



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:16 AM GMT

PDB ID : 3DVA
Title : Snapshots of catalysis in the E1 subunit of the pyruvate dehydrogenase multi-enzyme complex
Authors : Pei, X.Y.; Titman, C.M.; Frank, R.A.W.; Leeper, F.J.; Luisi, B.F.
Deposited on : 2008-07-18
Resolution : 2.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

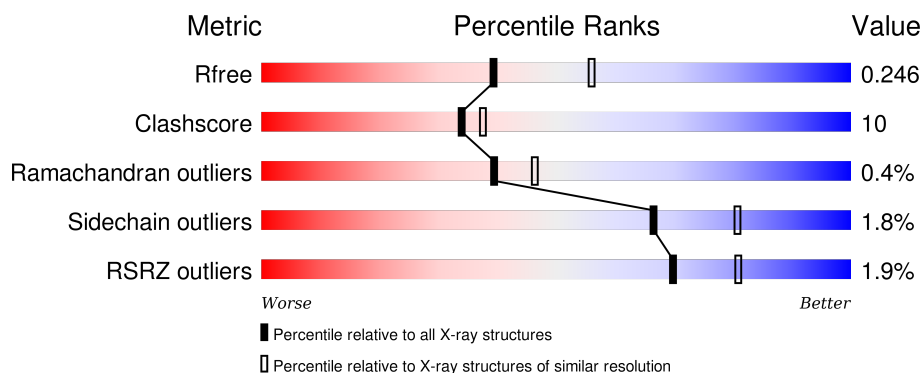
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



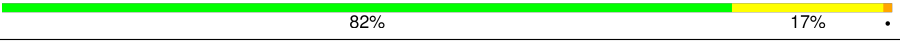



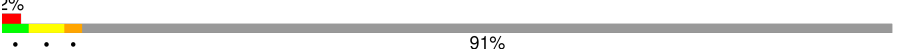
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	369	<div> <div>5%</div> <div>79%</div> <div>19%</div> <div>..</div> </div>
1	C	369	<div> <div>2%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>
1	E	369	<div> <div>2%</div> <div>82%</div> <div>14%</div> <div>.</div> </div>
1	G	369	<div> <div>%</div> <div>80%</div> <div>18%</div> <div>..</div> </div>
2	B	325	<div> <div>77%</div> <div>22%</div> <div>.</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	325	
2	F	325	
2	H	325	
3	I	428	
3	J	428	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MG	A	1326	-	-	-	X
4	MG	E	369	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 23282 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 Pyruvate dehydrogenase E1 component subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	0	0
			2895	1850	491	546	8			
1	C	365	Total	C	N	O	S	0	0	0
			2895	1850	491	546	8			
1	E	354	Total	C	N	O	S	0	0	0
			2798	1791	473	526	8			
1	G	365	Total	C	N	O	S	0	0	0
			2895	1850	491	546	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	206	ALA	ILE	ENGINEERED	UNP P21873
C	206	ALA	ILE	ENGINEERED	UNP P21873
E	206	ALA	ILE	ENGINEERED	UNP P21873
G	206	ALA	ILE	ENGINEERED	UNP P21873

- Molecule 2 is a protein called Pyruvate dehydrogenase E1 component subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	324	Total	C	N	O	S	0	0	0
			2488	1586	424	470	8			
2	D	324	Total	C	N	O	S	0	0	0
			2488	1586	424	470	8			
2	F	324	Total	C	N	O	S	0	0	0
			2488	1586	424	470	8			
2	H	324	Total	C	N	O	S	0	0	0
			2488	1586	424	470	8			

- Molecule 3 is a protein called Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	42	Total	C	N	O	S	0	0	0
			314	195	62	56	1			
3	J	40	Total	C	N	O	S	0	0	0
			294	180	59	54	1			

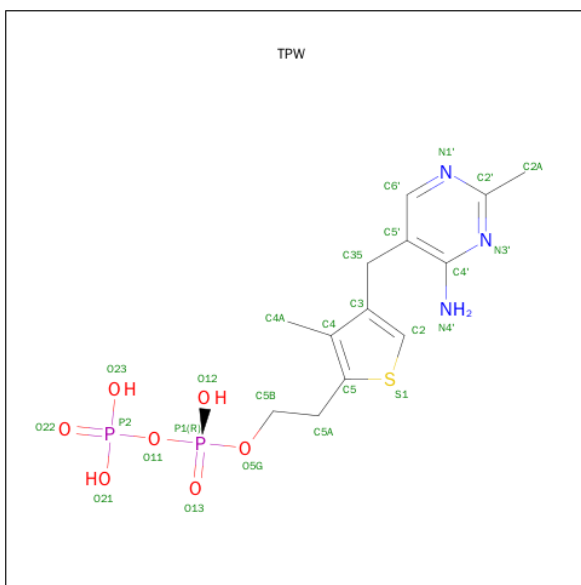
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Mg	0	0
			1	1		
4	A	2	Total	Mg	0	0
			2	2		
4	C	1	Total	Mg	0	0
			1	1		
4	E	2	Total	Mg	0	0
			2	2		

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	K	0	0
			1	1		
5	D	1	Total	K	0	0
			1	1		

- Molecule 6 is 2-{4-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-3-METHYLTHIOPHEN-2-YL}ETHYL TRIHYDROGEN DIPHOSPHATE (three-letter code: TPW) (formula: C₁₃H₁₉N₃O₇P₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total 26	C 13	N 3	O 7	P 2	S 1	0	0
6	C	1	Total 26	C 13	N 3	O 7	P 2	S 1	0	0
6	E	1	Total 26	C 13	N 3	O 7	P 2	S 1	0	0
6	G	1	Total 26	C 13	N 3	O 7	P 2	S 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	150	Total O 150 150	0	0
7	B	139	Total O 139 139	0	0
7	C	148	Total O 148 148	0	0
7	D	161	Total O 161 161	0	0
7	E	100	Total O 100 100	0	0
7	F	126	Total O 126 126	0	0
7	G	139	Total O 139 139	0	0
7	H	155	Total O 155 155	0	0

Continued on next page...

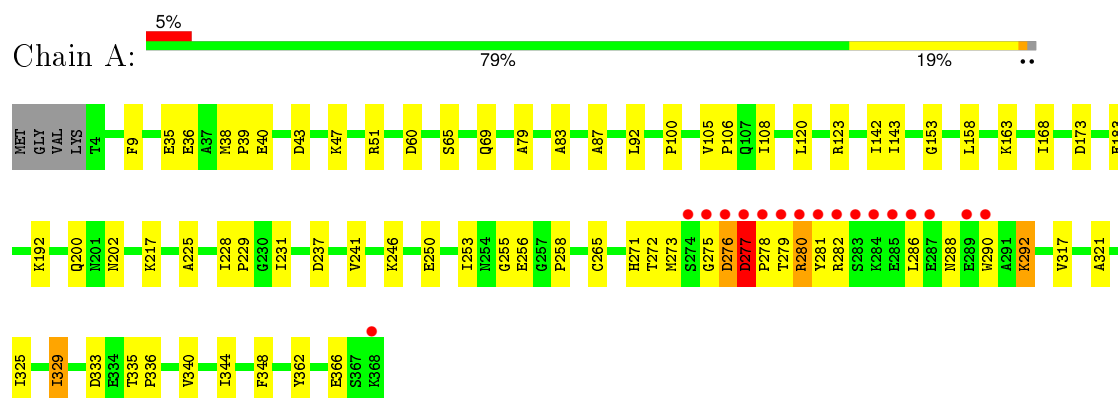
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	I	5	Total	O	0	0
			5	5		
7	J	4	Total	O	0	0
			4	4		

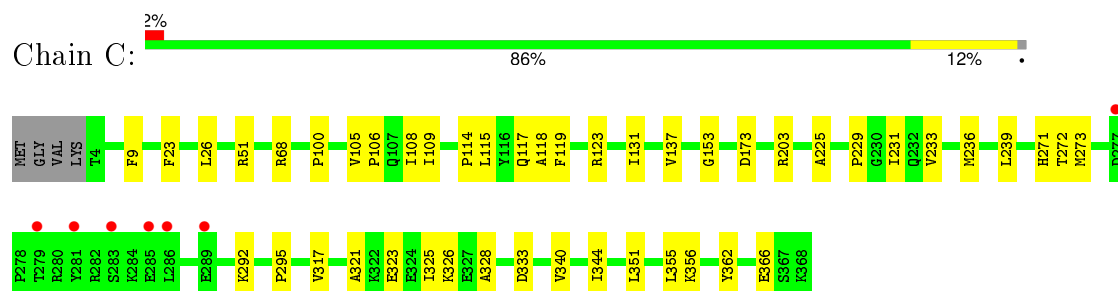
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

