLU:HG3	2.03	0.41
1:C:212:LEU:O	1:C:213:ASP:C	2.64	0.41
1:E:147:ASP:OD1	1:E:147:ASP:N	2.53	0.41
1:F:380:GLY:O	1:F:383:LEU:HA	2.21	0.41
1:C:55:LYS:NZ	1:C:209:GLU:OE1	2.52	0.41
1:C:203:THR:HG22	1:C:269:LEU:HB3	2.03	0.41
1:C:224:GLY:HA3	1:C:343:MET:SD	2.60	0.41
1:E:171:PHE:CD1	1:E:171:PHE:C	2.99	0.41
1:F:42:TYR:O	1:F:43:PRO:C	2.63	0.41
1:B:274:MET:HE2	1:F:339:GLU:HG3	2.02	0.41
1:B:311:GLY:HA2	1:B:342:ASN:ND2	2.35	0.41
1:A:123:TRP:CZ3	1:A:130:ILE:HD11	2.56	0.41
1:B:336:ILE:HD11	1:B:354:GLN:HB2	2.02	0.41
1:E:42:TYR:N	1:E:43:PRO:CD	2.84	0.41
1:F:285:ILE:HG12	1:F:289:LEU:CD1	2.51	0.41
1:A:298:SER:N	1:A:299:PRO:CD	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:ARG:HA	1:B:9:ARG:HD3	1.89	0.41
1:B:135:PHE:HA	1:B:195:VAL:O	2.21	0.41
1:B:44:GLU:OE1	1:B:44:GLU:N	2.53	0.40
1:D:24:CYS:O	1:D:230:VAL:HA	2.21	0.40
1:F:320:GLU:OE2	1:F:330:MET:HB2	2.21	0.40
1:C:347:SER:O	1:C:351:VAL:HG23	2.22	0.40
1:E:92:TYR:O	1:E:93:MET:HG2	2.21	0.40
1:F:337:LEU:HD12	1:F:341:GLY:HA2	2.02	0.40
1:A:173:GLY:O	1:A:176:VAL:HG22	2.20	0.40
1:A:212:LEU:CD1	1:A:213:ASP:N	2.84	0.40
1:C:289:LEU:HD23	1:C:289:LEU:HA	1.89	0.40
1:F:193:LEU:HD23	1:F:193:LEU:HA	1.87	0.40
1:A:250:GLU:O	1:B:159:THR:HA	2.21	0.40
1:B:52:CYS:SG	1:B:55:LYS:NZ	2.81	0.40
1:C:272:HIS:C	1:C:273:LEU:HD12	2.46	0.40
1:A:285:ILE:HD12	1:A:385:LEU:HD21	2.04	0.40
1:B:141:VAL:HG12	1:B:166:TYR:CG	2.56	0.40
1:B:240:LYS:HG3	1:B:240:LYS:O	2.22	0.40
1:E:391:ARG:HH12	1:F:12:LEU:HD23	1.85	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:ARG:HH21	1:D:18:ARG:HE[1_455]	1.31	0.29

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	385/397 (97%)	362 (94%)	22 (6%)	1 (0%)	36 56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	385/397 (97%)	363 (94%)	21 (6%)	1 (0%)	36	56
1	C	385/397 (97%)	363 (94%)	21 (6%)	1 (0%)	36	56
1	D	385/397 (97%)	364 (94%)	20 (5%)	1 (0%)	36	56
1	E	385/397 (97%)	360 (94%)	24 (6%)	1 (0%)	36	56
1	F	385/397 (97%)	361 (94%)	21 (6%)	3 (1%)	16	31
All	All	2310/2382 (97%)	2173 (94%)	129 (6%)	8 (0%)	36	56

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	276	ASP
1	F	300	ALA
1	F	383	LEU
1	C	17	PRO
1	E	14	ARG
1	A	53	GLY
1	D	296	VAL
1	B	298	SER

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	308/314 (98%)	299 (97%)	9 (3%)	37	63
1	B	308/314 (98%)	296 (96%)	12 (4%)	28	53
1	C	308/314 (98%)	300 (97%)	8 (3%)	40	66
1	D	308/314 (98%)	297 (96%)	11 (4%)	31	56
1	E	308/314 (98%)	298 (97%)	10 (3%)	34	60
1	F	308/314 (98%)	300 (97%)	8 (3%)	40	66
All	All	1848/1884 (98%)	1790 (97%)	58 (3%)	35	61

