



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 17, 2023 – 10:55 AM EST

PDB ID : 2GB3
Title : Crystal structure of Aspartate aminotransferase (tm1698) from *Thermotoga maritima* at 2.50 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2006-03-09
Resolution : 2.50 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.2
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) : 2.31.2

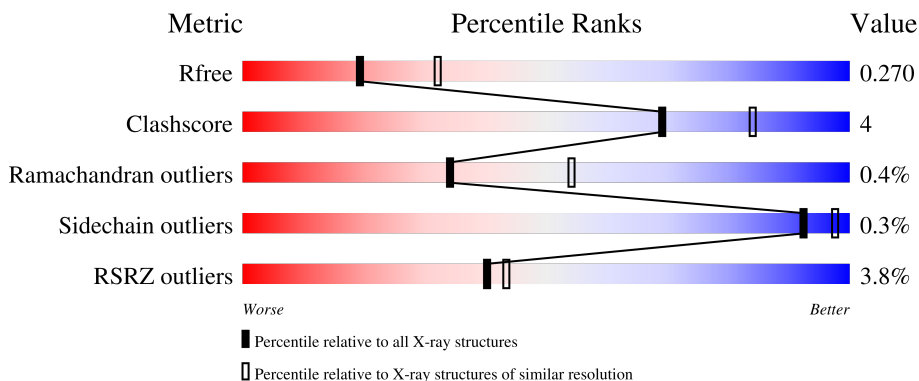
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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.



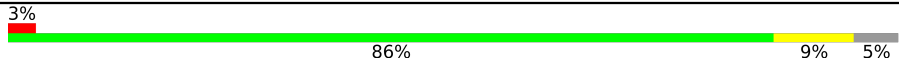
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	409	
1	B	409	
1	C	409	
1	D	409	
1	E	409	

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Mol	Chain	Length	Quality of chain
1	F	409	 <p>3% 86% 9% 5%</p>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 18415 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 aspartate aminotransferase.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S	Se			
1	A	389	3047	1968	513	551	1	5	9	0	3	0
1	B	394	3070	1985	514	556	1	5	9	0	1	0
1	C	391	3047	1969	508	556	1	5	8	0	1	0
1	D	390	3012	1943	495	562	1	4	7	0	0	0
1	E	393	3031	1959	502	557	1	5	7	0	0	0
1	F	389	3018	1953	504	547	1	5	8	0	0	0

There are 138 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MSE	-	expression tag	GB 4982275
A	-10	GLY	-	expression tag	GB 4982275
A	-9	SER	-	expression tag	GB 4982275
A	-8	ASP	-	expression tag	GB 4982275
A	-7	LYS	-	expression tag	GB 4982275
A	-6	ILE	-	expression tag	GB 4982275
A	-5	HIS	-	expression tag	GB 4982275
A	-4	HIS	-	expression tag	GB 4982275
A	-3	HIS	-	expression tag	GB 4982275
A	-2	HIS	-	expression tag	GB 4982275
A	-1	HIS	-	expression tag	GB 4982275
A	0	HIS	-	expression tag	GB 4982275
A	1	MSE	MET	modified residue	GB 4982275
A	25	MSE	MET	modified residue	GB 4982275
A	145	MSE	MET	modified residue	GB 4982275
A	184	MSE	MET	modified residue	GB 4982275
A	232	LLP	LYS	modified residue	GB 4982275

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Chain	Residue	Modelled	Actual	Comment	Reference
A	256	MSE	MET	modified residue	GB 4982275
A	335	MSE	MET	modified residue	GB 4982275
A	341	MSE	MET	modified residue	GB 4982275
A	347	MSE	MET	modified residue	GB 4982275
A	384	MSE	MET	modified residue	GB 4982275
A	389	MSE	MET	modified residue	GB 4982275
B	-11	MSE	-	expression tag	GB 4982275
B	-10	GLY	-	expression tag	GB 4982275
B	-9	SER	-	expression tag	GB 4982275
B	-8	ASP	-	expression tag	GB 4982275
B	-7	LYS	-	expression tag	GB 4982275
B	-6	ILE	-	expression tag	GB 4982275
B	-5	HIS	-	expression tag	GB 4982275
B	-4	HIS	-	expression tag	GB 4982275
B	-3	HIS	-	expression tag	GB 4982275
B	-2	HIS	-	expression tag	GB 4982275
B	-1	HIS	-	expression tag	GB 4982275
B	0	HIS	-	expression tag	GB 4982275
B	1	MSE	MET	modified residue	GB 4982275
B	25	MSE	MET	modified residue	GB 4982275
B	145	MSE	MET	modified residue	GB 4982275
B	184	MSE	MET	modified residue	GB 4982275
B	232	LLP	LYS	modified residue	GB 4982275
B	256	MSE	MET	modified residue	GB 4982275
B	335	MSE	MET	modified residue	GB 4982275
B	341	MSE	MET	modified residue	GB 4982275
B	347	MSE	MET	modified residue	GB 4982275
B	384	MSE	MET	modified residue	GB 4982275
B	389	MSE	MET	modified residue	GB 4982275
C	-11	MSE	-	expression tag	GB 4982275
C	-10	GLY	-	expression tag	GB 4982275
C	-9	SER	-	expression tag	GB 4982275
C	-8	ASP	-	expression tag	GB 4982275
C	-7	LYS	-	expression tag	GB 4982275
C	-6	ILE	-	expression tag	GB 4982275
C	-5	HIS	-	expression tag	GB 4982275
C	-4	HIS	-	expression tag	GB 4982275
C	-3	HIS	-	expression tag	GB 4982275
C	-2	HIS	-	expression tag	GB 4982275
C	-1	HIS	-	expression tag	GB 4982275
C	0	HIS	-	expression tag	GB 4982275
C	1	MSE	MET	modified residue	GB 4982275

