



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 8, 2021 – 02:21 PM JST

PDB ID : 7BUV
Title : Eucommia ulmoides TPT3, crystal form 2
Authors : Kajiura, H.; Yoshizawa, T.; Tokumoto, Y.; Suzuki, N.; Takeno, S.; Takeno, K.J.; Yamashita, T.; Tanaka, S.; Kaneko, Y.; Fujiyama, K.; Matsumura, H.; Nakazawa, Y.
Deposited on : 2020-04-08
Resolution : 3.30 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	:	2.16
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)	:	2.16

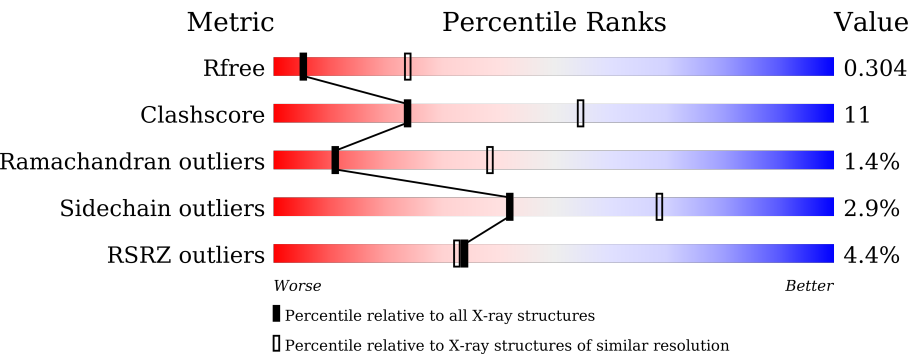
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	364	
1	B	364	
1	C	364	
1	D	364	
1	E	364	
1	F	364	

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Mol	Chain	Length	Quality of chain
1	G	364	<div><div></div><div>2%</div><div>68%</div><div>21%</div><div>10%</div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 18385 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 FPS3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2674	1721	436	503	14			
1	B	321	Total	C	N	O	S	0	0	0
			2605	1678	422	491	14			
1	C	322	Total	C	N	O	S	0	0	0
			2603	1673	425	491	14			
1	D	325	Total	C	N	O	S	0	0	0
			2633	1696	429	494	14			
1	E	316	Total	C	N	O	S	0	0	0
			2569	1655	417	483	14			
1	F	329	Total	C	N	O	S	0	0	0
			2663	1714	432	502	15			
1	G	326	Total	C	N	O	S	0	0	0
			2638	1699	432	492	15			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP A0A1L3KPU1
A	-14	ASN	-	expression tag	UNP A0A1L3KPU1
A	-13	HIS	-	expression tag	UNP A0A1L3KPU1
A	-12	LYS	-	expression tag	UNP A0A1L3KPU1
A	-11	VAL	-	expression tag	UNP A0A1L3KPU1
A	-10	HIS	-	expression tag	UNP A0A1L3KPU1
A	-9	HIS	-	expression tag	UNP A0A1L3KPU1
A	-8	HIS	-	expression tag	UNP A0A1L3KPU1
A	-7	HIS	-	expression tag	UNP A0A1L3KPU1
A	-6	HIS	-	expression tag	UNP A0A1L3KPU1
A	-5	HIS	-	expression tag	UNP A0A1L3KPU1
A	-4	ILE	-	expression tag	UNP A0A1L3KPU1
A	-3	GLU	-	expression tag	UNP A0A1L3KPU1
A	-2	GLY	-	expression tag	UNP A0A1L3KPU1
A	-1	ARG	-	expression tag	UNP A0A1L3KPU1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP A0A1L3KPU1
B	-15	MET	-	initiating methionine	UNP A0A1L3KPU1
B	-14	ASN	-	expression tag	UNP A0A1L3KPU1
B	-13	HIS	-	expression tag	UNP A0A1L3KPU1
B	-12	LYS	-	expression tag	UNP A0A1L3KPU1
B	-11	VAL	-	expression tag	UNP A0A1L3KPU1
B	-10	HIS	-	expression tag	UNP A0A1L3KPU1
B	-9	HIS	-	expression tag	UNP A0A1L3KPU1
B	-8	HIS	-	expression tag	UNP A0A1L3KPU1
B	-7	HIS	-	expression tag	UNP A0A1L3KPU1
B	-6	HIS	-	expression tag	UNP A0A1L3KPU1
B	-5	HIS	-	expression tag	UNP A0A1L3KPU1
B	-4	ILE	-	expression tag	UNP A0A1L3KPU1
B	-3	GLU	-	expression tag	UNP A0A1L3KPU1
B	-2	GLY	-	expression tag	UNP A0A1L3KPU1
B	-1	ARG	-	expression tag	UNP A0A1L3KPU1
B	0	HIS	-	expression tag	UNP A0A1L3KPU1
C	-15	MET	-	initiating methionine	UNP A0A1L3KPU1
C	-14	ASN	-	expression tag	UNP A0A1L3KPU1
C	-13	HIS	-	expression tag	UNP A0A1L3KPU1
C	-12	LYS	-	expression tag	UNP A0A1L3KPU1
C	-11	VAL	-	expression tag	UNP A0A1L3KPU1
C	-10	HIS	-	expression tag	UNP A0A1L3KPU1
C	-9	HIS	-	expression tag	UNP A0A1L3KPU1
C	-8	HIS	-	expression tag	UNP A0A1L3KPU1
C	-7	HIS	-	expression tag	UNP A0A1L3KPU1
C	-6	HIS	-	expression tag	UNP A0A1L3KPU1
C	-5	HIS	-	expression tag	UNP A0A1L3KPU1
C	-4	ILE	-	expression tag	UNP A0A1L3KPU1
C	-3	GLU	-	expression tag	UNP A0A1L3KPU1
C	-2	GLY	-	expression tag	UNP A0A1L3KPU1
C	-1	ARG	-	expression tag	UNP A0A1L3KPU1
C	0	HIS	-	expression tag	UNP A0A1L3KPU1
D	-15	MET	-	initiating methionine	UNP A0A1L3KPU1
D	-14	ASN	-	expression tag	UNP A0A1L3KPU1
D	-13	HIS	-	expression tag	UNP A0A1L3KPU1
D	-12	LYS	-	expression tag	UNP A0A1L3KPU1
D	-11	VAL	-	expression tag	UNP A0A1L3KPU1
D	-10	HIS	-	expression tag	UNP A0A1L3KPU1
D	-9	HIS	-	expression tag	UNP A0A1L3KPU1
D	-8	HIS	-	expression tag	UNP A0A1L3KPU1
D	-7	HIS	-	expression tag	UNP A0A1L3KPU1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	HIS	-	expression tag	UNP A0A1L3KPU1
D	-5	HIS	-	expression tag	UNP A0A1L3KPU1
D	-4	ILE	-	expression tag	UNP A0A1L3KPU1
D	-3	GLU	-	expression tag	UNP A0A1L3KPU1
D	-2	GLY	-	expression tag	UNP A0A1L3KPU1
D	-1	ARG	-	expression tag	UNP A0A1L3KPU1
D	0	HIS	-	expression tag	UNP A0A1L3KPU1
E	-15	MET	-	initiating methionine	UNP A0A1L3KPU1
E	-14	ASN	-	expression tag	UNP A0A1L3KPU1
E	-13	HIS	-	expression tag	UNP A0A1L3KPU1
E	-12	LYS	-	expression tag	UNP A0A1L3KPU1
E	-11	VAL	-	expression tag	UNP A0A1L3KPU1
E	-10	HIS	-	expression tag	UNP A0A1L3KPU1
E	-9	HIS	-	expression tag	UNP A0A1L3KPU1
E	-8	HIS	-	expression tag	UNP A0A1L3KPU1
E	-7	HIS	-	expression tag	UNP A0A1L3KPU1
E	-6	HIS	-	expression tag	UNP A0A1L3KPU1
E	-5	HIS	-	expression tag	UNP A0A1L3KPU1
E	-4	ILE	-	expression tag	UNP A0A1L3KPU1
E	-3	GLU	-	expression tag	UNP A0A1L3KPU1
E	-2	GLY	-	expression tag	UNP A0A1L3KPU1
E	-1	ARG	-	expression tag	UNP A0A1L3KPU1
E	0	HIS	-	expression tag	UNP A0A1L3KPU1
F	-15	MET	-	initiating methionine	UNP A0A1L3KPU1
F	-14	ASN	-	expression tag	UNP A0A1L3KPU1
F	-13	HIS	-	expression tag	UNP A0A1L3KPU1
F	-12	LYS	-	expression tag	UNP A0A1L3KPU1
F	-11	VAL	-	expression tag	UNP A0A1L3KPU1
F	-10	HIS	-	expression tag	UNP A0A1L3KPU1
F	-9	HIS	-	expression tag	UNP A0A1L3KPU1
F	-8	HIS	-	expression tag	UNP A0A1L3KPU1
F	-7	HIS	-	expression tag	UNP A0A1L3KPU1
F	-6	HIS	-	expression tag	UNP A0A1L3KPU1
F	-5	HIS	-	expression tag	UNP A0A1L3KPU1
F	-4	ILE	-	expression tag	UNP A0A1L3KPU1
F	-3	GLU	-	expression tag	UNP A0A1L3KPU1
F	-2	GLY	-	expression tag	UNP A0A1L3KPU1
F	-1	ARG	-	expression tag	UNP A0A1L3KPU1
F	0	HIS	-	expression tag	UNP A0A1L3KPU1
G	-15	MET	-	initiating methionine	UNP A0A1L3KPU1
G	-14	ASN	-	expression tag	UNP A0A1L3KPU1
G	-13	HIS	-	expression tag	UNP A0A1L3KPU1

