Full wwPDB X-ray Structure Validation Report (i)

Sep 5, 2023 – 04:16 AM EDT

PDB ID	:	3U3X
Title	:	Crystal structure of a putative oxidoreductase from Sinorhizobium meliloti 1021
Authors	:	Agarwal, R.; Chamala, S.; Evans, B.; Foti, R.; Gizzi, A.; Hillerich, B.; Kar, A.; LaFleur, J.; Seidel, R.; Villigas, G.; Zencheck, W.; Almo, S.C.; Swaminathan, S.; New York Structural Genomics Research Consortium (NYSGRC)
Deposited on	:	2011-10-06
Resolution	:	2.79 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 (i) 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 (i)) were used in the production of this report:

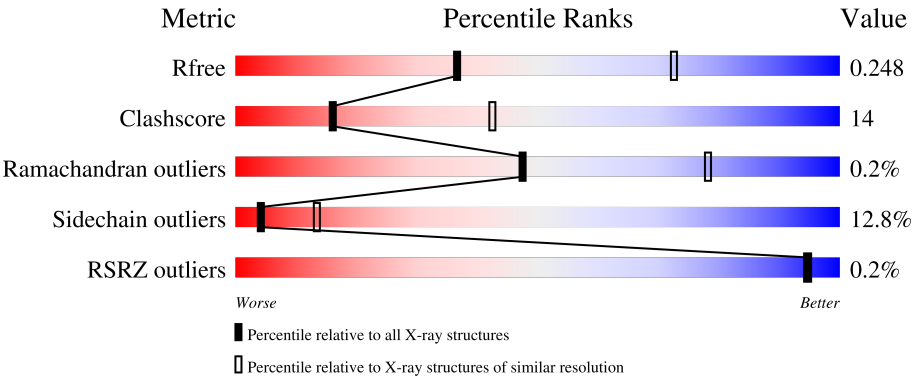
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.79 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 <=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	361	67% 20% • • 9%
1	D	361	65% 21% • • 9%
1	G	361	65% 20% 5% 9%
1	J	361	70% 20% • 9%

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Mol	Chain	Length	Quality of chain
1	M	361	

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
2	ACT	G	362	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12240 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 Oxidoreductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	Se	0	0	0
			2453	1540	445	458	4	6			
1	D	330	Total	C	N	O	S	Se	0	0	0
			2401	1513	431	447	4	6			
1	G	330	Total	C	N	O	S	Se	0	0	0
			2430	1527	440	453	4	6			
1	J	330	Total	C	N	O	S	Se	0	0	0
			2420	1521	437	452	4	6			
1	M	330	Total	C	N	O	S	Se	0	0	0
			2433	1529	442	452	4	6			

There are 115 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	expression tag	UNP Q92T66
A	2	HIS	-	expression tag	UNP Q92T66
A	3	HIS	-	expression tag	UNP Q92T66
A	4	HIS	-	expression tag	UNP Q92T66
A	5	HIS	-	expression tag	UNP Q92T66
A	6	HIS	-	expression tag	UNP Q92T66
A	7	HIS	-	expression tag	UNP Q92T66
A	8	SER	-	expression tag	UNP Q92T66
A	9	SER	-	expression tag	UNP Q92T66
A	10	GLY	-	expression tag	UNP Q92T66
A	11	VAL	-	expression tag	UNP Q92T66
A	12	ASP	-	expression tag	UNP Q92T66
A	13	LEU	-	expression tag	UNP Q92T66
A	14	GLY	-	expression tag	UNP Q92T66
A	15	THR	-	expression tag	UNP Q92T66
A	16	GLU	-	expression tag	UNP Q92T66
A	17	ASN	-	expression tag	UNP Q92T66
A	18	LEU	-	expression tag	UNP Q92T66
A	19	TYR	-	expression tag	UNP Q92T66

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Chain	Residue	Modelled	Actual	Comment	Reference
A	20	PHE	-	expression tag	UNP Q92T66
A	21	GLN	-	expression tag	UNP Q92T66
A	22	SER	-	expression tag	UNP Q92T66
A	23	MSE	-	expression tag	UNP Q92T66
D	1	MSE	-	expression tag	UNP Q92T66
D	2	HIS	-	expression tag	UNP Q92T66
D	3	HIS	-	expression tag	UNP Q92T66
D	4	HIS	-	expression tag	UNP Q92T66
D	5	HIS	-	expression tag	UNP Q92T66
D	6	HIS	-	expression tag	UNP Q92T66
D	7	HIS	-	expression tag	UNP Q92T66
D	8	SER	-	expression tag	UNP Q92T66
D	9	SER	-	expression tag	UNP Q92T66
D	10	GLY	-	expression tag	UNP Q92T66
D	11	VAL	-	expression tag	UNP Q92T66
D	12	ASP	-	expression tag	UNP Q92T66
D	13	LEU	-	expression tag	UNP Q92T66
D	14	GLY	-	expression tag	UNP Q92T66
D	15	THR	-	expression tag	UNP Q92T66
D	16	GLU	-	expression tag	UNP Q92T66
D	17	ASN	-	expression tag	UNP Q92T66
D	18	LEU	-	expression tag	UNP Q92T66
D	19	TYR	-	expression tag	UNP Q92T66
D	20	PHE	-	expression tag	UNP Q92T66
D	21	GLN	-	expression tag	UNP Q92T66
D	22	SER	-	expression tag	UNP Q92T66
D	23	MSE	-	expression tag	UNP Q92T66
G	1	MSE	-	expression tag	UNP Q92T66
G	2	HIS	-	expression tag	UNP Q92T66
G	3	HIS	-	expression tag	UNP Q92T66
G	4	HIS	-	expression tag	UNP Q92T66
G	5	HIS	-	expression tag	UNP Q92T66
G	6	HIS	-	expression tag	UNP Q92T66
G	7	HIS	-	expression tag	UNP Q92T66
G	8	SER	-	expression tag	UNP Q92T66
G	9	SER	-	expression tag	UNP Q92T66
G	10	GLY	-	expression tag	UNP Q92T66
G	11	VAL	-	expression tag	UNP Q92T66
G	12	ASP	-	expression tag	UNP Q92T66
G	13	LEU	-	expression tag	UNP Q92T66
G	14	GLY	-	expression tag	UNP Q92T66
G	15	THR	-	expression tag	UNP Q92T66