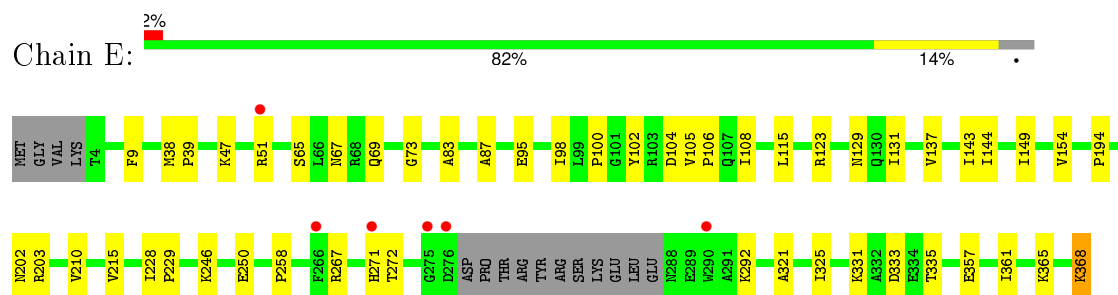
- Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha



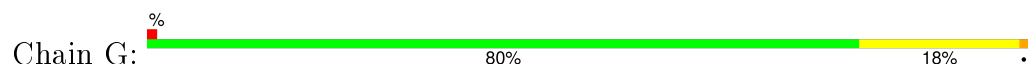
- Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha

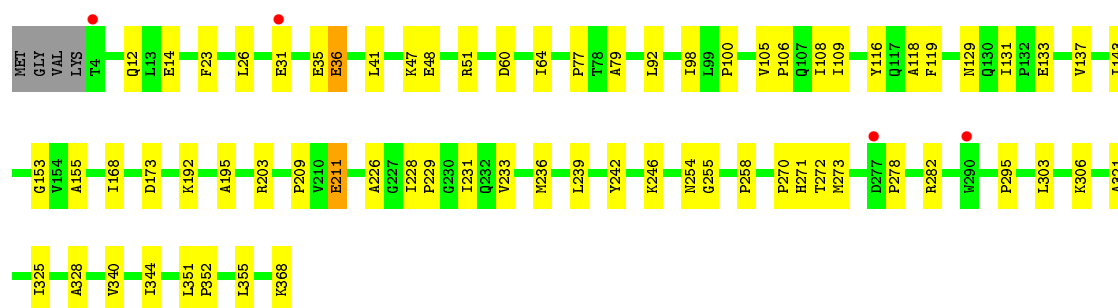


- Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha



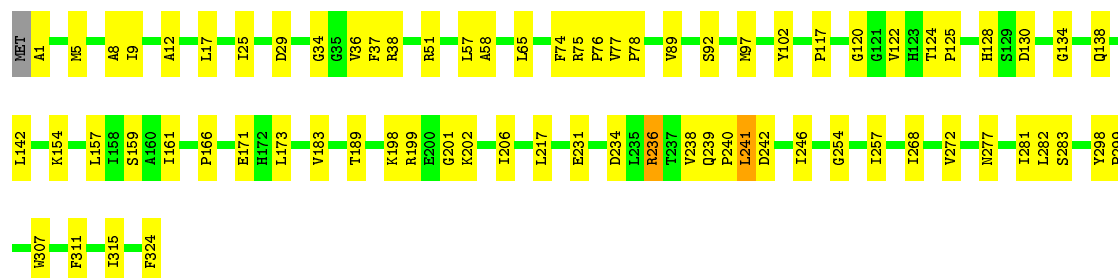
- Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha





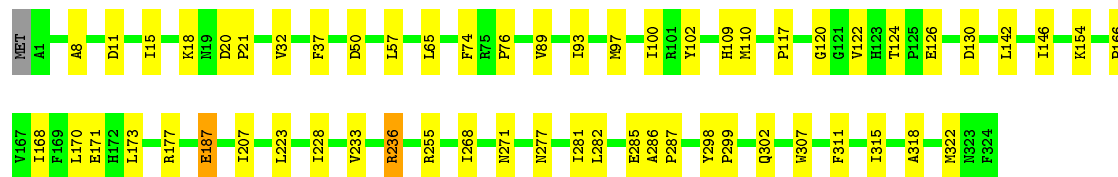
- Molecule 2: Pyruvate dehydrogenase E1 component subunit beta

Chain B:



- Molecule 2: Pyruvate dehydrogenase E1 component subunit beta

Chain D:



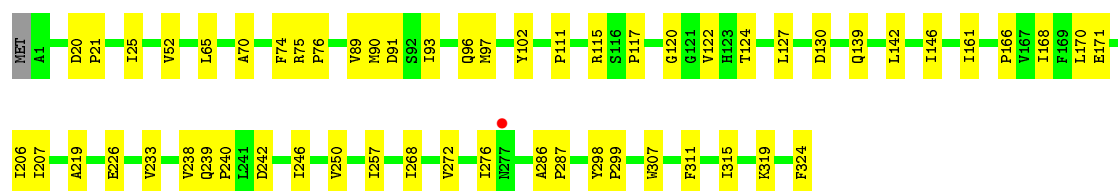
- Molecule 2: Pyruvate dehydrogenase E1 component subunit beta

Chain F:

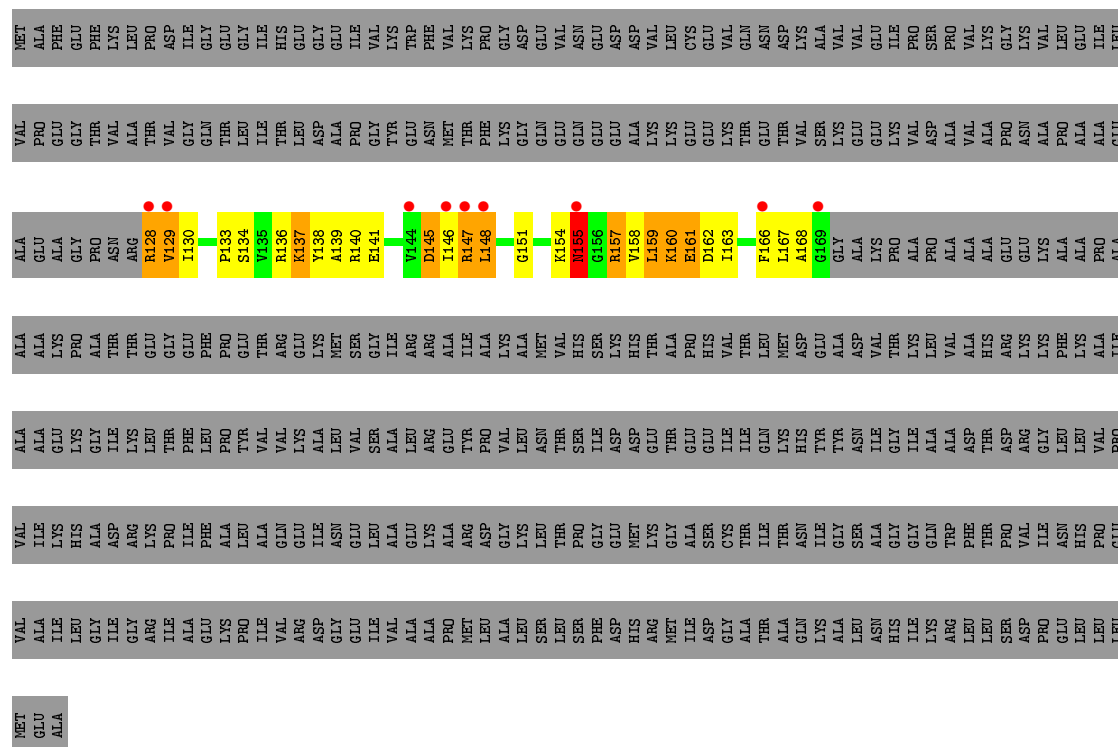


- Molecule 2: Pyruvate dehydrogenase E1 component subunit beta

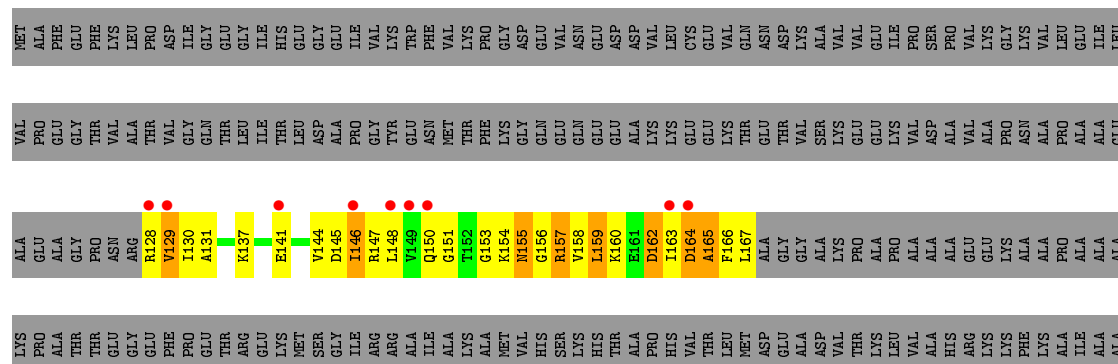
Chain H:



- Molecule 3: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex



- Molecule 3: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex



ILE	LYS	GLU
LEU	HIS	LYS
GLY	ALA	GLY
ILE	ASP	ILE
GLY	ARG	LYS
ILE	PRO	LEU
ALA	ILE	THR
GLU	PHE	PHE
LYS	ALA	LEU
PRO	LEU	PRO
ILE	ALA	TYR
VAL	GLN	VAL
ARG	GLU	VAL
ASP	ILE	LYS
GLY	ASN	ALA
ILE	GLU	LEU
VAL	LEU	VAL
ALA	ALA	SER
ALA	GLU	ALA
ALA	LYS	LEU
PRO	ALA	ARG
MET	ARG	GLU
LEU	ASP	TYR
ALA	GLY	PRO
LEU	LYS	VAL
SER	LEU	LEU
LEU	THR	ASN
SER	PRO	THR
PHE	GLY	SER
ASP	GLU	ILE
HIS	MET	ASP
ARG	LYS	ASP
MET	GLY	GLU
ILE	ALA	THR
ASP	SER	GLU
GLY	CYS	GLU
ALA	THR	ILE
THR	ILE	ILE
ALA	THR	GLN
GLN	LYS	LYS
LYS	ILE	HIS
ALA	ILE	TYR
LEU	SER	ASN
ASN	ALA	ILE
HIS	GLY	ILE
ILE	GLY	GLY
LYS	GLN	ALA
ARG	TRP	ALA
LEU	PHE	ASP
LEU	THR	THR
SER	PRO	ASP
ASP	VAL	ARG
PRO	ILE	GLY
GLU	ASN	LEU
LEU	HIS	LEU
LEU	PRO	VAL
MET	GLU	PRO
GLU	VAL	VAL
	ALA	ILE

ALA

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.67Å 232.29Å 91.94Å 90.00° 91.20° 90.00°	Depositor
Resolution (Å)	72.17 – 2.35 72.08 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.9 (72.17-2.35) 98.9 (72.08-2.35)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.04 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.190 , 0.247 0.191 , 0.246	Depositor DCC
R_{free} test set	5906 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.1	EDS
Estimated twinning fraction	0.049 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 117882 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	23282	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TPW, K, MG

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	0.38	0/2958	0.53	1/3995 (0.0%)
1	C	0.35	0/2958	0.48	0/3995
1	E	0.33	0/2858	0.45	0/3859
1	G	0.31	0/2958	0.47	0/3995
2	B	0.40	0/2534	0.55	2/3437 (0.1%)
2	D	0.27	0/2534	0.53	1/3437 (0.0%)
2	F	0.26	0/2534	0.52	1/3437 (0.0%)
2	H	0.28	0/2534	0.51	0/3437
3	I	1.44	1/316 (0.3%)	1.17	1/421 (0.2%)
3	J	1.54	0/295	1.16	1/395 (0.3%)
All	All	0.41	1/22479 (0.0%)	0.53	7/30408 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	138	TYR	CD2-CE2	-5.70	1.30	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	ASP	CB-CG-OD1	-7.67	111.40	118.30
2	B	234	ASP	CB-CG-OD1	6.80	124.42	118.30
2	B	236	ARG	CB-CA-C	-5.90	98.59	110.40
2	D	236	ARG	CB-CA-C	-5.84	98.72	110.40
3	J	162	ASP	CB-CG-OD1	-5.63	113.23	118.30
2	F	236	ARG	CB-CA-C	-5.61	99.18	110.40
3	I	145	ASP	N-CA-C	-5.16	97.08	111.00

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	2895	0	2871	73	0
1	C	2895	0	2871	34	0
1	E	2798	0	2776	44	0
1	G	2895	0	2871	64	0
2	B	2488	0	2515	47	0
2	D	2488	0	2515	46	0
2	F	2488	0	2515	58	0
2	H	2488	0	2515	47	0
3	I	314	0	322	40	0
3	J	294	0	291	36	0
4	A	2	0	0	0	0
4	C	1	0	0	0	0
4	E	2	0	0	0	0
4	G	1	0	0	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	A	26	0	16	1	0
6	C	26	0	16	3	0
6	E	26	0	16	1	0
6	G	26	0	16	3	0
7	A	150	0	0	3	0
7	B	139	0	0	5	0
7	C	148	0	0	3	0
7	D	161	0	0	7	0
7	E	100	0	0	6	0
7	F	126	0	0	5	0
7	G	139	0	0	10	0
7	H	155	0	0	2	0
7	I	5	0	0	0	0
7	J	4	0	0	2	0
All	All	23282	0	22126	449	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 10.