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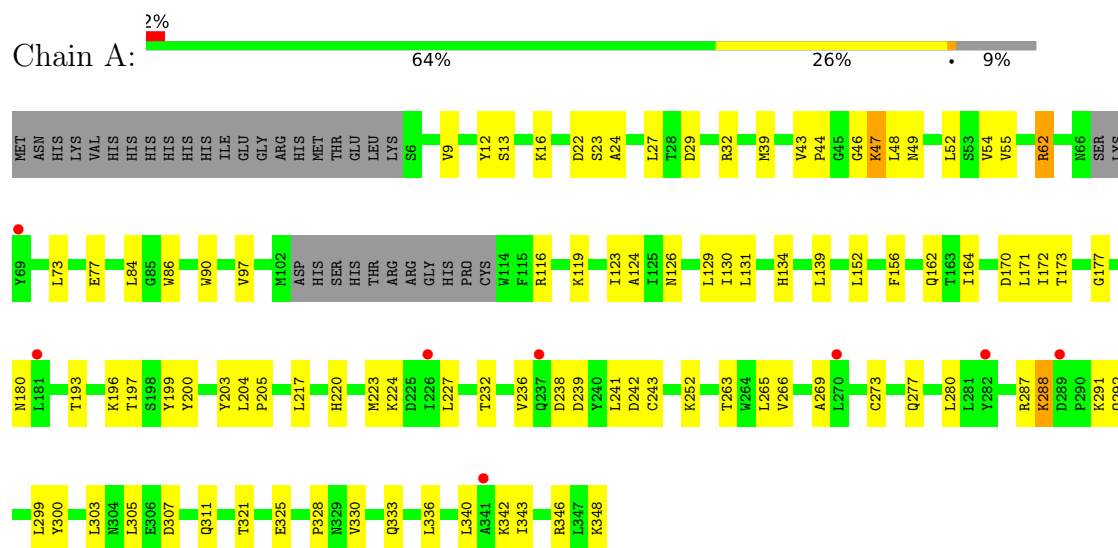
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Chain	Residue	Modelled	Actual	Comment	Reference
G	-12	LYS	-	expression tag	UNP A0A1L3KPU1
G	-11	VAL	-	expression tag	UNP A0A1L3KPU1
G	-10	HIS	-	expression tag	UNP A0A1L3KPU1
G	-9	HIS	-	expression tag	UNP A0A1L3KPU1
G	-8	HIS	-	expression tag	UNP A0A1L3KPU1
G	-7	HIS	-	expression tag	UNP A0A1L3KPU1
G	-6	HIS	-	expression tag	UNP A0A1L3KPU1
G	-5	HIS	-	expression tag	UNP A0A1L3KPU1
G	-4	ILE	-	expression tag	UNP A0A1L3KPU1
G	-3	GLU	-	expression tag	UNP A0A1L3KPU1
G	-2	GLY	-	expression tag	UNP A0A1L3KPU1
G	-1	ARG	-	expression tag	UNP A0A1L3KPU1
G	0	HIS	-	expression tag	UNP A0A1L3KPU1

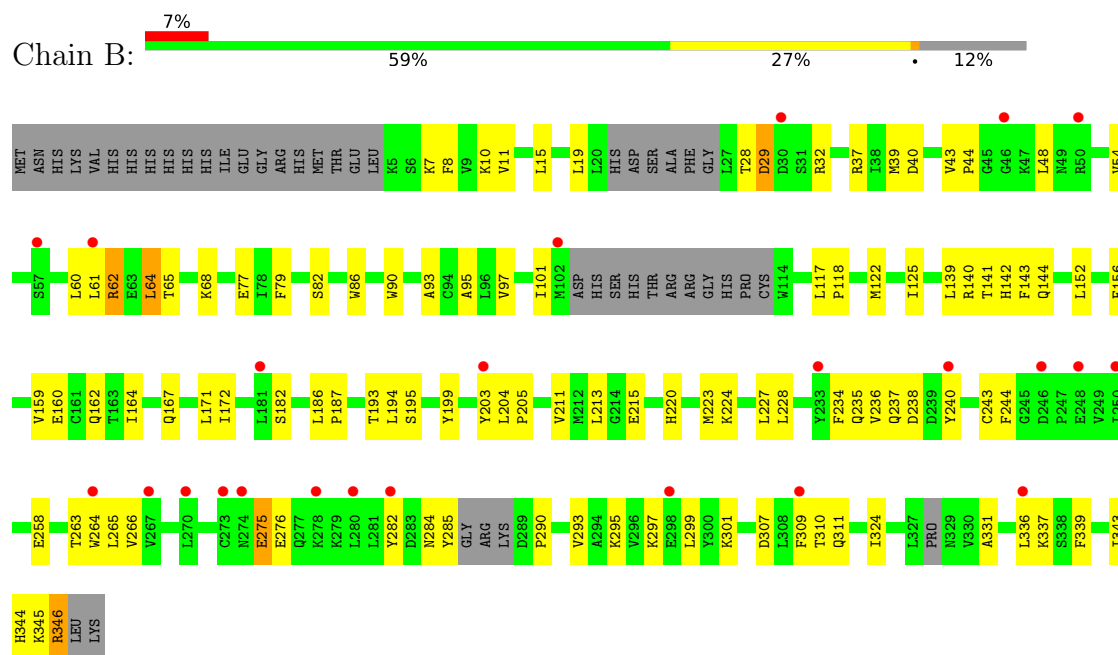
3 Residue-property plots [i](#)

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: FPS3

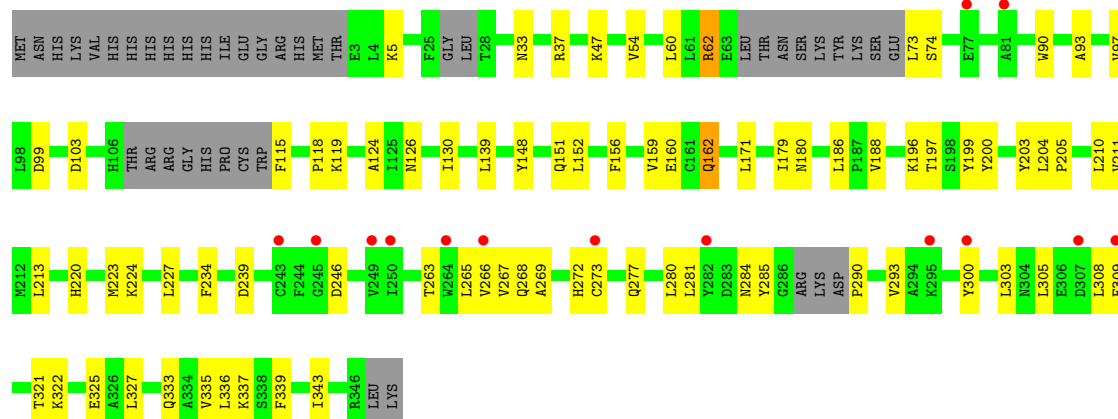


• Molecule 1: FPS3



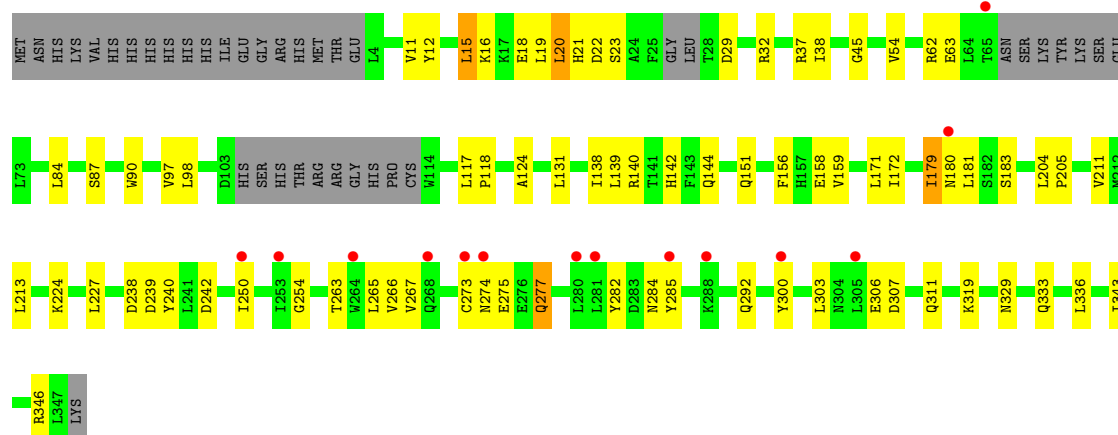
• Molecule 1: FPS3

Chain C: 