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Chain	Residue	Modelled	Actual	Comment	Reference
C	25	MSE	MET	modified residue	GB 4982275
C	145	MSE	MET	modified residue	GB 4982275
C	184	MSE	MET	modified residue	GB 4982275
C	232	LLP	LYS	modified residue	GB 4982275
C	256	MSE	MET	modified residue	GB 4982275
C	335	MSE	MET	modified residue	GB 4982275
C	341	MSE	MET	modified residue	GB 4982275
C	347	MSE	MET	modified residue	GB 4982275
C	384	MSE	MET	modified residue	GB 4982275
C	389	MSE	MET	modified residue	GB 4982275
D	-11	MSE	-	expression tag	GB 4982275
D	-10	GLY	-	expression tag	GB 4982275
D	-9	SER	-	expression tag	GB 4982275
D	-8	ASP	-	expression tag	GB 4982275
D	-7	LYS	-	expression tag	GB 4982275
D	-6	ILE	-	expression tag	GB 4982275
D	-5	HIS	-	expression tag	GB 4982275
D	-4	HIS	-	expression tag	GB 4982275
D	-3	HIS	-	expression tag	GB 4982275
D	-2	HIS	-	expression tag	GB 4982275
D	-1	HIS	-	expression tag	GB 4982275
D	0	HIS	-	expression tag	GB 4982275
D	1	MSE	MET	modified residue	GB 4982275
D	25	MSE	MET	modified residue	GB 4982275
D	145	MSE	MET	modified residue	GB 4982275
D	184	MSE	MET	modified residue	GB 4982275
D	232	LLP	LYS	modified residue	GB 4982275
D	256	MSE	MET	modified residue	GB 4982275
D	335	MSE	MET	modified residue	GB 4982275
D	341	MSE	MET	modified residue	GB 4982275
D	347	MSE	MET	modified residue	GB 4982275
D	384	MSE	MET	modified residue	GB 4982275
D	389	MSE	MET	modified residue	GB 4982275
E	-11	MSE	-	expression tag	GB 4982275
E	-10	GLY	-	expression tag	GB 4982275
E	-9	SER	-	expression tag	GB 4982275
E	-8	ASP	-	expression tag	GB 4982275
E	-7	LYS	-	expression tag	GB 4982275
E	-6	ILE	-	expression tag	GB 4982275
E	-5	HIS	-	expression tag	GB 4982275
E	-4	HIS	-	expression tag	GB 4982275
E	-3	HIS	-	expression tag	GB 4982275

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	HIS	-	expression tag	GB 4982275
E	-1	HIS	-	expression tag	GB 4982275
E	0	HIS	-	expression tag	GB 4982275
E	1	MSE	MET	modified residue	GB 4982275
E	25	MSE	MET	modified residue	GB 4982275
E	145	MSE	MET	modified residue	GB 4982275
E	184	MSE	MET	modified residue	GB 4982275
E	232	LLP	LYS	modified residue	GB 4982275
E	256	MSE	MET	modified residue	GB 4982275
E	335	MSE	MET	modified residue	GB 4982275
E	341	MSE	MET	modified residue	GB 4982275
E	347	MSE	MET	modified residue	GB 4982275
E	384	MSE	MET	modified residue	GB 4982275
E	389	MSE	MET	modified residue	GB 4982275
F	-11	MSE	-	expression tag	GB 4982275
F	-10	GLY	-	expression tag	GB 4982275
F	-9	SER	-	expression tag	GB 4982275
F	-8	ASP	-	expression tag	GB 4982275
F	-7	LYS	-	expression tag	GB 4982275
F	-6	ILE	-	expression tag	GB 4982275
F	-5	HIS	-	expression tag	GB 4982275
F	-4	HIS	-	expression tag	GB 4982275
F	-3	HIS	-	expression tag	GB 4982275
F	-2	HIS	-	expression tag	GB 4982275
F	-1	HIS	-	expression tag	GB 4982275
F	0	HIS	-	expression tag	GB 4982275
F	1	MSE	MET	modified residue	GB 4982275
F	25	MSE	MET	modified residue	GB 4982275
F	145	MSE	MET	modified residue	GB 4982275
F	184	MSE	MET	modified residue	GB 4982275
F	232	LLP	LYS	modified residue	GB 4982275
F	256	MSE	MET	modified residue	GB 4982275
F	335	MSE	MET	modified residue	GB 4982275
F	341	MSE	MET	modified residue	GB 4982275
F	347	MSE	MET	modified residue	GB 4982275
F	384	MSE	MET	modified residue	GB 4982275
F	389	MSE	MET	modified residue	GB 4982275