All (449) 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:281:TYR:CB	1:A:282:ARG:HA	1.57	1.34
2:D:285:GLU:HG3	3:I:140:ARG:NH2	1.56	1.18
3:J:160:LYS:O	3:J:160:LYS:HG2	1.43	1.17
1:A:281:TYR:HB3	1:A:282:ARG:HA	1.30	1.11
1:A:281:TYR:HB2	1:A:282:ARG:HA	1.30	1.07
2:F:127:LEU:HD13	1:G:143:ILE:HD11	1.32	1.06
3:I:154:LYS:O	3:I:155:ASN:HB2	1.62	0.98
3:I:160:LYS:HG2	3:I:160:LYS:O	1.60	0.98
3:I:160:LYS:O	3:I:161:GLU:HG3	1.61	0.98
1:A:281:TYR:CB	1:A:282:ARG:CA	2.44	0.96
2:D:285:GLU:HG3	3:I:140:ARG:HH22	1.25	0.93
1:A:277:ASP:N	1:A:278:PRO:CD	2.30	0.91
3:I:160:LYS:C	3:I:161:GLU:HG3	1.87	0.91
3:J:154:LYS:C	3:J:156:GLY:H	1.74	0.89
3:I:151:GLY:HA2	3:I:162:ASP:OD2	1.73	0.89
3:J:164:ASP:O	3:J:165:ALA:HB2	1.73	0.89
3:I:159:LEU:HB2	3:I:161:GLU:OE1	1.74	0.88
2:F:152:ASP:HB2	7:F:1357:HOH:O	1.73	0.87
1:C:273:MET:HE2	7:C:1510:HOH:O	1.74	0.86
3:I:166:PHE:C	3:I:168:ALA:H	1.80	0.84
1:E:368:LYS:HA	1:E:368:LYS:NZ	1.93	0.84
2:F:247:ILE:HD11	2:F:279:ARG:HD2	1.59	0.83
1:C:321:ALA:O	1:C:325:ILE:HG12	1.77	0.83
1:A:277:ASP:N	1:A:278:PRO:HD2	1.91	0.82
1:A:277:ASP:H	1:A:278:PRO:CD	1.91	0.82
1:A:231:ILE:HD11	1:C:9:PHE:HE1	1.43	0.81
1:A:273:MET:HA	1:A:273:MET:HE2	1.59	0.81
2:D:285:GLU:CG	3:I:140:ARG:NH2	2.41	0.81
3:I:159:LEU:CB	3:I:161:GLU:OE1	2.29	0.80
3:I:160:LYS:O	3:I:161:GLU:CG	2.30	0.80
2:H:122:VAL:HG23	2:H:124:THR:HG23	1.65	0.79
3:J:157:ARG:HG2	3:J:158:VAL:N	1.97	0.79
3:I:160:LYS:O	3:I:160:LYS:CG	2.29	0.78
2:D:32:VAL:HG23	7:D:1518:HOH:O	1.81	0.78
1:A:281:TYR:HB3	1:A:282:ARG:CA	2.09	0.78
1:E:365:LYS:HE3	7:E:1497:HOH:O	1.85	0.77
3:J:144:VAL:HG12	3:J:145:ASP:N	1.98	0.77
2:D:122:VAL:HG23	2:D:124:THR:HG23	1.67	0.77
2:B:198:LYS:HB3	2:B:217:LEU:HD21	1.65	0.77
1:G:23:PHE:HB3	1:G:233:VAL:HG12	1.67	0.76
1:A:277:ASP:HB2	1:A:278:PRO:HD3	1.67	0.76
1:E:321:ALA:O	1:E:325:ILE:HG12	1.86	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:137:LYS:O	3:I:137:LYS:HG3	1.86	0.76
3:J:164:ASP:O	3:J:165:ALA:CB	2.30	0.76
2:H:286:ALA:HB1	2:H:287:PRO:HD2	1.66	0.76
1:E:115:LEU:HD21	1:E:325:ILE:HD13	1.66	0.75
1:C:123:ARG:NH1	1:C:333:ASP:OD1	2.20	0.75
1:A:231:ILE:HD11	1:C:9:PHE:CE1	2.21	0.74
1:A:246:LYS:HE2	1:A:250:GLU:OE1	1.88	0.74
2:D:285:GLU:HG3	3:I:140:ARG:HH21	1.52	0.73
2:F:127:LEU:CD1	1:G:143:ILE:HD11	2.15	0.72
3:J:154:LYS:C	3:J:156:GLY:N	2.41	0.72
1:G:36:GLU:HG3	7:G:1416:HOH:O	1.88	0.72
3:I:166:PHE:C	3:I:168:ALA:N	2.44	0.71
2:F:100:ILE:HG13	2:F:110:MET:HE3	1.71	0.70
1:C:109:ILE:HD11	1:C:118:ALA:HB2	1.70	0.70
1:A:292:LYS:HD2	1:A:292:LYS:N	2.07	0.69
2:F:302:GLN:HE21	2:F:302:GLN:HA	1.55	0.69
1:E:9:PHE:HZ	1:G:231:ILE:HD11	1.57	0.69
2:D:271:ASN:ND2	7:D:1427:HOH:O	2.25	0.69
3:J:144:VAL:CG1	3:J:145:ASP:N	2.55	0.68
2:B:89:VAL:HG22	2:B:89:VAL:O	1.94	0.68
1:E:9:PHE:CD1	1:G:229:PRO:HB3	2.29	0.68
1:A:281:TYR:HB2	1:A:282:ARG:CA	2.14	0.67
2:H:324:PHE:O	3:J:137:LYS:HE2	1.93	0.67
2:F:120:GLY:HA3	2:F:298:TYR:OH	1.95	0.67
1:E:131:ILE:H	1:E:131:ILE:HD12	1.60	0.66
2:H:311:PHE:O	2:H:315:ILE:HG12	1.95	0.66
3:I:139:ALA:HB2	3:I:163:ILE:HD12	1.77	0.66
3:J:154:LYS:O	3:J:156:GLY:N	2.29	0.66
2:D:298:TYR:CG	2:D:299:PRO:HD2	2.31	0.66
1:G:129:ASN:O	1:G:131:ILE:HD12	1.96	0.66
2:F:5:MET:O	2:F:9:ILE:HG12	1.95	0.65
1:A:348:PHE:HE1	7:B:1328:HOH:O	1.78	0.65
3:J:163:ILE:HD13	3:J:163:ILE:N	2.10	0.65
2:H:272:VAL:O	2:H:276:ILE:HG12	1.96	0.65
2:H:168:ILE:HD12	2:H:168:ILE:N	2.12	0.65
1:A:277:ASP:H	1:A:278:PRO:HD2	1.55	0.64
1:E:368:LYS:HA	1:E:368:LYS:HZ3	1.62	0.64
1:G:109:ILE:HD11	1:G:118:ALA:HB2	1.79	0.64
1:C:115:LEU:HD21	1:C:325:ILE:HD13	1.79	0.64
2:F:67:ILE:HG23	2:F:110:MET:CE	2.28	0.64
2:D:285:GLU:CG	3:I:140:ARG:HH21	2.08	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:286:ALA:HB1	2:D:287:PRO:HD2	1.81	0.63
1:E:129:ASN:O	1:E:131:ILE:HD12	1.98	0.63
1:A:92:LEU:HD11	1:A:168:ILE:HG21	1.80	0.63
2:B:120:GLY:HA3	2:B:298:TYR:OH	1.99	0.62
2:D:277:ASN:O	2:D:281:ILE:HB	1.99	0.62
1:E:267:ARG:NH2	7:E:1518:HOH:O	2.32	0.62
1:G:192:LYS:HE2	1:G:255:GLY:O	1.99	0.62
3:J:156:GLY:O	3:J:157:ARG:C	2.36	0.62
2:H:319:LYS:HE3	7:H:1574:HOH:O	2.00	0.62
1:E:368:LYS:HA	1:E:368:LYS:HZ2	1.64	0.61
2:F:89:VAL:O	2:F:89:VAL:HG22	2.00	0.61
2:D:142:LEU:HD13	2:D:168:ILE:HD11	1.82	0.61
1:A:40:GLU:CD	1:A:40:GLU:H	2.02	0.61
1:C:123:ARG:NH2	1:C:333:ASP:OD1	2.32	0.61
2:F:25:ILE:HD13	2:F:77:VAL:HB	1.83	0.61
2:H:93:ILE:HA	2:H:97:MET:HG2	1.83	0.60
2:F:296:THR:CG2	1:G:344:ILE:HD13	2.31	0.60
1:A:277:ASP:H	1:A:278:PRO:HD3	1.65	0.60
3:J:156:GLY:C	3:J:157:ARG:O	2.35	0.60
2:B:117:PRO:HA	2:B:171:GLU:O	2.02	0.60
3:J:157:ARG:HG2	3:J:158:VAL:H	1.66	0.59
2:H:298:TYR:CG	2:H:299:PRO:HD2	2.37	0.59
2:B:74:PHE:O	2:B:76:PRO:HD3	2.03	0.59
2:H:89:VAL:HG22	2:H:89:VAL:O	2.02	0.59
2:H:117:PRO:HA	2:H:171:GLU:O	2.03	0.59
1:G:14:GLU:HG3	7:G:1448:HOH:O	2.01	0.59
1:A:273:MET:HE2	1:A:273:MET:CA	2.33	0.59
1:G:64:ILE:HG23	1:G:273:MET:HE3	1.84	0.59
2:D:89:VAL:O	2:D:89:VAL:HG22	2.03	0.58
2:B:57:LEU:HD11	6:C:1370:TPW:H4A3	1.85	0.58
2:F:32:VAL:HG23	7:F:1328:HOH:O	2.02	0.58
2:B:241:LEU:HD21	2:B:272:VAL:HG22	1.84	0.58
3:J:157:ARG:HD2	3:J:159:LEU:HD23	1.86	0.58
2:F:102:TYR:OH	2:H:299:PRO:HA	2.04	0.57
1:A:292:LYS:HD2	1:A:292:LYS:H	1.67	0.57
2:F:37:PHE:CZ	2:F:173:LEU:HD22	2.39	0.57
1:A:9:PHE:CD1	1:C:229:PRO:HB3	2.39	0.57
1:A:142:ILE:HG12	2:D:126:GLU:HB3	1.85	0.57
2:F:67:ILE:HG23	2:F:110:MET:HE3	1.85	0.57
1:A:65:SER:O	1:A:69:GLN:HG3	2.05	0.57
2:B:122:VAL:HG23	2:B:124:THR:HG23	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:ARG:CZ	1:C:333:ASP:OD1	2.53	0.57
2:H:120:GLY:HA3	2:H:298:TYR:OH	2.04	0.56
1:A:246:LYS:O	1:A:250:GLU:HG3	2.05	0.56
2:F:298:TYR:CG	2:F:299:PRO:HD2	2.41	0.56
1:G:352:PRO:HB3	2:H:240:PRO:HG3	1.86	0.56
1:G:60:ASP:OD2	1:G:79:ALA:HB2	2.06	0.56
2:B:281:ILE:O	2:B:281:ILE:HG13	2.05	0.56
2:F:311:PHE:O	2:F:315:ILE:HG12	2.05	0.56
2:B:102:TYR:OH	2:D:299:PRO:HA	2.06	0.56
2:H:206:ILE:HD12	2:H:257:ILE:HD11	1.88	0.56
3:J:160:LYS:O	3:J:160:LYS:CG	2.30	0.55
2:F:299:PRO:HA	2:H:102:TYR:OH	2.06	0.55
2:B:37:PHE:CZ	2:B:173:LEU:HD22	2.41	0.55
2:F:247:ILE:HD11	2:F:279:ARG:CD	2.35	0.55
2:H:207:ILE:HA	2:H:233:VAL:HG13	1.89	0.55
1:C:109:ILE:HD11	1:C:118:ALA:CB	2.36	0.55
1:C:23:PHE:HB3	1:C:233:VAL:HG12	1.89	0.55
3:J:166:PHE:O	3:J:167:LEU:CB	2.54	0.55
3:J:151:GLY:CA	3:J:158:VAL:HG22	2.37	0.55
2:H:250:VAL:HG21	2:H:276:ILE:HD12	1.88	0.55
3:I:145:ASP:OD2	3:I:147:ARG:HB2	2.07	0.55
2:B:311:PHE:O	2:B:315:ILE:HG12	2.06	0.55
3:I:159:LEU:O	3:I:161:GLU:N	2.39	0.55
2:D:223:LEU:HB3	2:D:228:ILE:HB	1.89	0.55
3:J:154:LYS:O	3:J:155:ASN:HB2	2.07	0.55
1:E:194:PRO:HG2	7:E:1444:HOH:O	2.07	0.55
2:F:100:ILE:HG13	2:F:110:MET:CE	2.36	0.55
1:A:329:ILE:HD13	1:A:329:ILE:O	2.06	0.55
1:A:153:GLY:HA2	2:B:65:LEU:HD12	1.89	0.55
1:C:271:HIS:CD2	1:C:272:THR:HG23	2.41	0.55
1:A:43:ASP:O	1:A:47:LYS:HG3	2.07	0.54
2:F:241:LEU:HD21	7:F:1373:HOH:O	2.07	0.54
2:D:100:ILE:HG13	2:D:110:MET:HE3	1.88	0.54
1:A:281:TYR:HB2	1:A:282:ARG:HG2	1.89	0.54
1:A:9:PHE:HZ	1:C:231:ILE:HD11	1.72	0.54
1:A:192:LYS:HE2	1:A:256:GLU:HA	1.88	0.54
1:A:60:ASP:OD2	1:A:79:ALA:HB2	2.08	0.54
1:A:277:ASP:CB	1:A:278:PRO:HD3	2.34	0.54
2:B:254:GLY:HA2	2:B:283:SER:O	2.08	0.54
2:F:246:ILE:CG2	2:F:276:ILE:HD11	2.38	0.54
3:J:151:GLY:HA3	3:J:158:VAL:HG22	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:120:GLY:HA3	2:D:298:TYR:OH	2.08	0.54
2:H:238:VAL:HB	2:H:268:ILE:HG12	1.90	0.54
3:J:157:ARG:HD3	7:J:432:HOH:O	2.08	0.54
2:D:142:LEU:HD23	2:D:166:PRO:HB2	1.90	0.53
1:G:271:HIS:CD2	1:G:272:THR:HG23	2.44	0.53
1:G:47:LYS:HG2	7:G:1474:HOH:O	2.07	0.53
2:F:117:PRO:HA	2:F:171:GLU:O	2.08	0.53
1:G:77:PRO:HG3	1:G:273:MET:HE1	1.90	0.53
7:B:1370:HOH:O	3:I:134:SER:HB3	2.07	0.53
2:F:122:VAL:HG23	2:F:124:THR:HG23	1.91	0.53
1:G:35:GLU:H	1:G:35:GLU:CD	2.11	0.53
3:J:147:ARG:HG3	3:J:147:ARG:HH21	1.74	0.53
1:E:144:ILE:HG12	6:E:1370:TPW:N3'	2.24	0.53
6:C:1370:TPW:H2	7:C:1455:HOH:O	2.09	0.53
3:I:129:VAL:CG2	3:I:130:ILE:N	2.72	0.53
3:I:137:LYS:HA	3:I:140:ARG:NH1	2.23	0.52
2:B:5:MET:O	2:B:9:ILE:HG12	2.09	0.52
2:B:298:TYR:CG	2:B:299:PRO:HD2	2.44	0.52
2:F:168:ILE:HD12	2:F:168:ILE:N	2.25	0.52
3:J:157:ARG:CD	7:J:432:HOH:O	2.58	0.52
2:F:100:ILE:HG21	2:F:110:MET:HE2	1.91	0.52
3:J:147:ARG:HG3	3:J:147:ARG:NH2	2.25	0.52
2:H:242:ASP:O	2:H:246:ILE:HG13	2.10	0.52
1:G:77:PRO:HG2	1:G:270:PRO:HD2	1.92	0.51
1:E:102:TYR:HE2	1:E:144:ILE:CD1	2.22	0.51
2:F:14:ARG:NH1	2:F:46:GLU:OE1	2.42	0.51
2:D:271:ASN:HB3	7:D:1420:HOH:O	2.09	0.51
1:G:368:LYS:HB3	1:G:368:LYS:NZ	2.26	0.51
1:E:271:HIS:CD2	1:E:272:THR:HG23	2.45	0.51
2:B:34:GLY:O	2:B:38:ARG:HA	2.11	0.51
1:G:100:PRO:HG3	1:G:108:ILE:HG21	1.93	0.51
1:A:83:ALA:O	1:A:87:ALA:HB3	2.10	0.51
2:H:75:ARG:HD3	2:H:161:ILE:O	2.10	0.51
1:A:100:PRO:HG3	1:A:108:ILE:HG21	1.92	0.51
1:C:100:PRO:HG3	1:C:108:ILE:HG21	1.93	0.51
1:G:153:GLY:HA2	2:H:65:LEU:HD12	1.92	0.51
2:F:125:PRO:HG2	2:F:128:HIS:CE1	2.45	0.51
2:H:146:ILE:HG12	2:H:170:LEU:HB2	1.93	0.51
1:G:109:ILE:HD11	1:G:118:ALA:CB	2.41	0.51
1:G:303:LEU:HD13	7:G:1474:HOH:O	2.10	0.51
2:D:298:TYR:CD2	2:D:299:PRO:HD2	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:LYS:HE2	1:A:255:GLY:O	2.11	0.51
1:A:158:LEU:HD23	1:A:163:LYS:HD2	1.93	0.51
1:E:65:SER:O	1:E:69:GLN:HG3	2.10	0.51
7:B:1406:HOH:O	3:I:133:PRO:HD2	2.11	0.50
1:A:286:LEU:O	1:A:290:TRP:HD1	1.94	0.50
1:C:105:VAL:O	1:C:109:ILE:HG12	2.12	0.50
1:G:233:VAL:HB	7:G:1441:HOH:O	2.10	0.50
1:G:271:HIS:CE1	6:G:1370:TPW:H5A2	2.46	0.50
3:J:156:GLY:O	3:J:157:ARG:O	2.29	0.50
2:F:198:LYS:HB3	2:F:217:LEU:HD21	1.93	0.50
1:E:203:ARG:HB2	7:E:1453:HOH:O	2.11	0.50
1:G:352:PRO:HD2	1:G:355:LEU:HB2	1.93	0.50
2:F:246:ILE:HG22	2:F:276:ILE:HD11	1.93	0.50
3:J:154:LYS:O	3:J:155:ASN:CB	2.59	0.50
3:I:148:LEU:O	3:I:166:PHE:CZ	2.64	0.50
1:A:272:THR:O	1:A:273:MET:HE2	2.13	0.49
1:A:142:ILE:HD12	1:A:143:ILE:HG12	1.93	0.49
1:E:215:VAL:HG12	1:G:226:ALA:O	2.12	0.49
2:H:74:PHE:O	2:H:76:PRO:HD3	2.11	0.49
2:B:134:GLY:O	2:B:138:GLN:HG3	2.12	0.49
1:G:254:ASN:ND2	7:G:1447:HOH:O	2.45	0.49
2:F:36:VAL:HG23	2:F:37:PHE:CD2	2.47	0.49
1:A:183:GLU:OE1	2:B:58:ALA:HB1	2.12	0.49
1:C:68:ARG:HG3	7:C:1510:HOH:O	2.11	0.49