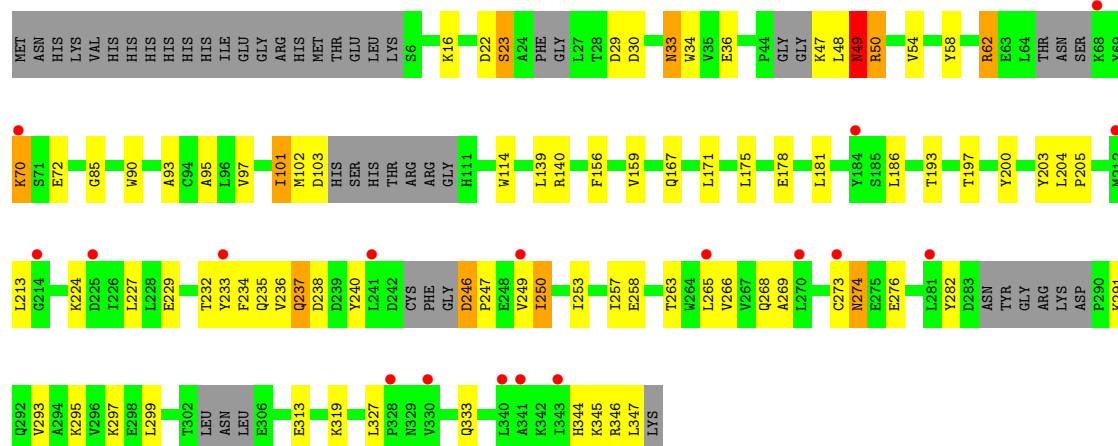
• Molecule 1: FPS3

Chain D: 

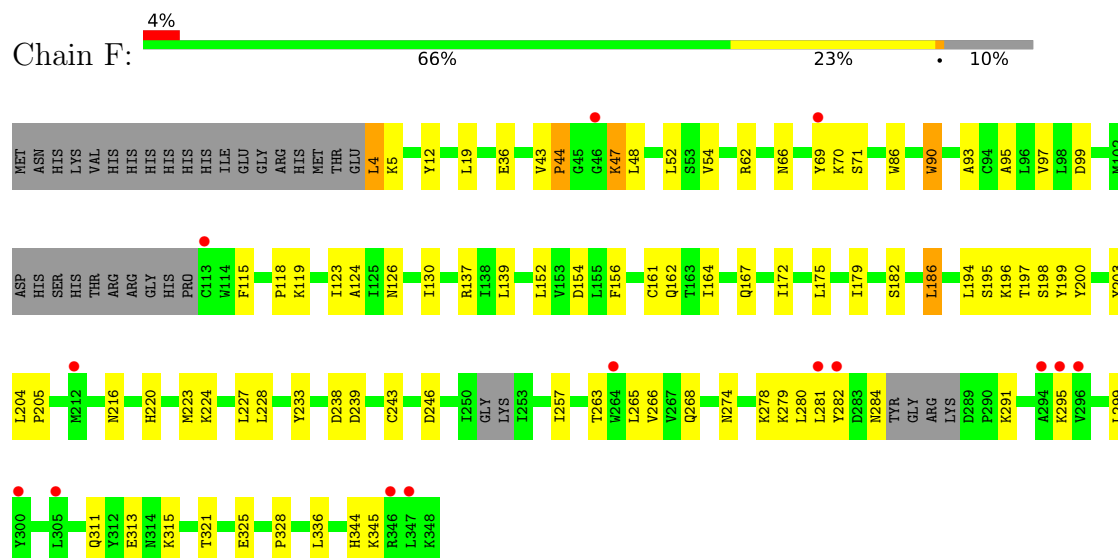


• Molecule 1: FPS3

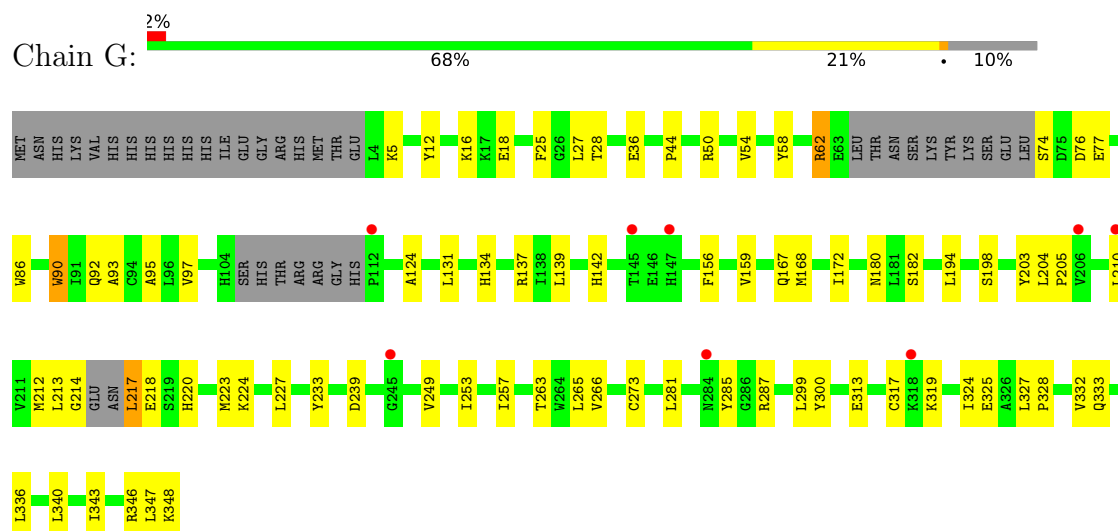
Chain E: 



- Molecule 1: FPS3



- Molecule 1: FPS3



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	234.39Å 131.06Å 103.92Å 90.00° 111.98° 90.00°	Depositor
Resolution (Å)	48.19 – 3.30 48.19 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.19-3.30) 99.9 (48.19-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.282 , 0.304 0.282 , 0.304	Depositor DCC
R_{free} test set	2193 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	116.1	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 71.9	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	0.91	EDS
Total number of atoms	18385	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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	0.27	0/2725	0.45	0/3684
1	B	0.29	0/2651	0.49	0/3582
1	C	0.27	0/2651	0.46	0/3582
1	D	0.26	0/2682	0.44	0/3627
1	E	0.27	0/2614	0.47	0/3530
1	F	0.26	0/2712	0.47	0/3666
1	G	0.27	0/2689	0.47	0/3633
All	All	0.27	0/18724	0.46	0/25304

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	2674	0	2690	64	0
1	B	2605	0	2626	79	0
1	C	2603	0	2607	60	0
1	D	2633	0	2651	49	0
1	E	2569	0	2585	61	0
1	F	2663	0	2682	57	0
1	G	2638	0	2657	56	0
All	All	18385	0	18498	410	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 11.