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	SER
1	A	44	GLU
1	A	138	THR
1	A	152	LYS
1	A	212	LEU
1	A	227	VAL
1	A	347	SER
1	A	367	LEU
1	A	383	LEU
1	B	18	ARG
1	B	63	LYS
1	B	94	GLU
1	B	99	VAL
1	B	138	THR
1	B	177	LEU
1	B	203	THR
1	B	237	GLU
1	B	282	SER
1	B	298	SER
1	B	349	LEU
1	B	387	VAL
1	C	18	ARG
1	C	86	ASN
1	C	199	VAL
1	C	227	VAL
1	C	257	ASP
1	C	274	MET
1	C	282	SER
1	C	383	LEU
1	D	38	LEU
1	D	105	VAL
1	D	106	VAL
1	D	127	LYS
1	D	134	VAL
1	D	138	THR
1	D	177	LEU
1	D	215	LEU
1	D	218	SER
1	D	244	GLU
1	D	349	LEU
1	E	93	MET
1	E	177	LEU
1	E	193	LEU

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Mol	Chain	Res	Type
1	E	203	THR
1	E	215	LEU
1	E	232	SER
1	E	261	ASP
1	E	324	LYS
1	E	344	SER
1	E	383	LEU
1	F	18	ARG
1	F	138	THR
1	F	177	LEU
1	F	199	VAL
1	F	293	ARG
1	F	330	MET
1	F	349	LEU
1	F	387	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	272	HIS
1	A	357	HIS
1	B	86	ASN
1	B	148	HIS
1	B	272	HIS
1	C	101	HIS
1	C	272	HIS
1	C	395	ASN
1	D	16	GLN
1	D	272	HIS
1	E	187	ASN
1	E	309	HIS
1	E	318	GLN
1	E	342	ASN
1	F	16	GLN
1	F	318	GLN

5.3.3 RNA ⓘ

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	387/397 (97%)	-0.26	8 (2%) 63 59	31, 54, 119, 174	0
1	B	387/397 (97%)	-0.31	3 (0%) 82 80	35, 60, 100, 190	0
1	C	387/397 (97%)	-0.11	9 (2%) 61 56	35, 62, 124, 188	0
1	D	387/397 (97%)	-0.21	4 (1%) 79 76	37, 64, 105, 160	0
1	E	387/397 (97%)	0.03	8 (2%) 63 59	44, 72, 115, 244	0
1	F	387/397 (97%)	-0.06	7 (1%) 67 63	34, 68, 121, 143	0
All	All	2322/2382 (97%)	-0.15	39 (1%) 69 65	31, 64, 117, 244	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	299	PRO	4.4
1	A	212	LEU	3.9
1	A	298	SER	3.3
1	D	263	HIS	3.2
1	C	216	VAL	3.2
1	C	143	MET	3.1
1	E	11	ALA	2.9
1	C	81	GLU	2.8
1	D	38	LEU	2.8
1	E	9	ARG	2.8
1	F	257	ASP	2.6
1	A	324	LYS	2.6
1	A	48	ASN	2.6
1	E	10	ALA	2.5
1	F	273	LEU	2.5
1	E	238	VAL	2.5
1	C	205	ARG	2.4
1	E	395	ASN	2.4
1	E	13	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	377	ILE	2.4
1	B	240	LYS	2.3
1	F	299	PRO	2.3
1	C	10	ALA	2.2
1	A	205	ARG	2.2
1	E	146	ALA	2.2
1	C	56	GLU	2.2
1	D	395	ASN	2.2
1	D	240	LYS	2.2
1	C	217	GLY	2.2
1	A	274	MET	2.1
1	F	385	LEU	2.1
1	C	367	LEU	2.1
1	B	355	ILE	2.1
1	A	45	PHE	2.1
1	C	206	ALA	2.1
1	B	300	ALA	2.1
1	F	359	SER	2.1
1	F	240	LYS	2.0
1	E	12	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.