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	33	Total O 33 33	0	0

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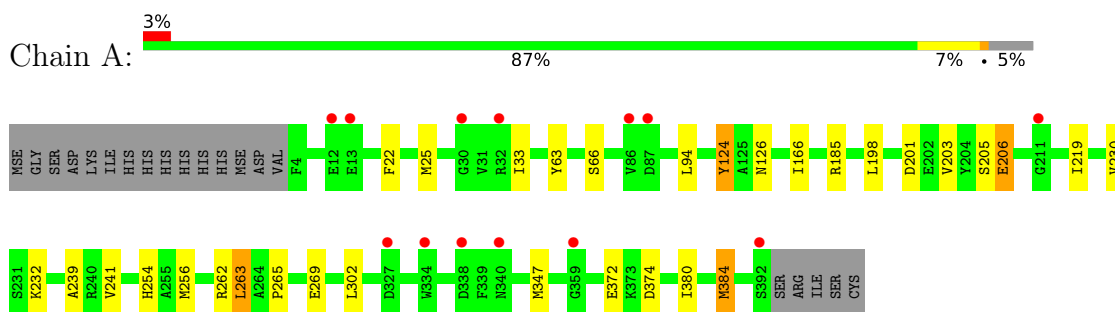
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	38	Total O 38 38	0	0
2	C	31	Total O 31 31	0	0
2	D	18	Total O 18 18	0	0
2	E	28	Total O 28 28	0	0
2	F	42	Total O 42 42	0	0

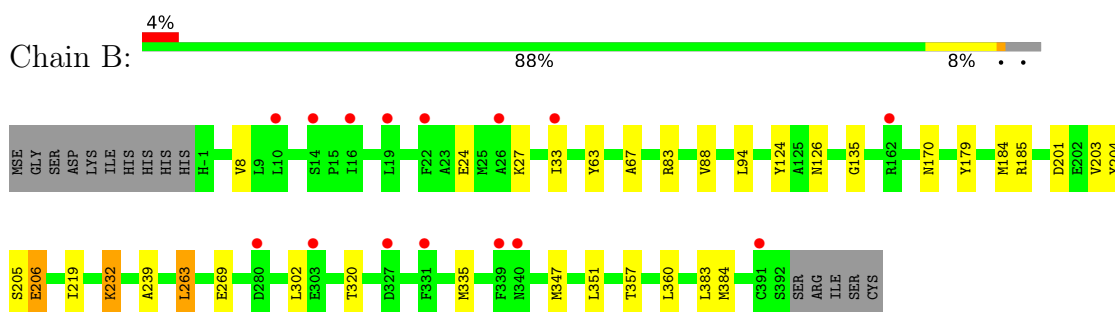
3 Residue-property plots [i](#)

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.

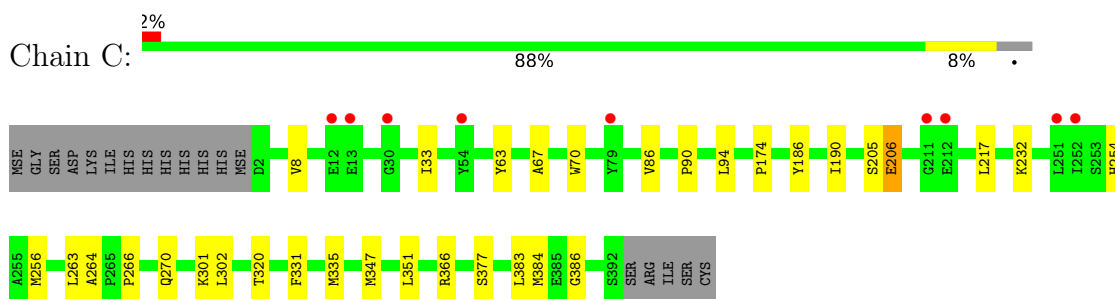
- Molecule 1: aspartate aminotransferase



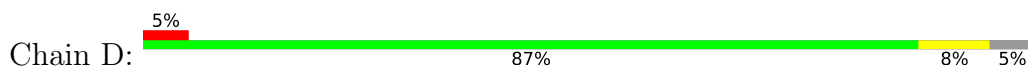
- Molecule 1: aspartate aminotransferase

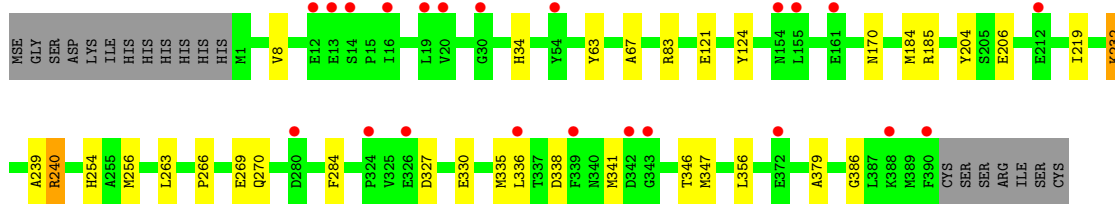


- Molecule 1: aspartate aminotransferase

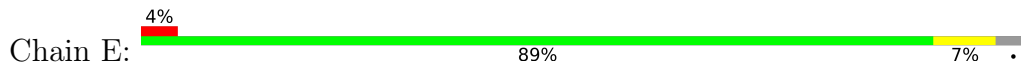


- Molecule 1: aspartate aminotransferase

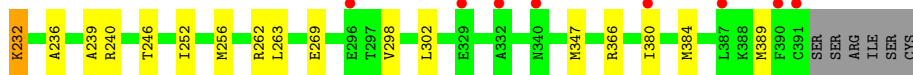
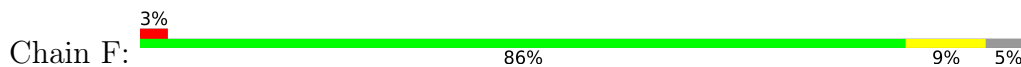