All (410) 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:G:58:TYR:CE1	1:G:213:LEU:HD21	1.79	1.15
1:G:58:TYR:HE1	1:G:213:LEU:HD21	0.89	1.03
1:A:346:ARG:HG2	1:A:348:LYS:H	1.35	0.92
1:G:212:MET:C	1:G:213:LEU:HD23	1.90	0.91
1:F:43:VAL:HB	1:F:44:PRO:HD3	1.54	0.89
1:B:62:ARG:HG2	1:B:62:ARG:HH11	1.37	0.87
1:B:61:LEU:HB3	1:B:213:LEU:HD11	1.59	0.85
1:C:179:ILE:HD11	1:D:179:ILE:HD11	1.63	0.81
1:D:263:THR:HB	1:D:266:VAL:HG23	1.63	0.78
1:B:28:THR:H	1:B:32:ARG:HH21	1.31	0.77
1:G:131:LEU:HA	1:G:134:HIS:HD2	1.50	0.77
1:A:263:THR:HB	1:A:266:VAL:HG23	1.66	0.76
1:G:58:TYR:HE1	1:G:213:LEU:CD2	1.85	0.75
1:D:263:THR:HG22	1:D:265:LEU:H	1.50	0.75
1:A:263:THR:HG22	1:A:265:LEU:H	1.52	0.75
1:G:217:LEU:HD12	1:G:217:LEU:N	2.02	0.75
1:G:213:LEU:HD23	1:G:213:LEU:N	2.01	0.73
1:F:263:THR:HG22	1:F:265:LEU:H	1.51	0.73
1:B:8:PHE:CE1	1:B:82:SER:HB3	2.24	0.73
1:D:239:ASP:HB3	1:D:263:THR:HG23	1.72	0.72
1:B:48:LEU:HD13	1:B:86:TRP:CZ2	2.25	0.72
1:F:280:LEU:O	1:F:284:ASN:ND2	2.23	0.71
1:C:227:LEU:HD21	1:C:336:LEU:HD22	1.71	0.71
1:G:263:THR:HB	1:G:266:VAL:HG23	1.71	0.70
1:G:95:ALA:HA	1:G:167:GLN:HE21	1.57	0.70
1:F:62:ARG:NH1	1:F:70:LYS:O	2.24	0.69
1:B:8:PHE:HE1	1:B:82:SER:HB3	1.56	0.69
1:B:263:THR:HG22	1:B:265:LEU:H	1.56	0.69
1:G:263:THR:HG22	1:G:265:LEU:H	1.56	0.69
1:G:266:VAL:HG21	1:G:285:TYR:OH	1.92	0.69
1:F:263:THR:HB	1:F:266:VAL:HG23	1.75	0.68
1:E:139:LEU:HD11	1:E:156:PHE:CD2	2.28	0.68
1:C:280:LEU:O	1:C:284:ASN:ND2	2.22	0.68
1:C:263:THR:HB	1:C:266:VAL:HG23	1.75	0.68
1:E:263:THR:HG22	1:E:265:LEU:H	1.59	0.68
1:B:290:PRO:HA	1:B:293:VAL:HB	1.73	0.68
1:E:257:ILE:HD13	1:E:297:LYS:HE2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:131:LEU:HA	1:G:134:HIS:CD2	2.29	0.67
1:C:99:ASP:OD1	1:C:196:LYS:NZ	2.25	0.67
1:F:139:LEU:HD11	1:F:156:PHE:CD2	2.30	0.67
1:G:18:GLU:OE1	1:G:142:HIS:NE2	2.27	0.67
1:E:95:ALA:HA	1:E:167:GLN:HE21	1.61	0.66
1:D:284:ASN:HB2	1:D:292:GLN:HB3	1.77	0.66
1:A:12:TYR:HB3	1:A:86:TRP:CZ2	2.30	0.66
1:B:8:PHE:CZ	1:B:10:LYS:HB2	2.30	0.66
1:B:263:THR:HB	1:B:266:VAL:HG23	1.77	0.65
1:E:16:LYS:HD2	1:E:36:GLU:HG3	1.78	0.65
1:F:99:ASP:OD1	1:F:196:LYS:NZ	2.24	0.65
1:A:139:LEU:HD11	1:A:156:PHE:CD2	2.32	0.64
1:D:158:GLU:OE2	1:D:224:LYS:NZ	2.26	0.64
1:F:95:ALA:HA	1:F:167:GLN:HE21	1.61	0.64
1:E:327:LEU:O	1:E:333:GLN:NE2	2.31	0.64
1:B:62:ARG:HG2	1:B:62:ARG:NH1	2.10	0.64
1:B:95:ALA:HA	1:B:167:GLN:HE21	1.63	0.64
1:D:139:LEU:HD11	1:D:156:PHE:HD2	1.63	0.64
1:D:343:ILE:O	1:D:346:ARG:HG2	1.98	0.64
1:G:139:LEU:HD11	1:G:156:PHE:CD2	2.33	0.64
1:E:29:ASP:O	1:E:33:ASN:ND2	2.30	0.63
1:G:223:MET:HG3	1:G:336:LEU:HD11	1.80	0.63
1:A:131:LEU:HA	1:A:134:HIS:HD2	1.63	0.63
1:D:139:LEU:HD11	1:D:156:PHE:CD2	2.34	0.63
1:A:287:ARG:CB	1:A:292:GLN:OE1	2.46	0.63
1:B:10:LYS:HD3	1:B:79:PHE:HD1	1.63	0.63
1:F:239:ASP:HB3	1:F:263:THR:HG23	1.80	0.63
1:G:156:PHE:HE1	1:G:204:LEU:HD11	1.62	0.63
1:E:269:ALA:O	1:E:273:CYS:N	2.33	0.62
1:C:139:LEU:HD11	1:C:156:PHE:CD2	2.35	0.62
1:C:327:LEU:O	1:C:333:GLN:NE2	2.32	0.62
1:B:223:MET:HG3	1:B:336:LEU:HD11	1.81	0.62
1:G:239:ASP:HB3	1:G:263:THR:HG23	1.80	0.62
1:C:277:GLN:HA	1:C:280:LEU:HD12	1.82	0.62
1:G:227:LEU:HD21	1:G:336:LEU:HD22	1.81	0.61
1:B:139:LEU:HD22	1:B:152:LEU:HD23	1.82	0.61
1:B:28:THR:O	1:B:29:ASP:C	2.38	0.61
1:E:247:PRO:HB3	1:E:253:ILE:HA	1.80	0.61
1:G:62:ARG:NH2	1:G:77:GLU:OE1	2.33	0.61
1:F:220:HIS:HB3	1:F:223:MET:HE2	1.81	0.61
1:B:43:VAL:HB	1:B:44:PRO:HD3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:ARG:HE	1:F:123:ILE:HD12	1.65	0.61
1:A:39:MET:O	1:A:43:VAL:HG23	2.00	0.60
1:D:156:PHE:HE1	1:D:204:LEU:HD11	1.66	0.60
1:B:139:LEU:HD11	1:B:156:PHE:CD2	2.36	0.60
1:A:49:ASN:N	1:A:49:ASN:OD1	2.30	0.60
1:D:156:PHE:CE1	1:D:204:LEU:HD11	2.37	0.60
1:G:95:ALA:HA	1:G:167:GLN:NE2	2.17	0.60
1:B:95:ALA:HA	1:B:167:GLN:NE2	2.15	0.59
1:F:156:PHE:CE1	1:F:204:LEU:HD11	2.37	0.59
1:C:339:PHE:O	1:C:343:ILE:HG12	2.02	0.59
1:A:342:LYS:O	1:A:346:ARG:NH2	2.35	0.59
1:B:60:LEU:O	1:B:64:LEU:HD22	2.02	0.59
1:E:156:PHE:HE1	1:E:204:LEU:HD11	1.68	0.59
1:C:139:LEU:HD11	1:C:156:PHE:HD2	1.67	0.59
1:A:156:PHE:CE1	1:A:204:LEU:HD11	2.38	0.58
1:G:54:VAL:HG22	1:G:205:PRO:HA	1.85	0.58
1:B:258:GLU:HG2	1:B:293:VAL:HG21	1.86	0.58
1:F:156:PHE:HE1	1:F:204:LEU:HD11	1.69	0.58
1:C:62:ARG:CG	1:C:62:ARG:HH11	2.17	0.58
1:D:11:VAL:O	1:D:15:LEU:HG	2.04	0.58
1:G:156:PHE:CE1	1:G:204:LEU:HD11	2.38	0.57
1:B:159:VAL:HG13	1:B:199:TYR:HB3	1.86	0.57
1:A:43:VAL:HB	1:A:44:PRO:HD3	1.86	0.57