1:A:228:ILE:HG21	1:A:258:PRO:HG2	1.94	0.49
2:H:142:LEU:HD22	2:H:168:ILE:HD11	1.95	0.49
1:A:123:ARG:HB3	2:D:302:GLN:HE21	1.78	0.49
2:B:201:GLY:H	2:B:231:GLU:HB2	1.76	0.49
2:D:146:ILE:HG12	2:D:170:LEU:HB2	1.92	0.49
2:D:207:ILE:HA	2:D:233:VAL:HG13	1.94	0.49
1:A:288:ASN:N	1:A:288:ASN:HD22	2.10	0.49
1:G:133:GLU:HG2	7:H:1500:HOH:O	2.13	0.49
2:F:17:LEU:O	2:F:51:ARG:NH1	2.45	0.49
1:A:335:THR:HG22	7:A:1501:HOH:O	2.13	0.49
1:E:331:LYS:O	1:E:335:THR:HG23	2.12	0.49
2:F:170:LEU:HD13	7:F:1332:HOH:O	2.13	0.48
2:H:226:GLU:OE1	2:H:319:LYS:NZ	2.45	0.48
1:E:100:PRO:HB2	1:E:104:ASP:HB2	1.95	0.48
2:D:117:PRO:HA	2:D:171:GLU:O	2.12	0.48
6:A:1370:TPW:H4A3	2:D:57:LEU:HD11	1.95	0.48
2:H:299:PRO:HD3	2:H:307:TRP:CD2	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:228:ILE:HG21	1:E:258:PRO:HG2	1.95	0.48
1:E:357:GLU:O	1:E:361:ILE:HG12	2.13	0.48
2:F:98:ALA:HB2	2:F:142:LEU:HD21	1.95	0.48
1:C:105:VAL:N	1:C:106:PRO:CD	2.77	0.48
2:B:299:PRO:HA	2:D:102:TYR:OH	2.14	0.48
2:D:11:ASP:O	2:D:15:ILE:HG12	2.13	0.48
2:F:4:THR:OG1	2:F:7:GLN:HG3	2.13	0.48
2:B:36:VAL:HG23	2:B:37:PHE:CD2	2.48	0.48
1:E:228:ILE:HB	1:E:229:PRO:HD2	1.96	0.48
1:A:51:ARG:HG3	1:A:317:VAL:HG22	1.96	0.48
1:G:271:HIS:HE1	6:G:1370:TPW:H5A2	1.78	0.48
3:J:129:VAL:HG11	3:J:146:ILE:HG23	1.95	0.48
2:D:311:PHE:O	2:D:315:ILE:HG13	2.14	0.48
1:G:278:PRO:HB3	1:G:282:ARG:HE	1.79	0.48
2:D:109:HIS:HE1	7:D:1436:HOH:O	1.96	0.48
1:G:143:ILE:HD12	2:H:96:GLN:NE2	2.29	0.47
2:F:8:ALA:HB1	2:F:154:LYS:HB2	1.96	0.47
1:G:143:ILE:HD13	2:H:91:ASP:OD1	2.14	0.47
2:B:324:PHE:O	3:I:157:ARG:NH2	2.40	0.47
3:I:162:ASP:N	3:I:162:ASP:OD1	2.44	0.47
2:B:125:PRO:HG2	2:B:128:HIS:CE1	2.49	0.47
2:F:93:ILE:HA	2:F:97:MET:HG2	1.96	0.47
1:A:228:ILE:HB	1:A:229:PRO:HD2	1.96	0.47
1:G:340:VAL:O	1:G:344:ILE:HG12	2.14	0.47
1:A:123:ARG:NH2	1:A:329:ILE:HD11	2.29	0.47
1:A:51:ARG:HG3	1:A:317:VAL:CG2	2.45	0.47
1:A:271:HIS:CD2	1:A:272:THR:HG23	2.50	0.47
2:D:299:PRO:HD3	2:D:307:TRP:CD2	2.49	0.47
1:G:31:GLU:OE1	1:G:31:GLU:N	2.48	0.47
2:B:206:ILE:HD12	2:B:257:ILE:HD11	1.97	0.47
3:J:144:VAL:CG1	3:J:145:ASP:H	2.25	0.47
1:E:202:ASN:O	1:E:203:ARG:HB3	2.15	0.47
1:C:119:PHE:HE2	1:C:328:ALA:HB3	1.80	0.47
1:E:100:PRO:HG3	1:E:108:ILE:HG21	1.97	0.47
1:E:246:LYS:NZ	1:E:250:GLU:OE2	2.48	0.47
2:F:212:MET:HE2	2:F:212:MET:HA	1.97	0.46
1:G:119:PHE:HE2	1:G:328:ALA:HB3	1.80	0.46
1:A:278:PRO:O	1:A:279:THR:CG2	2.63	0.46
1:A:278:PRO:C	1:A:279:THR:HG23	2.35	0.46
2:H:142:LEU:HD23	2:H:166:PRO:HB2	1.97	0.46
2:D:8:ALA:HB1	2:D:154:LYS:HB2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:15:ILE:HG21	2:D:187:GLU:HB3	1.98	0.46
1:E:143:ILE:HD11	2:H:127:LEU:HD13	1.98	0.46
2:F:268:ILE:HD12	2:F:268:ILE:C	2.36	0.46
1:E:47:LYS:HE3	1:E:51:ARG:HH12	1.80	0.46
2:D:318:ALA:O	2:D:322:MET:HG2	2.16	0.46
1:G:321:ALA:O	1:G:325:ILE:HG13	2.16	0.46
1:A:38:MET:SD	1:A:39:PRO:HD2	2.55	0.46
2:B:159:SER:OG	2:B:189:THR:HB	2.16	0.46
1:C:26:LEU:HG	1:C:239:LEU:HD12	1.98	0.46
1:G:64:ILE:HG12	1:G:273:MET:CE	2.45	0.46
3:J:130:ILE:O	3:J:131:ALA:HB2	2.15	0.46
1:G:105:VAL:N	1:G:106:PRO:CD	2.78	0.46
2:F:147:PRO:HD2	2:F:170:LEU:O	2.16	0.46
2:B:1:ALA:N	2:B:183:VAL:O	2.48	0.46
1:C:362:TYR:O	1:C:366:GLU:HG3	2.16	0.46
1:E:292:LYS:H	1:E:292:LYS:HD2	1.80	0.46
2:D:177:ARG:HD3	7:D:1466:HOH:O	2.16	0.46
1:A:123:ARG:NH2	1:A:333:ASP:OD1	2.46	0.46
2:B:268:ILE:HD12	2:B:268:ILE:C	2.36	0.46
2:B:75:ARG:HD3	2:B:161:ILE:O	2.16	0.45
2:F:90:MET:HG3	2:H:90:MET:HG3	1.98	0.45
1:E:9:PHE:CZ	1:G:231:ILE:HD11	2.44	0.45
2:F:102:TYR:HH	2:H:299:PRO:HA	1.79	0.45
3:J:157:ARG:HD2	3:J:159:LEU:CD2	2.46	0.45
1:G:105:VAL:O	1:G:108:ILE:HG12	2.17	0.45
1:A:280:ARG:HA	1:A:280:ARG:HD3	1.72	0.45
1:E:149:ILE:HG21	7:E:1527:HOH:O	2.16	0.45
1:G:41:LEU:HD21	1:G:242:TYR:CZ	2.52	0.45
2:D:282:LEU:HG	7:D:1485:HOH:O	2.16	0.45
1:G:98:ILE:HB	1:G:137:VAL:HG12	1.99	0.45
1:C:340:VAL:O	1:C:344:ILE:HG13	2.16	0.45
1:A:105:VAL:N	1:A:106:PRO:CD	2.79	0.45
2:D:37:PHE:CZ	2:D:173:LEU:HD22	2.52	0.45
2:B:299:PRO:HD3	2:B:307:TRP:CD2	2.52	0.45
1:E:100:PRO:HG3	1:E:108:ILE:CG2	2.47	0.45
2:F:143:LYS:HB2	2:F:167:VAL:HG22	1.99	0.45
2:H:286:ALA:HB1	2:H:287:PRO:CD	2.43	0.45
1:C:109:ILE:CD1	1:C:118:ALA:HB2	2.44	0.45
2:H:298:TYR:CD2	2:H:299:PRO:HD2	2.52	0.45
2:B:25:ILE:HD13	2:B:77:VAL:HB	1.98	0.45
3:J:137:LYS:O	3:J:141:GLU:HG3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:115:ARG:NE	2:H:171:GLU:OE2	2.48	0.45
2:D:93:ILE:HA	2:D:97:MET:HG2	1.99	0.45
1:A:225:ALA:HB2	1:C:225:ALA:HB2	1.98	0.45
3:I:166:PHE:O	3:I:168:ALA:N	2.50	0.44
1:G:155:ALA:HB2	1:G:195:ALA:HB2	1.98	0.44
1:C:51:ARG:HG2	1:C:317:VAL:HG21	1.99	0.44
1:E:67:ASN:ND2	1:E:73:GLY:O	2.51	0.44
3:I:157:ARG:HG2	3:I:159:LEU:HD23	2.00	0.44
2:B:8:ALA:HB1	2:B:154:LYS:HB2	1.98	0.44
1:C:351:LEU:O	1:C:356:LYS:HE3	2.17	0.44
2:H:268:ILE:C	2:H:268:ILE:HD12	2.37	0.44
2:F:1:ALA:HB3	7:F:1442:HOH:O	2.17	0.44
1:E:105:VAL:N	1:E:106:PRO:CD	2.79	0.44
2:F:98:ALA:HB2	2:F:142:LEU:CD2	2.48	0.44
2:F:162:ARG:NH2	2:F:187:GLU:OE1	2.47	0.44
2:D:74:PHE:O	2:D:76:PRO:HD3	2.18	0.44
2:D:268:ILE:HD12	2:D:268:ILE:C	2.37	0.44
2:F:238:VAL:HB	2:F:268:ILE:HG12	1.99	0.44
2:F:34:GLY:O	2:F:38:ARG:HA	2.17	0.44
1:G:306:LYS:NZ	1:G:306:LYS:HB3	2.33	0.44
2:F:202:LYS:HB3	2:F:202:LYS:NZ	2.33	0.44
7:E:1463:HOH:O	1:G:12:GLN:HB2	2.17	0.44
2:H:168:ILE:H	2:H:168:ILE:HD12	1.83	0.44
3:I:128:ARG:HB3	3:I:129:VAL:H	1.53	0.44
1:G:254:ASN:HB3	7:G:1465:HOH:O	2.16	0.44
2:B:12:ALA:HB3	2:B:157:LEU:HD23	1.99	0.44
1:C:236:MET:CE	1:C:295:PRO:HD3	2.48	0.44
1:C:153:GLY:HA2	2:D:65:LEU:HD12	2.00	0.44
1:G:209:PRO:HB2	1:G:211:GLU:OE2	2.18	0.44
3:I:159:LEU:CD1	3:I:161:GLU:OE1	2.66	0.43
2:B:17:LEU:O	2:B:51:ARG:NH1	2.46	0.43
2:H:70:ALA:HB1	2:H:111:PRO:HD2	2.00	0.43
1:A:202:ASN:HA	1:A:265:CYS:O	2.18	0.43
3:I:146:ILE:HD11	3:I:158:VAL:HG22	2.00	0.43
1:E:123:ARG:NH2	1:E:333:ASP:OD1	2.49	0.43
1:E:131:ILE:HD13	2:F:108:TYR:HE2	1.84	0.43
2:B:277:ASN:O	2:B:281:ILE:HB	2.17	0.43
1:E:203:ARG:O	1:E:210:VAL:N	2.50	0.43
2:D:20:ASP:HA	2:D:21:PRO:HD2	1.88	0.43
2:D:277:ASN:HB2	7:D:1494:HOH:O	2.19	0.43
2:F:299:PRO:HA	2:H:102:TYR:HH	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:147:ARG:HE	3:I:147:ARG:HB3	1.12	0.43
1:G:211:GLU:CD	1:G:211:GLU:H	2.22	0.43
1:A:362:TYR:O	1:A:366:GLU:HG3	2.19	0.43
2:H:20:ASP:HA	2:H:21:PRO:HD2	1.87	0.43
2:B:29:ASP:HB3	7:B:1373:HOH:O	2.19	0.43
1:C:131:ILE:HD13	1:C:137:VAL:HG23	2.01	0.43
1:G:92:LEU:HD11	1:G:168:ILE:HG21	2.01	0.43
2:B:124:THR:HB	2:B:125:PRO:HD2	1.99	0.43
1:E:98:ILE:HB	1:E:137:VAL:HG12	2.00	0.43
1:G:271:HIS:CE1	6:G:1370:TPW:S1	3.12	0.43
1:E:38:MET:SD	1:E:39:PRO:HD2	2.59	0.43
2:B:202:LYS:HG3	7:B:1454:HOH:O	2.19	0.42
1:A:217:LYS:HA	1:A:217:LYS:HD3	1.79	0.42
1:G:228:ILE:HG21	1:G:258:PRO:HG2	2.01	0.42
1:G:246:LYS:HE3	7:G:1478:HOH:O	2.19	0.42
1:A:200:GLN:NE2	7:A:1378:HOH:O	2.52	0.42
1:E:95:GLU:H	1:E:95:GLU:HG2	1.60	0.42
1:A:321:ALA:O	1:A:325:ILE:HG13	2.19	0.42
3:I:154:LYS:O	3:I:155:ASN:CB	2.46	0.42
3:J:146:ILE:CG2	3:J:147:ARG:N	2.81	0.42
1:A:275:GLY:HA2	1:A:276:ASP:HA	1.54	0.42
3:J:153:GLY:O	3:J:156:GLY:N	2.52	0.42
1:G:60:ASP:O	1:G:64:ILE:HG13	2.19	0.42
3:I:129:VAL:HG22	3:I:130:ILE:N	2.34	0.42
2:F:308:LEU:HA	2:F:309:PRO:HD3	1.91	0.42
1:A:237:ASP:O	1:A:241:VAL:HG23	2.20	0.42
2:D:255:ARG:NH2	2:D:285:GLU:HG2	2.35	0.42
3:J:131:ALA:HA	3:J:157:ARG:HG3	2.01	0.42
2:D:18:LYS:HA	2:D:18:LYS:HE3	2.01	0.42
1:C:114:PRO:HD2	1:C:117:GLN:OE1	2.19	0.42
2:H:219:ALA:HA	2:H:315:ILE:HD11	2.02	0.42
1:A:255:GLY:HA2	7:A:1498:HOH:O	2.20	0.42
1:G:116:TYR:OH	7:G:1489:HOH:O	2.21	0.42
1:A:253:ILE:C	1:A:253:ILE:HD12	2.40	0.42
1:C:355:LEU:HD23	1:C:355:LEU:HA	1.94	0.42
3:I:159:LEU:HB3	3:I:161:GLU:OE1	2.15	0.42
2:B:199:ARG:O	2:B:231:GLU:HA	2.20	0.42
1:A:120:LEU:HD11	1:A:335:THR:HG21	2.00	0.42
1:A:292:LYS:N	1:A:292:LYS:CD	2.77	0.42
2:F:82:PHE:HB2	2:F:85:PHE:CE2	2.55	0.42
2:B:242:ASP:O	2:B:246:ILE:HG13	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:THR:HA	1:A:336:PRO:HD3	1.91	0.41
1:C:203:ARG:HD2	1:C:203:ARG:HA	1.83	0.41
1:A:229:PRO:HB2	1:C:9:PHE:CD1	2.56	0.41
2:B:238:VAL:HB	2:B:268:ILE:HG12	2.01	0.41
2:F:58:ALA:O	2:F:62:ILE:HG13	2.19	0.41
1:E:83:ALA:O	1:E:87:ALA:HB3	2.21	0.41
2:H:139:GLN:HB3	2:H:142:LEU:HD12	2.02	0.41
2:H:168:ILE:CD1	2:H:168:ILE:N	2.82	0.41
1:G:351:LEU:HA	1:G:352:PRO:HD3	1.86	0.41
2:B:201:GLY:N	2:B:231:GLU:HB2	2.35	0.41
1:G:129:ASN:O	1:G:131:ILE:CD1	2.67	0.41
2:D:281:ILE:HG23	2:D:282:LEU:N	2.35	0.41
2:H:25:ILE:O	2:H:52:VAL:HA	2.21	0.41
3:J:162:ASP:OD1	3:J:162:ASP:N	2.50	0.41
1:G:143:ILE:HD12	2:H:96:GLN:HE21	1.85	0.41
2:F:16:GLU:OE2	2:F:158:ILE:HG23	2.20	0.41
3:J:145:ASP:OD1	3:J:145:ASP:C	2.58	0.41
1:A:123:ARG:HH21	1:A:329:ILE:HD11	1.86	0.41
2:B:282:LEU:HA	3:I:134:SER:HB2	2.03	0.41
1:G:26:LEU:HG	1:G:239:LEU:HD12	2.03	0.41
1:G:64:ILE:HG12	1:G:273:MET:HE2	2.03	0.41
1:G:48:GLU:HG3	1:G:51:ARG:HH21	1.86	0.40
1:G:236:MET:CE	1:G:295:PRO:HD3	2.50	0.40
1:E:123:ARG:NH1	1:E:333:ASP:OD1	2.51	0.40
1:G:203:ARG:HG3	7:G:1399:HOH:O	2.21	0.40
1:A:340:VAL:O	1:A:344:ILE:HG13	2.22	0.40
2:H:239:GLN:HA	2:H:240:PRO:HA	1.97	0.40
2:B:92:SER:O	2:B:97:MET:HG2	2.22	0.40
2:B:142:LEU:HD23	2:B:166:PRO:HB2	2.04	0.40
3:I:157:ARG:HH11	3:I:157:ARG:HD2	1.73	0.40
3:I:157:ARG:HG2	3:I:159:LEU:CD2	2.52	0.40
2:B:57:LEU:CD1	6:C:1370:TPW:H4A3	2.51	0.40
1:E:102:TYR:HE2	1:E:144:ILE:HD11	1.87	0.40
2:F:92:SER:O	2:F:97:MET:HG2	2.21	0.40
1:C:323:GLU:O	1:C:326:LYS:HB3	2.21	0.40
3:I:139:ALA:HB2	3:I:163:ILE:CD1	2.46	0.40
2:B:239:GLN:HA	2:B:240:PRO:HA	1.84	0.40
1:E:154:VAL:HG13	2:F:72:GLN:HE21	1.86	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	363/369 (98%)	352 (97%)	11 (3%)	0	100	100
1	C	363/369 (98%)	350 (96%)	13 (4%)	0	100	100
1	E	350/369 (95%)	339 (97%)	11 (3%)	0	100	100
1	G	363/369 (98%)	353 (97%)	10 (3%)	0	100	100
2	B	322/325 (99%)	315 (98%)	6 (2%)	1 (0%)	46	55
2	D	322/325 (99%)	312 (97%)	9 (3%)	1 (0%)	46	55
2	F	322/325 (99%)	307 (95%)	12 (4%)	3 (1%)	21	22
2	H	322/325 (99%)	307 (95%)	15 (5%)	0	100	100
3	I	40/428 (9%)	31 (78%)	4 (10%)	5 (12%)	0	0
3	J	38/428 (9%)	30 (79%)	6 (16%)	2 (5%)	2	0
All	All	2805/3632 (77%)	2696 (96%)	97 (4%)	12 (0%)	39	46