• Molecule 1: aspartate aminotransferase



• Molecule 1: aspartate aminotransferase



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.09Å 214.05Å 76.84Å 90.00° 112.31° 90.00°	Depositor
Resolution (Å)	107.03 – 2.50 107.03 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.5 (107.03-2.50) 97.8 (107.03-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.48Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.229 , 0.266 0.237 , 0.270	Depositor DCC
R_{free} test set	3791 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	36.8	Xtrriage
Anisotropy	0.536	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 66.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.000 for l,-k,h	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18415	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 75.86 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1638e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LLP

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	0.43	0/3083	0.74	1/4163 (0.0%)
1	B	0.42	0/3104	0.75	0/4191
1	C	0.44	0/3077	0.73	0/4157
1	D	0.39	0/3042	0.72	1/4118 (0.0%)
1	E	0.43	0/3062	0.74	1/4143 (0.0%)
1	F	0.46	0/3048	0.75	0/4119
All	All	0.43	0/18416	0.74	3/24891 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	240	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	E	7	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	384	MSE	CA-CB-CG	-5.15	104.55	113.30

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	3047	0	3008	21	0
1	B	3070	0	3025	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3047	0	2997	26	0
1	D	3012	0	2914	22	0
1	E	3031	0	2938	19	0
1	F	3018	0	2974	29	0
2	A	33	0	0	0	0
2	B	38	0	0	1	0
2	C	31	0	0	0	0
2	D	18	0	0	0	0
2	E	28	0	0	1	0
2	F	42	0	0	1	0
All	All	18415	0	17856	133	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 4.