1:A:62:ARG:NH2	1:A:77:GLU:OE1	2.36	0.57
1:B:62:ARG:HH11	1:B:62:ARG:CG	2.14	0.57
1:B:10:LYS:HD3	1:B:79:PHE:CD1	2.39	0.57
1:B:156:PHE:CE1	1:B:204:LEU:HD11	2.39	0.57
1:D:12:TYR:HA	1:D:15:LEU:HD11	1.86	0.57
1:C:265:LEU:HG	1:C:309:PHE:HZ	1.70	0.57
1:G:233:TYR:HE1	1:G:313:GLU:HG3	1.70	0.57
1:D:266:VAL:HG21	1:D:285:TYR:OH	2.05	0.57
1:E:101:ILE:HG12	1:E:101:ILE:O	2.04	0.57
1:E:181:LEU:HD12	1:E:282:TYR:HA	1.86	0.57
1:A:54:VAL:HG22	1:A:205:PRO:HA	1.86	0.57
1:G:203:TYR:CE1	1:G:224:LYS:HG2	2.40	0.57
1:C:54:VAL:HG22	1:C:205:PRO:HA	1.87	0.56
1:B:54:VAL:HG22	1:B:205:PRO:HA	1.86	0.56
1:C:188:VAL:HG21	1:D:118:PRO:HB2	1.87	0.56
1:G:97:VAL:HG12	1:G:124:ALA:HB1	1.88	0.56
1:B:227:LEU:HD21	1:B:336:LEU:HD22	1.86	0.56
1:B:156:PHE:HE1	1:B:204:LEU:HD11	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:156:PHE:CE1	1:E:204:LEU:HD11	2.40	0.56
1:F:95:ALA:HA	1:F:167:GLN:NE2	2.19	0.56
1:A:220:HIS:HB3	1:A:223:MET:HE2	1.88	0.56
1:D:277:GLN:NE2	1:D:303:LEU:HD21	2.21	0.56
1:E:193:THR:HG22	1:E:235:GLN:HG2	1.88	0.56
1:C:156:PHE:CE1	1:C:204:LEU:HD11	2.41	0.56
1:E:229:GLU:OE1	1:E:319:LYS:NZ	2.39	0.56
1:F:344:HIS:CE1	1:F:345:LYS:HG3	2.41	0.56
1:G:233:TYR:CE1	1:G:313:GLU:HG3	2.41	0.56
1:F:203:TYR:CE1	1:F:224:LYS:HG2	2.41	0.55
1:F:48:LEU:O	1:F:52:LEU:HD12	2.07	0.55
1:A:9:VAL:HG12	1:A:86:TRP:HE1	1.71	0.55
1:C:239:ASP:HB3	1:C:263:THR:HG23	1.89	0.55
1:D:54:VAL:HG22	1:D:205:PRO:HA	1.88	0.55
1:A:303:LEU:HB2	1:A:305:LEU:HG	1.88	0.55
1:F:119:LYS:H	1:F:119:LYS:HD2	1.71	0.55
1:A:330:VAL:HG13	1:A:333:GLN:NE2	2.22	0.54
1:C:263:THR:HG22	1:C:265:LEU:H	1.72	0.54
1:E:236:VAL:C	1:E:238:ASP:H	2.11	0.54
1:B:8:PHE:CD2	1:B:11:VAL:HG23	2.42	0.54
1:F:4:LEU:HD22	1:F:5:LYS:H	1.73	0.54
1:A:171:LEU:HD21	1:B:172:ILE:HD11	1.90	0.54
1:E:258:GLU:HG2	1:E:293:VAL:HG11	1.89	0.54
1:C:159:VAL:HG13	1:C:199:TYR:HB3	1.89	0.54
1:F:182:SER:HB3	1:F:282:TYR:OH	2.07	0.54
1:A:340:LEU:HD12	1:A:343:ILE:HD11	1.90	0.54
1:C:115:PHE:HD1	1:D:180:ASN:HD22	1.54	0.54
1:A:197:THR:HA	1:A:200:TYR:CE2	2.43	0.54
1:F:186:LEU:HD21	1:F:268:GLN:NE2	2.22	0.54
1:C:268:GLN:HG3	1:C:272:HIS:CD2	2.43	0.54
1:A:156:PHE:HE1	1:A:204:LEU:HD11	1.72	0.53
1:A:164:ILE:HG21	1:B:164:ILE:HD13	1.91	0.53
1:B:64:LEU:HD23	1:B:331:ALA:HB1	1.90	0.53
1:F:233:TYR:CE1	1:F:313:GLU:HG3	2.43	0.53
1:E:344:HIS:ND1	1:E:345:LYS:HG3	2.23	0.53
1:C:118:PRO:HG3	1:D:183:SER:HB3	1.91	0.53
1:E:114:TRP:HZ2	1:E:178:GLU:HG2	1.72	0.52
1:B:339:PHE:O	1:B:343:ILE:HG12	2.09	0.52
1:G:281:LEU:O	1:G:285:TYR:HB2	2.09	0.52
1:B:8:PHE:CE2	1:B:11:VAL:HG23	2.45	0.52
1:C:62:ARG:HG3	1:C:62:ARG:NH1	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:LEU:HD22	1:B:39:MET:SD	2.49	0.52
1:F:97:VAL:HG12	1:F:124:ALA:HB1	1.91	0.52
1:F:197:THR:HA	1:F:200:TYR:CE2	2.44	0.52
1:E:274:ASN:OD1	1:E:274:ASN:N	2.43	0.52
1:A:203:TYR:CE1	1:A:224:LYS:HG2	2.45	0.52
1:B:141:THR:HB	1:B:142:HIS:HD1	1.73	0.52
1:C:268:GLN:HG3	1:C:272:HIS:HD2	1.74	0.52
1:E:114:TRP:CZ2	1:E:178:GLU:HG2	2.44	0.52
1:F:139:LEU:HD11	1:F:156:PHE:HD2	1.71	0.52
1:B:203:TYR:CZ	1:B:224:LYS:HE2	2.45	0.52
1:E:295:LYS:O	1:E:299:LEU:HG	2.09	0.52
1:E:203:TYR:CE1	1:E:224:LYS:HG2	2.44	0.52
1:C:33:ASN:O	1:C:37:ARG:HG3	2.10	0.51
1:C:156:PHE:O	1:C:160:GLU:HB2	2.10	0.51
1:D:181:LEU:HB3	1:D:282:TYR:CE1	2.45	0.51
1:F:126:ASN:O	1:F:130:ILE:HG12	2.10	0.51
1:A:277:GLN:HA	1:A:280:LEU:HD12	1.92	0.51
1:B:193:THR:HG22	1:B:235:GLN:HG2	1.93	0.51
1:E:159:VAL:HG21	1:E:204:LEU:HD13	1.92	0.50
1:E:22:ASP:OD1	1:E:23:SER:N	2.44	0.50
1:A:139:LEU:HD11	1:A:156:PHE:HD2	1.73	0.50
1:C:148:TYR:HD2	1:C:152:LEU:HD13	1.76	0.50
1:C:269:ALA:O	1:C:273:CYS:N	2.43	0.50
1:A:280:LEU:HD13	1:A:299:LEU:HD21	1.93	0.50
1:D:16:LYS:O	1:D:20:LEU:HG	2.11	0.50
1:B:220:HIS:HB3	1:B:223:MET:HE2	1.93	0.50
1:A:16:LYS:HG2	1:A:39:MET:HE1	1.93	0.50
1:A:170:ASP:OD2	1:A:196:LYS:NZ	2.30	0.50
1:E:140:ARG:NH2	1:F:154:ASP:OD1	2.44	0.50
1:C:156:PHE:HE1	1:C:204:LEU:HD11	1.74	0.50
1:C:305:LEU:HD23	1:C:308:LEU:HD12	1.94	0.50
1:D:20:LEU:HD13	1:D:32:ARG:HG3	1.94	0.50
1:F:161:CYS:O	1:F:164:ILE:HG13	2.12	0.50
1:G:340:LEU:HA	1:G:343:ILE:HG12	1.94	0.50
1:A:239:ASP:HB3	1:A:263:THR:HG23	1.94	0.49
1:E:263:THR:HB	1:E:266:VAL:HG23	1.94	0.49
1:F:19:LEU:O	1:F:137:ARG:NH2	2.44	0.49
1:E:234:PHE:O	1:E:237:GLN:HB2	2.13	0.49
1:A:266:VAL:HG22	1:A:300:TYR:OH	2.12	0.49
1:C:97:VAL:HG12	1:C:124:ALA:HB1	1.93	0.49
1:F:321:THR:O	1:F:325:GLU:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:THR:O	1:A:177:GLY:N	2.45	0.49
1:B:152:LEU:HD12	1:B:211:VAL:HG11	1.95	0.49