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	236	ARG
3	J	165	ALA
2	F	301	ALA
3	I	161	GLU
3	I	167	LEU
2	D	236	ARG
2	F	236	ARG
3	I	136	ARG
3	I	160	LYS
3	I	155	ASN
3	J	157	ARG
2	F	31	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	301/304 (99%)	293 (97%)	8 (3%)	52	67
1	C	301/304 (99%)	299 (99%)	2 (1%)	88	95
1	E	290/304 (95%)	289 (100%)	1 (0%)	94	98
1	G	301/304 (99%)	298 (99%)	3 (1%)	82	91
2	B	263/264 (100%)	260 (99%)	3 (1%)	80	90
2	D	263/264 (100%)	260 (99%)	3 (1%)	80	90
2	F	263/264 (100%)	260 (99%)	3 (1%)	80	90
2	H	263/264 (100%)	262 (100%)	1 (0%)	93	97
3	I	30/341 (9%)	21 (70%)	9 (30%)	0	0
3	J	28/341 (8%)	20 (71%)	8 (29%)	0	0
All	All	2303/2954 (78%)	2262 (98%)	41 (2%)	66	81

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	GLU
1	A	36	GLU
1	A	173	ASP
1	A	276	ASP
1	A	277	ASP
1	A	280	ARG
1	A	292	LYS
1	A	329	ILE
2	B	78	PRO
2	B	130	ASP
2	B	241	LEU
1	C	173	ASP
1	C	292	LYS
2	D	50	ASP
2	D	130	ASP
2	D	187	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	368	LYS
2	F	50	ASP
2	F	130	ASP
2	F	302	GLN
1	G	36	GLU
1	G	173	ASP
1	G	211	GLU
2	H	130	ASP
3	I	128	ARG
3	I	129	VAL
3	I	137	LYS
3	I	141	GLU
3	I	147	ARG
3	I	148	LEU
3	I	155	ASN
3	I	157	ARG
3	I	159	LEU
3	J	128	ARG
3	J	129	VAL
3	J	146	ILE
3	J	148	LEU
3	J	150	GLN
3	J	155	ASN
3	J	159	LEU
3	J	164	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	288	ASN
2	B	33	ASN
2	B	123	HIS
2	B	239	GLN
1	C	19	GLN
1	C	69	GLN
2	D	72	GLN
2	D	109	HIS
2	D	123	HIS
2	D	271	ASN
1	E	81	GLN
1	E	288	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	72	GLN
2	F	214	HIS
2	F	302	GLN
1	G	69	GLN
1	G	271	HIS
2	H	271	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	TPW	A	1370	4	22,27,27	1.30	2 (9%)	31,40,40	1.72	8 (25%)
6	TPW	C	1370	4	22,27,27	1.35	2 (9%)	31,40,40	1.82	8 (25%)
6	TPW	E	1370	4	22,27,27	1.38	3 (13%)	31,40,40	1.77	10 (32%)
6	TPW	G	1370	4	22,27,27	1.35	3 (13%)	31,40,40	1.74	8 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	TPW	A	1370	4	-	0/15/17/17	0/2/2/2
6	TPW	C	1370	4	-	0/15/17/17	0/2/2/2
6	TPW	E	1370	4	-	0/15/17/17	0/2/2/2
6	TPW	G	1370	4	-	0/15/17/17	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	1370	TPW	C2-C3	-3.65	1.34	1.37
6	C	1370	TPW	C2-C3	-3.50	1.34	1.37
6	G	1370	TPW	C2-C3	-3.39	1.35	1.37
6	A	1370	TPW	C2-C3	-3.14	1.35	1.37
6	G	1370	TPW	P2-O23	2.08	1.62	1.54
6	E	1370	TPW	P2-O23	2.15	1.62	1.54
6	A	1370	TPW	P2-O22	3.07	1.61	1.51
6	C	1370	TPW	P2-O22	3.08	1.61	1.51
6	G	1370	TPW	P2-O22	3.14	1.61	1.51
6	E	1370	TPW	P2-O22	3.22	1.61	1.51