All (133) 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:D:346:THR:HG21	1:D:379:ALA:O	1.86	0.75
1:D:34:HIS:HB2	1:D:346:THR:HG22	1.70	0.73
1:B:33:ILE:HG21	1:B:347:MSE:HE3	1.71	0.71
1:E:112:ASN:HD22	1:E:113:PRO:HD2	1.54	0.70
1:C:254:HIS:HB3	1:D:8:VAL:HG21	1.77	0.66
1:F:33:ILE:HG21	1:F:347:MSE:HE3	1.78	0.65
1:A:254:HIS:HB3	1:B:8:VAL:HG21	1.77	0.65
1:A:33:ILE:HG21	1:A:347:MSE:HE3	1.78	0.65
1:C:331:PHE:CZ	1:C:335:MSE:HE2	2.31	0.65
1:C:301:LYS:NZ	1:C:377:SER:OG	2.30	0.64
1:F:67:ALA:HB2	1:F:256:MSE:SE	2.48	0.64
1:D:336:LEU:HD21	1:D:347:MSE:CG	2.28	0.64
1:F:184:MSE:HA	1:F:184:MSE:HE2	1.78	0.63
1:F:389:MSE:HA	1:F:389:MSE:HE2	1.79	0.63
1:B:83:ARG:HG2	1:B:206:GLU:OE2	1.99	0.62
1:C:33:ILE:HG21	1:C:347:MSE:HE3	1.83	0.61
1:C:335:MSE:HE3	1:C:383:LEU:HD12	1.83	0.60
1:F:230:VAL:HG12	1:F:236:ALA:HB3	1.83	0.60
1:E:336:LEU:HD21	1:E:347:MSE:CG	2.32	0.59
1:B:302:LEU:CD2	1:B:384:MSE:HE3	2.33	0.59
1:A:239:ALA:O	1:A:269:GLU:HG2	2.03	0.59
1:E:112:ASN:HD22	1:E:113:PRO:CD	2.14	0.58
1:C:335:MSE:HE1	1:C:386:GLY:HA3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:298:VAL:HG22	1:F:380:ILE:HD11	1.87	0.56
1:F:33:ILE:HG21	1:F:347:MSE:CE	2.36	0.56
1:A:63:TYR:CZ	1:A:263:LEU:HD13	2.41	0.55
1:B:335:MSE:HE2	1:B:383:LEU:HA	1.89	0.55
1:F:63:TYR:CZ	1:F:263:LEU:HD13	2.42	0.55
1:F:298:VAL:HG13	1:F:380:ILE:CD1	2.37	0.55
1:E:205:SER:O	1:E:206:GLU:CB	2.55	0.54
1:F:298:VAL:HG13	1:F:380:ILE:HD13	1.89	0.54
1:A:380:ILE:CG2	1:A:384:MSE:HE2	2.38	0.54
1:A:201:ASP:OD1	1:A:203:VAL:HG23	2.09	0.53
1:B:239:ALA:O	1:B:269:GLU:HG2	2.09	0.53
1:C:33:ILE:HG21	1:C:347:MSE:CE	2.39	0.53
1:A:269:GLU:N	1:A:269:GLU:OE1	2.41	0.53
1:C:302:LEU:HA	1:C:384:MSE:HE3	1.91	0.53
1:B:201:ASP:OD1	1:B:203:VAL:HG23	2.10	0.52
1:D:170:ASN:HD22	1:D:184:MSE:HE3	1.74	0.52
1:D:336:LEU:HD21	1:D:347:MSE:HG2	1.93	0.51
1:A:22:PHE:HA	1:A:25:MSE:HE2	1.93	0.51
1:B:185:ARG:HA	1:B:219:ILE:HD13	1.93	0.51
1:C:63:TYR:CZ	1:C:263:LEU:HD13	2.46	0.51
1:B:357:THR:OG1	1:B:360:LEU:HD12	2.10	0.51
1:A:124:TYR:CE2	1:A:126:ASN:HB2	2.46	0.51
1:C:8:VAL:HG21	1:D:254:HIS:HB3	1.93	0.51
1:E:266:PRO:O	1:E:270:GLN:HG3	2.11	0.50
1:B:269:GLU:N	1:B:269:GLU:OE1	2.45	0.50
1:D:170:ASN:ND2	1:D:184:MSE:HE3	2.26	0.50
1:F:298:VAL:HG22	1:F:380:ILE:CD1	2.42	0.50
1:E:121:GLU:OE2	1:E:356:LEU:N	2.44	0.50
1:C:205:SER:O	1:C:206:GLU:HB2	2.12	0.49
1:D:327:ASP:O	1:D:330:GLU:HG2	2.12	0.49
1:B:67:ALA:HA	1:B:94:LEU:HD12	1.95	0.49
1:A:94:LEU:HD13	1:A:256:MSE:HE2	1.95	0.49
1:F:179:TYR:CB	1:F:184:MSE:HE3	2.43	0.48
1:A:380:ILE:HG22	1:A:384:MSE:HE2	1.95	0.48
1:F:302:LEU:HD23	1:F:384:MSE:HE2	1.96	0.48
1:B:33:ILE:HG21	1:B:347:MSE:CE	2.40	0.48
1:F:246:THR:CG2	1:F:252:ILE:HG23	2.44	0.48
1:C:67:ALA:HA	1:C:94:LEU:HD12	1.96	0.48
1:E:205:SER:O	1:E:206:GLU:HB2	2.13	0.47
1:B:63:TYR:CZ	1:B:263:LEU:HD13	2.49	0.47
1:F:179:TYR:HB3	1:F:184:MSE:HE3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:LEU:HA	1:A:384:MSE:HE1	1.96	0.47
1:C:186:TYR:CZ	1:C:190:ILE:HD11	2.50	0.47
1:E:254:HIS:HB3	1:F:8:VAL:HG21	1.97	0.47
1:D:185:ARG:HA	1:D:219:ILE:HD13	1.97	0.47
1:E:336:LEU:HD21	1:E:347:MSE:HG3	1.96	0.46
1:B:170:ASN:ND2	1:B:184:MSE:HE3	2.30	0.46
1:E:206:GLU:HG2	1:E:284:PHE:CD1	2.50	0.46
1:F:101:GLU:OE2	1:F:262:ARG:HD3	2.16	0.46
1:D:336:LEU:HD21	1:D:347:MSE:HG3	1.97	0.46
1:A:185[A]:ARG:HA	1:A:219:ILE:HD13	1.98	0.46
1:D:239:ALA:O	1:D:269:GLU:HG2	2.15	0.46
1:E:63:TYR:CZ	1:E:263:LEU:HD13	2.52	0.45
1:A:185[B]:ARG:HA	1:A:219:ILE:HD13	1.98	0.45
1:A:230:VAL:HG22	1:A:241:VAL:O	2.17	0.45
1:F:239:ALA:O	1:F:269:GLU:HG2	2.17	0.45
1:B:179:TYR:HB2	1:B:184:MSE:HE2	1.99	0.45
1:E:36:LEU:HD21	1:E:371:LEU:HD12	1.99	0.45
1:C:67:ALA:HB2	1:C:256:MSE:HE1	1.98	0.44
1:E:201:ASP:OD1	1:E:203:VAL:HG23	2.16	0.44
1:F:12:GLU:N	2:F:436:HOH:O	2.43	0.44
1:A:33:ILE:HG21	1:A:347:MSE:CE	2.46	0.44
1:C:266:PRO:O	1:C:270:GLN:HG3	2.17	0.44
1:B:205:SER:O	1:B:206:GLU:HB2	2.16	0.44
1:D:67:ALA:HB2	1:D:256:MSE:HE1	1.99	0.44
1:F:185:ARG:HA	1:F:219:ILE:HD13	1.98	0.44
1:A:205:SER:O	1:A:206:GLU:HB2	2.17	0.43
1:D:121:GLU:OE2	1:D:356:LEU:N	2.48	0.43
1:D:83:ARG:NH2	1:D:284:PHE:HB2	2.34	0.43
1:C:67:ALA:HB2	1:C:256:MSE:CE	2.49	0.43
1:F:205:SER:O	1:F:206:GLU:HB2	2.19	0.43
1:A:66:SER:O	1:A:262:ARG:NH2	2.51	0.43
1:F:174:PRO:HB3	1:F:366:ARG:HD3	2.01	0.43
1:D:239:ALA:HA	1:D:269:GLU:HG2	2.01	0.42
1:B:320:THR:HG23	1:B:351:LEU:HD22	2.01	0.42
1:C:205:SER:O	1:C:206:GLU:CB	2.67	0.42
1:F:240:ARG:HA	1:F:240:ARG:NH1	2.35	0.42
2:E:424:HOH:O	1:F:223:LYS:CE	2.67	0.42
1:B:124:TYR:CE2	1:B:126:ASN:HB2	2.54	0.42
1:C:302:LEU:HD23	1:C:384:MSE:CE	2.49	0.42
1:E:323:LEU:HD11	1:E:365:ILE:HD13	2.02	0.42
1:A:372:GLU:OE1	1:A:374:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:331:PHE:CZ	1:E:335:MSE:CE	3.02	0.42
1:F:201:ASP:OD2	1:F:232:LLP:N1	2.52	0.42
1:C:86:VAL:HG11	1:C:217:LEU:CB	2.49	0.42
1:C:86:VAL:HG11	1:C:217:LEU:HB2	2.02	0.42
1:F:118:LEU:HD23	1:F:139:ILE:HB	2.02	0.42
1:D:266:PRO:O	1:D:270:GLN:HG3	2.20	0.42
1:D:335:MSE:HE1	1:D:386:GLY:HA3	2.02	0.41
1:C:174:PRO:HB3	1:C:366:ARG:HD3	2.02	0.41
1:C:320:THR:HG23	1:C:351:LEU:HD22	2.02	0.41
1:D:63:TYR:CZ	1:D:263:LEU:HD13	2.55	0.41
1:E:124:TYR:CE2	1:E:126:ASN:HB2	2.55	0.41
1:F:63:TYR:CE1	1:F:263:LEU:HD13	2.55	0.41
1:B:204:TYR:CE1	1:B:232:LLP:HG2	2.55	0.41
1:C:264:ALA:O	1:D:240:ARG:CD	2.69	0.41
1:E:336:LEU:HD21	1:E:347:MSE:HG2	2.01	0.41
1:A:185[A]:ARG:NH1	1:A:219:ILE:HG23	2.36	0.41
1:B:135:GLY:HA2	2:B:402:HOH:O	2.21	0.41
1:C:70:TRP:CH2	1:C:90:PRO:HB2	2.55	0.41
1:E:217:LEU:HG	1:E:226:VAL:HG21	2.02	0.41
1:A:166:ILE:HG23	1:A:198:LEU:HD12	2.03	0.41
1:B:24:GLU:O	1:B:27:LYS:HG2	2.21	0.41
1:F:302:LEU:HA	1:F:384:MSE:HE3	2.02	0.41
1:E:186:TYR:CZ	1:E:190:ILE:HD11	2.56	0.41
1:C:63:TYR:CE1	1:C:263:LEU:HD13	2.56	0.40
1:B:205:SER:O	1:B:206:GLU:CB	2.69	0.40
1:F:217:LEU:HG	1:F:226:VAL:HG21	2.03	0.40
1:C:264:ALA:O	1:D:240:ARG:HD3	2.21	0.40
1:D:204:TYR:CE1	1:D:232:LLP:HG2	2.57	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	389/409 (95%)	376 (97%)	10 (3%)	3 (1%)	19	35
1	B	392/409 (96%)	380 (97%)	10 (3%)	2 (0%)	29	48
1	C	389/409 (95%)	376 (97%)	12 (3%)	1 (0%)	41	61
1	D	387/409 (95%)	373 (96%)	12 (3%)	2 (0%)	29	48
1	E	390/409 (95%)	377 (97%)	12 (3%)	1 (0%)	41	61
1	F	386/409 (94%)	372 (96%)	13 (3%)	1 (0%)	41	61
All	All	2333/2454 (95%)	2254 (97%)	69 (3%)	10 (0%)	34	54