1:B:344:HIS:CD2	1:B:345:LYS:HG3	2.48	0.49
1:A:280:LEU:HB3	1:A:299:LEU:HD11	1.95	0.49
1:B:237:GLN:HE21	1:B:346:ARG:HG2	1.78	0.49
1:B:237:GLN:NE2	1:B:346:ARG:HG2	2.27	0.49
1:B:307:ASP:O	1:B:311:GLN:HG3	2.12	0.49
1:G:93:ALA:O	1:G:97:VAL:HG23	2.13	0.49
1:B:240:TYR:HB2	1:B:309:PHE:CE1	2.48	0.49
1:D:117:LEU:N	1:D:118:PRO:HD2	2.28	0.49
1:A:287:ARG:HB3	1:A:292:GLN:OE1	2.12	0.48
1:B:194:LEU:HD11	1:B:228:LEU:HD13	1.94	0.48
1:C:62:ARG:CG	1:C:62:ARG:NH1	2.75	0.48
1:E:346:ARG:HG2	1:E:347:LEU:H	1.77	0.48
1:F:43:VAL:CB	1:F:44:PRO:HD3	2.29	0.48
1:A:193:THR:O	1:A:197:THR:OG1	2.29	0.48
1:B:140:ARG:O	1:B:144:GLN:HB2	2.13	0.48
1:B:62:ARG:CG	1:B:62:ARG:NH1	2.73	0.48
1:B:7:LYS:O	1:B:7:LYS:HG3	2.13	0.48
1:C:151:GLN:NE2	1:C:211:VAL:HG13	2.27	0.48
1:E:246:ASP:HB3	1:E:249:VAL:HB	1.95	0.48
1:C:119:LYS:NZ	1:F:36:GLU:OE2	2.47	0.48
1:A:203:TYR:OH	1:A:217:LEU:HD13	2.14	0.48
1:B:182:SER:HB3	1:B:282:TYR:OH	2.13	0.48
1:E:95:ALA:HA	1:E:167:GLN:NE2	2.28	0.48
1:F:47:LYS:HA	1:F:47:LYS:HD2	1.47	0.48
1:D:140:ARG:O	1:D:144:GLN:HB2	2.14	0.48
1:A:227:LEU:HD21	1:A:336:LEU:HD22	1.96	0.48
1:C:162:GLN:HG2	1:C:199:TYR:CE1	2.49	0.48
1:D:151:GLN:NE2	1:D:211:VAL:HG13	2.29	0.48
1:A:97:VAL:HG12	1:A:124:ALA:HB1	1.96	0.48
1:F:257:ILE:H	1:F:257:ILE:HD12	1.79	0.48
1:D:97:VAL:HG12	1:D:124:ALA:HB1	1.96	0.47
1:D:38:ILE:HG22	1:D:131:LEU:HD21	1.95	0.47
1:D:29:ASP:OD1	1:D:32:ARG:NH1	2.36	0.47
1:G:50:ARG:NH1	1:G:92:GLN:OE1	2.47	0.47
1:A:269:ALA:O	1:A:273:CYS:N	2.46	0.47
1:A:203:TYR:OH	1:A:224:LYS:HE2	2.15	0.47
1:A:241:LEU:C	1:A:243:CYS:H	2.18	0.47
1:C:73:LEU:HB3	1:C:74:SER:H	1.57	0.47
1:E:203:TYR:HA	1:E:227:LEU:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:25:PHE:CZ	1:G:137:ARG:HD2	2.50	0.47
1:A:172:ILE:CG1	1:B:171:LEU:HD21	2.45	0.47
1:E:175:LEU:HD12	1:F:175:LEU:HD12	1.97	0.47
1:C:171:LEU:HD21	1:D:172:ILE:HD11	1.97	0.47
1:D:62:ARG:O	1:D:63:GLU:HG3	2.14	0.47
1:E:30:ASP:HA	1:E:33:ASN:ND2	2.30	0.47
1:F:281:LEU:HD13	1:F:299:LEU:HD23	1.96	0.47
1:G:249:VAL:O	1:G:348:LYS:HD3	2.15	0.47
1:C:321:THR:HG23	1:C:337:LYS:NZ	2.30	0.47
1:D:227:LEU:HD21	1:D:336:LEU:HD22	1.97	0.47
1:G:317:CYS:SG	1:G:340:LEU:HD21	2.55	0.47
1:G:324:ILE:HG22	1:G:333:GLN:HG3	1.97	0.46
1:A:16:LYS:HZ1	1:A:44:PRO:HG3	1.80	0.46
1:B:64:LEU:HD23	1:B:331:ALA:CB	2.45	0.46
1:B:62:ARG:NH1	1:B:77:GLU:OE2	2.46	0.46
1:D:242:ASP:O	1:D:254:GLY:HA3	2.15	0.46
1:E:47:LYS:O	1:E:48:LEU:HD23	2.16	0.46
1:F:12:TYR:HB2	1:F:86:TRP:CE2	2.50	0.46
1:C:162:GLN:HG2	1:C:199:TYR:CD1	2.50	0.46
1:E:232:THR:O	1:E:236:VAL:HG23	2.15	0.46
1:G:266:VAL:HG22	1:G:300:TYR:OH	2.16	0.46
1:G:12:TYR:HB2	1:G:86:TRP:CE2	2.50	0.46
1:D:19:LEU:HD11	1:D:138:ILE:HD11	1.98	0.46
1:F:274:ASN:O	1:F:278:LYS:N	2.44	0.46
1:E:139:LEU:HD11	1:E:156:PHE:HD2	1.79	0.46
1:E:235:GLN:O	1:E:238:ASP:HB2	2.15	0.46
1:G:12:TYR:HB2	1:G:86:TRP:CZ2	2.51	0.46
1:A:139:LEU:HD21	1:A:156:PHE:CE2	2.50	0.46
1:F:62:ARG:HG3	1:F:71:SER:O	2.15	0.46
1:A:62:ARG:NH1	1:A:62:ARG:HG3	2.31	0.46
1:D:18:GLU:OE1	1:D:142:HIS:NE2	2.45	0.46
1:F:291:LYS:O	1:F:295:LYS:HG3	2.16	0.46
1:A:62:ARG:HH21	1:A:73:LEU:HA	1.81	0.46
1:E:171:LEU:HD21	1:F:172:ILE:HD11	1.96	0.46
1:A:273:CYS:SG	1:A:303:LEU:HD11	2.57	0.45
1:C:203:TYR:CE1	1:C:224:LYS:HG2	2.51	0.45
1:C:37:ARG:NE	1:F:123:ILE:HG23	2.31	0.45
1:E:257:ILE:HD12	1:E:257:ILE:H	1.81	0.45
1:G:159:VAL:HG21	1:G:204:LEU:HD13	1.98	0.45
1:E:233:TYR:CE1	1:E:313:GLU:HG3	2.51	0.45
1:G:257:ILE:HD12	1:G:257:ILE:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:LEU:HD13	1:B:86:TRP:HZ2	1.74	0.45
1:C:266:VAL:HG21	1:C:285:TYR:OH	2.16	0.45
1:C:126:ASN:O	1:C:130:ILE:HG13	2.16	0.45
1:A:12:TYR:CG	1:A:13:SER:N	2.85	0.45
1:B:243:CYS:SG	1:B:297:LYS:HE2	2.56	0.45
1:E:240:TYR:OH	1:E:347:LEU:HD23	2.17	0.45
1:F:12:TYR:HB2	1:F:86:TRP:CZ2	2.52	0.45
1:G:168:MET:O	1:G:172:ILE:HG13	2.15	0.45
1:G:325:GLU:HA	1:G:333:GLN:NE2	2.32	0.45
1:C:210:LEU:HD11	1:C:223:MET:HE2	1.99	0.45
1:B:122:MET:O	1:B:125:ILE:HG13	2.17	0.45
1:C:197:THR:HA	1:C:200:TYR:CE2	2.52	0.45
1:F:162:GLN:O	1:F:195:SER:HB2	2.16	0.45
1:A:52:LEU:O	1:A:55:VAL:N	2.50	0.45
1:E:50:ARG:CD	1:E:50:ARG:N	2.80	0.45
1:E:58:TYR:O	1:E:62:ARG:HB2	2.17	0.45
1:A:162:GLN:HG2	1:A:199:TYR:CD1	2.52	0.44
1:C:234:PHE:CE1	1:C:343:ILE:HD12	2.52	0.44
1:A:84:LEU:HD21	1:A:152:LEU:HD21	1.98	0.44
1:B:28:THR:O	1:B:29:ASP:O	2.35	0.44
1:G:16:LYS:HE3	1:G:36:GLU:HG3	1.99	0.44
1:A:29:ASP:OD1	1:A:32:ARG:NH1	2.49	0.44
1:F:203:TYR:HA	1:F:227:LEU:HD13	1.99	0.44