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1370	TPW	C3-C2-S1	-3.88	108.13	112.26
6	A	1370	TPW	C3-C2-S1	-3.61	108.42	112.26
6	G	1370	TPW	P1-O11-P2	-3.61	120.58	132.67
6	E	1370	TPW	C3-C2-S1	-3.59	108.44	112.26
6	C	1370	TPW	C35-C5'-C6'	-3.46	116.58	121.72
6	C	1370	TPW	P1-O11-P2	-3.45	121.10	132.67
6	G	1370	TPW	C3-C2-S1	-3.31	108.73	112.26
6	E	1370	TPW	P1-O11-P2	-3.28	121.66	132.67
6	A	1370	TPW	C35-C5'-C6'	-3.16	117.04	121.72
6	G	1370	TPW	C35-C5'-C6'	-3.09	117.14	121.72
6	E	1370	TPW	C35-C5'-C6'	-2.96	117.33	121.72
6	C	1370	TPW	N1'-C2'-N3'	-2.87	120.28	125.60
6	A	1370	TPW	P1-O11-P2	-2.87	123.03	132.67
6	E	1370	TPW	N1'-C2'-N3'	-2.81	120.41	125.60
6	A	1370	TPW	N1'-C2'-N3'	-2.74	120.53	125.60
6	G	1370	TPW	N1'-C2'-N3'	-2.57	120.84	125.60
6	E	1370	TPW	O23-P2-O22	-2.17	103.60	110.58
6	G	1370	TPW	O21-P2-O11	2.00	114.17	105.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1370	TPW	O21-P2-O11	2.05	114.40	105.09
6	E	1370	TPW	C2A-C2'-N1'	2.08	119.52	117.03
6	E	1370	TPW	O21-P2-O11	2.09	114.59	105.09
6	E	1370	TPW	C5A-C5-S1	2.10	123.18	120.24
6	C	1370	TPW	C5A-C5-S1	2.11	123.19	120.24
6	G	1370	TPW	C35-C5'-C4'	2.28	125.13	122.21
6	A	1370	TPW	O21-P2-O11	2.28	115.46	105.09
6	E	1370	TPW	C35-C5'-C4'	2.40	125.28	122.21
6	G	1370	TPW	C5A-C5-S1	2.49	123.72	120.24
6	A	1370	TPW	C2A-C2'-N1'	2.56	120.11	117.03
6	A	1370	TPW	C35-C5'-C4'	2.65	125.60	122.21
6	G	1370	TPW	C6'-N1'-C2'	2.89	120.83	115.77
6	A	1370	TPW	C6'-N1'-C2'	3.02	121.04	115.77
6	E	1370	TPW	C6'-N1'-C2'	3.12	121.22	115.77
6	C	1370	TPW	C35-C5'-C4'	3.14	126.22	122.21
6	C	1370	TPW	C6'-N1'-C2'	3.31	121.56	115.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1370	TPW	1	0
6	C	1370	TPW	3	0
6	E	1370	TPW	1	0
6	G	1370	TPW	3	0