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	GLU
1	B	206	GLU
1	C	206	GLU
1	E	206	GLU
1	F	206	GLU
1	D	206	GLU
1	A	124	TYR
1	D	124	TYR
1	A	263	LEU
1	B	263	LEU

5.3.2 Protein sidechains [i](#)

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	312/343 (91%)	311 (100%)	1 (0%)	92	97
1	B	314/343 (92%)	313 (100%)	1 (0%)	92	97
1	C	312/343 (91%)	312 (100%)	0	100	100
1	D	306/343 (89%)	304 (99%)	2 (1%)	84	94
1	E	306/343 (89%)	305 (100%)	1 (0%)	92	97
1	F	308/343 (90%)	308 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1858/2058 (90%)	1853 (100%)	5 (0%)	92 97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	265	PRO
1	B	88	VAL
1	D	338	ASP
1	D	341	MSE
1	E	112	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	HIS
1	C	126	ASN
1	D	92	ASN
1	D	126	ASN
1	E	112	ASN
1	F	65	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	LLP	D	232	1	23,24,25	1.79	4 (17%)	25,32,34	1.69	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	LLP	F	232	1	23,24,25	1.91	5 (21%)	25,32,34	1.64	4 (16%)
1	LLP	C	232	1	23,24,25	1.85	5 (21%)	25,32,34	1.55	5 (20%)
1	LLP	E	232	1	23,24,25	1.78	5 (21%)	25,32,34	1.82	4 (16%)
1	LLP	A	232	1	23,24,25	1.81	5 (21%)	25,32,34	1.60	2 (8%)
1	LLP	B	232	1	23,24,25	1.79	6 (26%)	25,32,34	1.84	5 (20%)