1:A:287:ARG:HB2	1:A:292:GLN:OE1	2.18	0.44
1:B:117:LEU:N	1:B:118:PRO:HD2	2.33	0.44
1:D:240:TYR:OH	1:D:306:GLU:OE2	2.35	0.44
1:E:236:VAL:C	1:E:238:ASP:N	2.71	0.44
1:E:276:GLU:O	1:E:276:GLU:HG2	2.18	0.44
1:B:162:GLN:O	1:B:195:SER:HB3	2.17	0.44
1:C:93:ALA:O	1:C:97:VAL:HG23	2.17	0.44
1:F:54:VAL:HG22	1:F:205:PRO:HA	2.00	0.44
1:G:327:LEU:HD13	1:G:332:VAL:HG12	1.99	0.44
1:G:5:LYS:HD2	1:G:5:LYS:N	2.32	0.44
1:E:197:THR:HA	1:E:200:TYR:CE2	2.53	0.44
1:A:116:ARG:HH22	1:D:45:GLY:HA2	1.82	0.44
1:A:126:ASN:O	1:A:130:ILE:HG13	2.18	0.44
1:A:16:LYS:NZ	1:A:44:PRO:HG3	2.33	0.44
1:C:152:LEU:HD12	1:C:211:VAL:HG11	2.00	0.44
1:A:288:LYS:HA	1:A:288:LYS:HD3	1.70	0.43
1:B:324:ILE:HG21	1:B:337:LYS:HG3	2.00	0.43
1:D:159:VAL:HG21	1:D:204:LEU:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:152:LEU:HD23	1:F:152:LEU:HA	1.90	0.43
1:C:148:TYR:CB	1:C:151:GLN:HE21	2.31	0.43
1:D:12:TYR:HA	1:D:15:LEU:CD1	2.47	0.43
1:G:210:LEU:HD21	1:G:220:HIS:ND1	2.33	0.43
1:D:22:ASP:HB3	1:D:23:SER:H	1.54	0.43
1:E:49:ASN:OD1	1:E:50:ARG:HD3	2.17	0.43
1:B:295:LYS:O	1:B:299:LEU:HG	2.19	0.43
1:F:198:SER:OG	1:F:228:LEU:O	2.32	0.43
1:E:54:VAL:HG22	1:E:205:PRO:HA	2.01	0.43
1:B:236:VAL:HG13	1:B:264:TRP:CG	2.54	0.43
1:E:240:TYR:OH	1:E:347:LEU:HA	2.18	0.43
1:E:93:ALA:O	1:E:97:VAL:HG23	2.19	0.43
1:G:210:LEU:HD21	1:G:220:HIS:CG	2.53	0.43
1:C:220:HIS:O	1:C:224:LYS:HG3	2.19	0.43
1:D:266:VAL:HG22	1:D:300:TYR:OH	2.19	0.43
1:A:119:LYS:O	1:A:123:ILE:HG13	2.19	0.42
1:B:93:ALA:O	1:B:97:VAL:HG23	2.17	0.42
1:E:54:VAL:HG21	1:E:85:GLY:HA2	1.99	0.42
1:F:233:TYR:OH	1:F:313:GLU:OE2	2.31	0.42
1:F:93:ALA:O	1:F:97:VAL:HG23	2.19	0.42
1:D:84:LEU:O	1:D:87:SER:OG	2.27	0.42
1:G:213:LEU:O	1:G:214:GLY:C	2.56	0.42
1:B:284:ASN:HB3	1:B:285:TYR:H	1.61	0.42
1:C:281:LEU:HD12	1:C:281:LEU:HA	1.92	0.42
1:C:60:LEU:HD22	1:C:335:VAL:HG23	2.01	0.42
1:B:234:PHE:HE1	1:B:343:ILE:HD12	1.84	0.42
1:D:29:ASP:HA	1:D:32:ARG:NH1	2.33	0.42
1:A:252:LYS:HA	1:A:252:LYS:HD2	1.90	0.42
1:G:227:LEU:HD23	1:G:227:LEU:HA	1.88	0.42
1:C:62:ARG:HG2	1:C:62:ARG:O	2.19	0.42
1:E:346:ARG:HG2	1:E:347:LEU:N	2.34	0.42
1:G:273:CYS:SG	1:G:299:LEU:HD11	2.60	0.42
1:A:46:GLY:O	1:A:48:LEU:N	2.53	0.42
1:E:186:LEU:HD21	1:E:268:GLN:NE2	2.35	0.42
1:G:249:VAL:HG11	1:G:347:LEU:HB2	2.02	0.42
1:G:76:ASP:OD1	1:G:77:GLU:N	2.52	0.42
1:A:232:THR:O	1:A:236:VAL:HG23	2.20	0.42
1:B:234:PHE:CZ	1:B:346:ARG:NH2	2.87	0.42
1:D:343:ILE:HA	1:D:346:ARG:HD3	2.02	0.42
1:G:203:TYR:OH	1:G:224:LYS:HE2	2.20	0.42
1:F:86:TRP:O	1:F:90:TRP:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:GLU:HB3	1:B:276:GLU:H	1.57	0.41
1:C:171:LEU:HA	1:C:171:LEU:HD12	1.88	0.41
1:C:290:PRO:HA	1:C:293:VAL:HB	2.00	0.41
1:D:319:LYS:HB3	1:D:319:LYS:HE2	1.77	0.41
1:E:240:TYR:CE2	1:E:250:ILE:HD12	2.56	0.41
1:F:279:LYS:HD3	1:F:279:LYS:HA	1.76	0.41
1:B:19:LEU:HB3	1:B:32:ARG:HD3	2.03	0.41
1:B:40:ASP:HA	1:B:44:PRO:HD2	2.02	0.41
1:C:273:CYS:SG	1:C:303:LEU:HD11	2.60	0.41
1:B:139:LEU:O	1:B:143:PHE:N	2.53	0.41
1:C:5:LYS:HB3	1:C:5:LYS:HE2	1.84	0.41
1:G:194:LEU:O	1:G:198:SER:OG	2.30	0.41
1:B:215:GLU:OE1	1:B:220:HIS:NE2	2.54	0.41
1:B:37:ARG:HD2	1:B:37:ARG:HA	1.62	0.41
1:F:311:GLN:O	1:F:315:LYS:HG3	2.21	0.41
1:A:307:ASP:O	1:A:311:GLN:HG3	2.21	0.41
1:F:194:LEU:O	1:F:199:TYR:HD1	2.03	0.41
1:C:186:LEU:HG	1:C:267:VAL:HG12	2.03	0.41
1:C:266:VAL:HG22	1:C:300:TYR:OH	2.21	0.41
1:F:115:PHE:O	1:F:118:PRO:HD2	2.20	0.41
1:A:321:THR:O	1:A:325:GLU:HG3	2.20	0.41
1:B:227:LEU:HA	1:B:227:LEU:HD23	1.87	0.41
1:B:64:LEU:HA	1:B:64:LEU:HD12	1.87	0.41
1:G:217:LEU:N	1:G:217:LEU:CD1	2.73	0.41
1:A:129:LEU:HD11	1:B:162:GLN:OE1	2.21	0.41
1:B:344:HIS:NE2	1:B:345:LYS:HG3	2.36	0.41
1:D:98:LEU:HD13	1:D:171:LEU:HD11	2.02	0.41
1:B:156:PHE:O	1:B:160:GLU:HB2	2.20	0.41
1:B:244:PHE:CE1	1:B:301:LYS:HE3	2.56	0.41
1:D:12:TYR:O	1:D:15:LEU:HD12	2.21	0.41
1:D:263:THR:O	1:D:267:VAL:HG23	2.21	0.41
1:D:266:VAL:HG11	1:D:285:TYR:CZ	2.56	0.41
1:G:74:SER:HB3	1:G:77:GLU:HB2	2.02	0.41
1:B:186:LEU:N	1:B:187:PRO:HD2	2.36	0.40
1:G:86:TRP:O	1:G:90:TRP:HE3	2.05	0.40
1:E:291:LYS:O	1:E:295:LYS:HG3	2.21	0.40
1:E:30:ASP:HA	1:E:33:ASN:HD21	1.85	0.40
1:C:322:LYS:O	1:C:325:GLU:HG2	2.21	0.40
1:D:307:ASP:O	1:D:311:GLN:HG3	2.22	0.40
1:E:50:ARG:HD2	1:E:50:ARG:HA	1.81	0.40
1:E:70:LYS:HD2	1:E:70:LYS:HA	1.58	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:238:ASP:C	1:E:240:TYR:H	2.24	0.40
1:E:62:ARG:HH22	1:E:72:GLU:H	1.70	0.40
1:F:216:ASN:O	1:F:220:HIS:ND1	2.50	0.40
1:F:223:MET:HG3	1:F:336:LEU:HD11	2.02	0.40