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	365/369 (98%)	0.10	17 (4%) 35 50	15, 25, 44, 58	2 (0%)
1	C	365/369 (98%)	-0.02	7 (1%) 70 81	14, 24, 45, 58	2 (0%)
1	E	354/369 (95%)	0.06	6 (1%) 73 83	21, 32, 48, 60	2 (0%)
1	G	365/369 (98%)	-0.03	4 (1%) 82 90	20, 29, 48, 55	2 (0%)
2	B	324/325 (99%)	-0.23	0 100 100	16, 24, 34, 38	0
2	D	324/325 (99%)	-0.18	0 100 100	15, 20, 27, 30	0
2	F	324/325 (99%)	-0.12	0 100 100	21, 27, 34, 36	0
2	H	324/325 (99%)	-0.12	1 (0%) 94 97	21, 25, 31, 32	0
3	I	42/428 (9%)	1.20	9 (21%) 1 2	22, 62, 70, 74	0
3	J	40/428 (9%)	1.06	9 (22%) 1 2	20, 53, 75, 78	0
All	All	2827/3632 (77%)	-0.03	53 (1%) 70 81	14, 26, 47, 78	8 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	283	SER	8.3
1	A	281	TYR	6.1
1	A	286	LEU	6.1
1	A	280	ARG	5.4
3	I	128	ARG	5.4
1	C	286	LEU	5.4
1	A	276	ASP	5.3
3	I	148	LEU	5.0
1	E	290	TRP	4.2
1	A	284	LYS	3.9
1	G	277	ASP	3.8
3	I	155	ASN	3.7
1	E	276	ASP	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	282	ARG	3.5
1	A	289	GLU	3.4
1	A	275	GLY	3.3
3	J	149	VAL	3.1
1	A	287	GLU	3.1
3	J	129	VAL	3.1
1	G	4	THR	3.0
1	A	274	SER	2.9
3	I	129	VAL	2.9
1	A	277	ASP	2.9
3	J	150	GLN	2.8
1	E	271	HIS	2.8
1	A	285	GLU	2.7
1	C	277	ASP	2.7
3	I	146	ILE	2.7
3	J	128	ARG	2.7
1	A	290	TRP	2.6
1	C	281	TYR	2.6
3	J	163	ILE	2.6
1	E	266	PHE	2.5
1	A	278	PRO	2.5
3	J	141	GLU	2.5
1	C	279	THR	2.5
1	E	51	ARG	2.4
1	E	275	GLY	2.4
1	A	368	LYS	2.4
1	G	31	GLU	2.3
3	I	169	GLY	2.3
1	C	283	SER	2.3
3	J	164	ASP	2.3
1	A	279	THR	2.3
1	C	285	GLU	2.3
3	J	148	LEU	2.2
3	I	147	ARG	2.2
3	I	144	VAL	2.2
1	C	289	GLU	2.2
3	J	146	ILE	2.2
1	G	290	TRP	2.1
3	I	166	PHE	2.0
2	H	277	ASN	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	MG	E	369	1/1	0.65	0.32	9.24	45,45,45,45	0
4	MG	A	1326	1/1	0.85	0.20	5.10	30,30,30,30	0
4	MG	A	1368	1/1	0.97	0.13	0.15	3,3,3,3	0
6	TPW	A	1370	26/26	0.98	0.12	-0.40	13,13,15,15	0
4	MG	C	1368	1/1	0.99	0.11	-0.45	7,7,7,7	0
6	TPW	G	1370	26/26	0.97	0.12	-0.55	23,23,24,24	0
4	MG	G	369	1/1	0.93	0.11	-0.71	16,16,16,16	0
6	TPW	C	1370	26/26	0.98	0.10	-0.74	12,12,13,13	0
6	TPW	E	1370	26/26	0.97	0.10	-0.76	19,20,20,20	0
5	K	D	1325	1/1	0.99	0.06	-3.63	10,10,10,10	0
4	MG	E	370	1/1	0.94	0.08	-4.14	33,33,33,33	0
5	K	B	1325	1/1	0.99	0.04	-4.59	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.