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
1	LLP	D	232	1	-	6/16/17/19	0/1/1/1
1	LLP	F	232	1	-	5/16/17/19	0/1/1/1
1	LLP	C	232	1	-	5/16/17/19	0/1/1/1
1	LLP	E	232	1	-	9/16/17/19	0/1/1/1
1	LLP	A	232	1	-	6/16/17/19	0/1/1/1
1	LLP	B	232	1	-	9/16/17/19	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	232	LLP	O3-C3	-6.00	1.23	1.37
1	C	232	LLP	O3-C3	-5.84	1.23	1.37
1	D	232	LLP	O3-C3	-5.81	1.23	1.37
1	F	232	LLP	O3-C3	-5.81	1.23	1.37
1	B	232	LLP	O3-C3	-5.79	1.23	1.37
1	E	232	LLP	O3-C3	-5.73	1.23	1.37
1	F	232	LLP	CE-NZ	3.09	1.53	1.46
1	D	232	LLP	C4-C4'	2.97	1.52	1.46
1	C	232	LLP	C4-C4'	2.88	1.52	1.46
1	A	232	LLP	C4-C4'	2.88	1.52	1.46
1	F	232	LLP	C4'-NZ	2.86	1.36	1.27
1	F	232	LLP	C4-C4'	2.84	1.52	1.46
1	E	232	LLP	C4-C4'	2.74	1.51	1.46
1	B	232	LLP	C4-C4'	2.66	1.51	1.46
1	D	232	LLP	C2-N1	2.65	1.38	1.33
1	C	232	LLP	C4'-NZ	2.55	1.35	1.27
1	A	232	LLP	C4'-NZ	2.46	1.35	1.27
1	E	232	LLP	CE-NZ	2.43	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	232	LLP	C2-N1	2.41	1.38	1.33
1	B	232	LLP	C2-N1	2.36	1.38	1.33
1	B	232	LLP	CE-NZ	2.33	1.51	1.46
1	C	232	LLP	CE-NZ	2.32	1.51	1.46
1	F	232	LLP	C2-N1	2.26	1.38	1.33
1	B	232	LLP	C4'-NZ	2.26	1.34	1.27
1	A	232	LLP	C2-N1	2.25	1.38	1.33
1	A	232	LLP	CE-NZ	2.21	1.51	1.46
1	E	232	LLP	C4'-NZ	2.19	1.34	1.27
1	E	232	LLP	C2-N1	2.15	1.37	1.33
1	D	232	LLP	C4'-NZ	2.12	1.34	1.27
1	B	232	LLP	C6-N1	2.07	1.38	1.34

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	232	LLP	OP4-C5'-C5	6.72	122.16	109.35
1	B	232	LLP	OP4-C5'-C5	6.14	121.06	109.35
1	D	232	LLP	OP4-C5'-C5	5.56	119.95	109.35
1	A	232	LLP	OP4-C5'-C5	5.50	119.82	109.35
1	F	232	LLP	OP4-C5'-C5	5.10	119.07	109.35
1	C	232	LLP	OP4-C5'-C5	4.36	117.67	109.35
1	F	232	LLP	C4-C4'-NZ	-3.60	107.80	124.31
1	C	232	LLP	C4-C4'-NZ	-3.59	107.84	124.31
1	B	232	LLP	OP2-P-OP4	-3.44	97.58	106.73
1	A	232	LLP	C4-C4'-NZ	-3.30	109.17	124.31
1	B	232	LLP	C4-C4'-NZ	-3.10	110.08	124.31
1	E	232	LLP	C4-C4'-NZ	-2.85	111.22	124.31
1	D	232	LLP	C5-C6-N1	-2.76	119.22	123.82
1	E	232	LLP	OP2-P-OP4	-2.72	99.49	106.73
1	F	232	LLP	OP3-P-OP4	-2.64	99.71	106.73
1	D	232	LLP	C4-C4'-NZ	-2.64	112.20	124.31
1	D	232	LLP	OP4-P-OP1	-2.56	99.29	106.47
1	B	232	LLP	C5-C6-N1	-2.48	119.69	123.82
1	E	232	LLP	C5-C6-N1	-2.47	119.71	123.82
1	C	232	LLP	OP3-P-OP4	-2.22	100.83	106.73
1	C	232	LLP	CD-CE-NZ	2.17	116.24	110.93
1	D	232	LLP	CE-NZ-C4'	-2.15	112.29	118.90
1	C	232	LLP	C5-C6-N1	-2.15	120.24	123.82
1	B	232	LLP	CE-NZ-C4'	-2.14	112.33	118.90
1	F	232	LLP	CD-CE-NZ	2.10	116.08	110.93

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	232	LLP	C5'-OP4-P-OP2
1	B	232	LLP	C5'-OP4-P-OP3
1	D	232	LLP	C5'-OP4-P-OP2
1	E	232	LLP	C5'-OP4-P-OP1
1	E	232	LLP	C5'-OP4-P-OP2
1	E	232	LLP	C5'-OP4-P-OP3
1	D	232	LLP	C4-C4'-NZ-CE
1	F	232	LLP	C4-C4'-NZ-CE
1	C	232	LLP	C4-C4'-NZ-CE
1	E	232	LLP	C4-C4'-NZ-CE
1	A	232	LLP	C4-C4'-NZ-CE
1	B	232	LLP	C4-C4'-NZ-CE
1	A	232	LLP	C3-C4-C4'-NZ
1	C	232	LLP	C3-C4-C4'-NZ
1	F	232	LLP	C3-C4-C4'-NZ
1	B	232	LLP	C3-C4-C4'-NZ
1	D	232	LLP	C3-C4-C4'-NZ
1	E	232	LLP	C3-C4-C4'-NZ
1	A	232	LLP	C5-C4-C4'-NZ
1	B	232	LLP	C5-C4-C4'-NZ
1	C	232	LLP	C5-C4-C4'-NZ
1	D	232	LLP	C5-C4-C4'-NZ
1	F	232	LLP	C5-C4-C4'-NZ
1	B	232	LLP	CD-CE-NZ-C4'
1	D	232	LLP	CD-CE-NZ-C4'
1	E	232	LLP	CD-CE-NZ-C4'
1	E	232	LLP	C5-C4-C4'-NZ
1	C	232	LLP	CA-CB-CG-CD
1	A	232	LLP	CD-CE-NZ-C4'
1	C	232	LLP	CD-CE-NZ-C4'
1	F	232	LLP	CD-CE-NZ-C4'
1	F	232	LLP	CA-CB-CG-CD
1	E	232	LLP	CA-CB-CG-CD
1	B	232	LLP	CG-CD-CE-NZ
1	A	232	LLP	C6-C5-C5'-OP4
1	D	232	LLP	C5'-OP4-P-OP3
1	B	232	LLP	C5'-OP4-P-OP1
1	E	232	LLP	CG-CD-CE-NZ
1	A	232	LLP	CA-CB-CG-CD
1	B	232	LLP	CA-CB-CG-CD