There are no symmetry-related clashes.

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	324/364 (89%)	300 (93%)	18 (6%)	6 (2%)	8	34
1	B	311/364 (85%)	291 (94%)	17 (6%)	3 (1%)	15	46
1	C	312/364 (86%)	292 (94%)	17 (5%)	3 (1%)	15	46
1	D	317/364 (87%)	292 (92%)	20 (6%)	5 (2%)	9	36
1	E	300/364 (82%)	273 (91%)	21 (7%)	6 (2%)	7	32
1	F	321/364 (88%)	300 (94%)	17 (5%)	4 (1%)	13	42
1	G	318/364 (87%)	294 (92%)	20 (6%)	4 (1%)	12	40
All	All	2203/2548 (86%)	2042 (93%)	130 (6%)	31 (1%)	11	38

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	29	ASP
1	A	47	LYS
1	A	242	ASP
1	C	47	LYS
1	D	20	LEU
1	D	329	ASN
1	E	49	ASN

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Mol	Chain	Res	Type
1	E	70	LYS
1	E	237	GLN
1	A	24	ALA
1	A	180	ASN
1	C	180	ASN
1	D	274	ASN
1	E	23	SER
1	F	69	TYR
1	G	44	PRO
1	G	253	ILE
1	A	23	SER
1	B	68	LYS
1	B	275	GLU
1	E	274	ASN
1	G	180	ASN
1	C	246	ASP
1	F	328	PRO
1	G	328	PRO
1	A	328	PRO
1	E	250	ILE
1	F	179	ILE
1	D	179	ILE
1	F	44	PRO
1	D	250	ILE

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	300/332 (90%)	292 (97%)	8 (3%)	44	71
1	B	294/332 (89%)	286 (97%)	8 (3%)	44	71
1	C	293/332 (88%)	288 (98%)	5 (2%)	60	78
1	D	296/332 (89%)	286 (97%)	10 (3%)	37	65
1	E	291/332 (88%)	280 (96%)	11 (4%)	33	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	301/332 (91%)	293 (97%)	8 (3%)	44	71
1	G	296/332 (89%)	286 (97%)	10 (3%)	37	65
All	All	2071/2324 (89%)	2011 (97%)	60 (3%)	42	69

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ASP
1	A	27	LEU
1	A	47	LYS
1	A	62	ARG
1	A	90	TRP
1	A	238	ASP
1	A	288	LYS
1	A	291	LYS
1	B	62	ARG
1	B	64	LEU
1	B	65	THR
1	B	90	TRP
1	B	101	ILE
1	B	238	ASP
1	B	310	THR
1	B	346	ARG
1	C	62	ARG
1	C	90	TRP
1	C	103	ASP
1	C	162	GLN
1	C	213	LEU
1	D	15	LEU
1	D	21	HIS
1	D	37	ARG
1	D	90	TRP
1	D	213	LEU
1	D	238	ASP
1	D	273	CYS
1	D	275	GLU
1	D	277	GLN
1	D	333	GLN
1	E	33	ASN
1	E	34	TRP
1	E	49	ASN

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Mol	Chain	Res	Type
1	E	50	ARG
1	E	62	ARG
1	E	90	TRP
1	E	101	ILE
1	E	102	MET
1	E	103	ASP
1	E	213	LEU
1	E	246	ASP
1	F	4	LEU
1	F	47	LYS
1	F	66	ASN
1	F	90	TRP
1	F	186	LEU
1	F	238	ASP
1	F	243	CYS
1	F	246	ASP
1	G	27	LEU
1	G	28	THR
1	G	62	ARG
1	G	90	TRP
1	G	182	SER
1	G	217	LEU
1	G	218	GLU
1	G	287	ARG
1	G	319	LYS
1	G	346	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	333	GLN
1	B	167	GLN
1	B	260	ASN
1	C	151	GLN
1	C	333	GLN
1	D	277	GLN
1	E	33	ASN
1	E	167	GLN
1	E	333	GLN
1	F	167	GLN
1	F	237	GLN

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Mol	Chain	Res	Type
1	G	167	GLN

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 monosaccharides 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	330/364 (90%)	0.27	8 (2%) 59 56	30, 115, 139, 162	0
1	B	321/364 (88%)	0.54	24 (7%) 14 13	77, 121, 149, 159	0
1	C	322/364 (88%)	0.46	14 (4%) 35 34	78, 120, 149, 166	0
1	D	325/364 (89%)	0.32	14 (4%) 35 34	81, 119, 143, 163	0
1	E	316/364 (86%)	0.43	18 (5%) 23 23	84, 120, 159, 170	0
1	F	329/364 (90%)	0.34	14 (4%) 35 34	30, 97, 135, 154	0
1	G	326/364 (89%)	0.29	8 (2%) 57 54	63, 103, 132, 158	0
All	All	2269/2548 (89%)	0.38	100 (4%) 34 33	30, 114, 149, 170	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	274	ASN	7.1
1	F	281	LEU	6.4
1	B	61	LEU	5.4
1	F	113	CYS	4.6
1	F	46	GLY	4.2
1	C	309	PHE	4.2
1	B	282	TYR	4.1
1	C	77	GLU	4.0
1	B	280	LEU	3.9
1	E	328	PRO	3.9
1	D	65	THR	3.8
1	C	243	CYS	3.8
1	D	250	ILE	3.7
1	E	273	CYS	3.5
1	B	336	LEU	3.4
1	A	270	LEU	3.3
1	G	145	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	57	SER	3.3
1	E	270	LEU	3.2
1	B	246	ASP	3.2
1	F	347	LEU	3.1
1	A	69	TYR	3.1
1	F	264	TRP	3.1
1	E	330	VAL	3.1
1	A	181	LEU	3.1
1	E	341	ALA	3.0
1	B	102	MET	3.0
1	E	70	LYS	3.0
1	F	300	TYR	2.9
1	G	245	GLY	2.9
1	B	273	CYS	2.9
1	C	250	ILE	2.9
1	E	340	LEU	2.9
1	E	343	ILE	2.9
1	F	346	ARG	2.9
1	E	241	LEU	2.8
1	F	282	TYR	2.8
1	C	264	TRP	2.8
1	B	274	ASN	2.8
1	D	300	TYR	2.7
1	A	282	TYR	2.7
1	B	203	TYR	2.7
1	E	184	TYR	2.7
1	D	273	CYS	2.7
1	E	214	GLY	2.6
1	A	237	GLN	2.6
1	C	273	CYS	2.6
1	F	295	LYS	2.6
1	G	112	PRO	2.6
1	F	305	LEU	2.6
1	B	233	TYR	2.6
1	C	245	GLY	2.6
1	G	284	ASN	2.6
1	B	30	ASP	2.5
1	B	50	ARG	2.5
1	C	282	TYR	2.5
1	D	288	LYS	2.5
1	A	289	ASP	2.5
1	D	285	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	307	ASP	2.4
1	C	300	TYR	2.4
1	B	270	LEU	2.4
1	F	69	TYR	2.4
1	B	250	ILE	2.4
1	B	46	GLY	2.4
1	C	81	ALA	2.4
1	A	226	ILE	2.4
1	A	341	ALA	2.3
1	F	294	ALA	2.3
1	B	278	LYS	2.3
1	B	181	LEU	2.3
1	G	206	VAL	2.3
1	D	253	ILE	2.3
1	C	249	VAL	2.3
1	D	305	LEU	2.3
1	E	281	LEU	2.3
1	D	281	LEU	2.3
1	E	233	TYR	2.3
1	G	210	LEU	2.2
1	F	296	VAL	2.2
1	B	309	PHE	2.2
1	E	212	MET	2.2
1	E	68	LYS	2.2
1	E	249	VAL	2.2
1	G	318	LYS	2.2
1	B	267	VAL	2.1
1	F	212	MET	2.1
1	B	264	TRP	2.1
1	G	147	HIS	2.1
1	E	225	ASP	2.1
1	D	180	ASN	2.1
1	E	265	LEU	2.1
1	D	280	LEU	2.1
1	B	240	TYR	2.1
1	B	248	GLU	2.1
1	D	264	TRP	2.1
1	B	298	GLU	2.1
1	C	266	VAL	2.1
1	D	268	GLN	2.1
1	C	295	LYS	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.