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	232	LLP	1	0
1	F	232	LLP	1	0
1	B	232	LLP	1	0

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	379/409 (92%)	0.24	13 (3%) 45 48	26, 30, 32, 39	0
1	B	383/409 (93%)	0.29	15 (3%) 39 42	21, 30, 32, 37	0
1	C	381/409 (93%)	0.33	9 (2%) 59 62	26, 30, 32, 38	0
1	D	379/409 (92%)	0.39	22 (5%) 23 24	27, 30, 32, 35	0
1	E	382/409 (93%)	0.29	16 (4%) 36 39	22, 30, 32, 39	0
1	F	379/409 (92%)	0.21	12 (3%) 47 51	27, 30, 32, 37	0
All	All	2283/2454 (93%)	0.29	87 (3%) 40 43	21, 30, 32, 39	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	16	ILE	5.6
1	A	340	ASN	4.9
1	C	212	GLU	4.8
1	E	191	ALA	4.2
1	E	16	ILE	4.1
1	E	385	GLU	3.8
1	E	22	PHE	3.8
1	D	20	VAL	3.7
1	D	390	PHE	3.6
1	D	19	LEU	3.6
1	D	212	GLU	3.5
1	B	16	ILE	3.5
1	F	28	LYS	3.5
1	F	340	ASN	3.5
1	B	14	SER	3.4
1	D	343	GLY	3.3
1	E	19	LEU	3.3
1	E	26	ALA	3.3
1	D	339	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	13	GLU	3.3
1	A	359	GLY	3.2
1	A	211	GLY	3.1
1	D	14	SER	3.1
1	B	19	LEU	3.0
1	E	30	GLY	3.0
1	B	10	LEU	2.9
1	A	86	VAL	2.9
1	A	12	GLU	2.8
1	A	338	ASP	2.8
1	D	336	LEU	2.8
1	D	155	LEU	2.7
1	C	211	GLY	2.6
1	D	154	ASN	2.6
1	E	154	ASN	2.6
1	E	187	LEU	2.5
1	D	30	GLY	2.5
1	E	339	PHE	2.5
1	F	390	PHE	2.5
1	D	388	LYS	2.5
1	A	13	GLU	2.5
1	A	392	SER	2.5
1	D	280	ASP	2.5
1	D	54	TYR	2.5
1	D	342	ASP	2.5
1	D	12	GLU	2.5
1	C	252	ILE	2.4
1	B	162	ARG	2.4
1	C	12	GLU	2.4
1	E	146	GLU	2.4
1	B	26	ALA	2.4
1	F	13	GLU	2.4
1	D	326	GLU	2.4
1	E	-1	HIS	2.4
1	F	332	ALA	2.4
1	C	13	GLU	2.4
1	B	33	ILE	2.4
1	B	280	ASP	2.3
1	D	161	GLU	2.3
1	D	372	GLU	2.3
1	B	391	CYS	2.3
1	E	15	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	14	SER	2.3
1	F	391	CYS	2.3
1	B	327	ASP	2.2
1	B	331	PHE	2.2
1	B	339	PHE	2.2
1	F	161	GLU	2.2
1	F	329	GLU	2.2
1	B	303	GLU	2.2
1	F	380	ILE	2.2
1	D	324	PRO	2.2
1	B	340	ASN	2.2
1	B	22	PHE	2.1
1	C	251	LEU	2.1
1	A	327	ASP	2.1
1	C	30	GLY	2.1
1	C	54	TYR	2.1
1	E	210	ARG	2.1
1	A	87	ASP	2.1
1	E	160	ASN	2.1
1	A	30	GLY	2.1
1	F	296	GLU	2.1
1	E	6	ASP	2.0
1	A	32	ARG	2.0
1	C	79	TYR	2.0
1	A	334	TRP	2.0
1	F	387	LEU	2.0

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

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. 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	B-factors(Å ²)	Q<0.9
1	LLP	C	232	24/25	0.94	0.15	29,31,33,34	0
1	LLP	F	232	24/25	0.95	0.16	28,32,33,35	0
1	LLP	E	232	24/25	0.96	0.14	27,30,33,34	0
1	LLP	D	232	24/25	0.96	0.14	28,31,33,33	0
1	LLP	A	232	24/25	0.97	0.14	29,31,33,34	0
1	LLP	B	232	24/25	0.97	0.14	28,31,33,33	0

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.