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Chain	Residue	Modelled	Actual	Comment	Reference
G	16	GLU	-	expression tag	UNP Q92T66
G	17	ASN	-	expression tag	UNP Q92T66
G	18	LEU	-	expression tag	UNP Q92T66
G	19	TYR	-	expression tag	UNP Q92T66
G	20	PHE	-	expression tag	UNP Q92T66
G	21	GLN	-	expression tag	UNP Q92T66
G	22	SER	-	expression tag	UNP Q92T66
G	23	MSE	-	expression tag	UNP Q92T66
J	1	MSE	-	expression tag	UNP Q92T66
J	2	HIS	-	expression tag	UNP Q92T66
J	3	HIS	-	expression tag	UNP Q92T66
J	4	HIS	-	expression tag	UNP Q92T66
J	5	HIS	-	expression tag	UNP Q92T66
J	6	HIS	-	expression tag	UNP Q92T66
J	7	HIS	-	expression tag	UNP Q92T66
J	8	SER	-	expression tag	UNP Q92T66
J	9	SER	-	expression tag	UNP Q92T66
J	10	GLY	-	expression tag	UNP Q92T66
J	11	VAL	-	expression tag	UNP Q92T66
J	12	ASP	-	expression tag	UNP Q92T66
J	13	LEU	-	expression tag	UNP Q92T66
J	14	GLY	-	expression tag	UNP Q92T66
J	15	THR	-	expression tag	UNP Q92T66
J	16	GLU	-	expression tag	UNP Q92T66
J	17	ASN	-	expression tag	UNP Q92T66
J	18	LEU	-	expression tag	UNP Q92T66
J	19	TYR	-	expression tag	UNP Q92T66
J	20	PHE	-	expression tag	UNP Q92T66
J	21	GLN	-	expression tag	UNP Q92T66
J	22	SER	-	expression tag	UNP Q92T66
J	23	MSE	-	expression tag	UNP Q92T66
M	1	MSE	-	expression tag	UNP Q92T66
M	2	HIS	-	expression tag	UNP Q92T66
M	3	HIS	-	expression tag	UNP Q92T66
M	4	HIS	-	expression tag	UNP Q92T66
M	5	HIS	-	expression tag	UNP Q92T66
M	6	HIS	-	expression tag	UNP Q92T66
M	7	HIS	-	expression tag	UNP Q92T66
M	8	SER	-	expression tag	UNP Q92T66
M	9	SER	-	expression tag	UNP Q92T66
M	10	GLY	-	expression tag	UNP Q92T66
M	11	VAL	-	expression tag	UNP Q92T66

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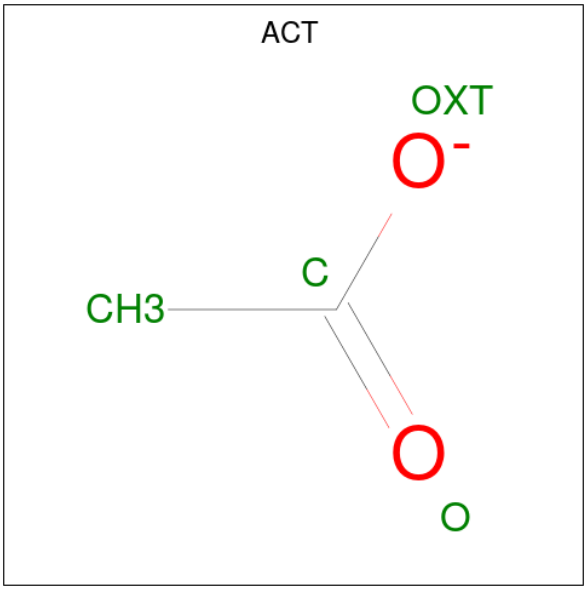
Chain	Residue	Modelled	Actual	Comment	Reference
M	12	ASP	-	expression tag	UNP Q92T66
M	13	LEU	-	expression tag	UNP Q92T66
M	14	GLY	-	expression tag	UNP Q92T66
M	15	THR	-	expression tag	UNP Q92T66
M	16	GLU	-	expression tag	UNP Q92T66
M	17	ASN	-	expression tag	UNP Q92T66
M	18	LEU	-	expression tag	UNP Q92T66
M	19	TYR	-	expression tag	UNP Q92T66
M	20	PHE	-	expression tag	UNP Q92T66
M	21	GLN	-	expression tag	UNP Q92T66
M	22	SER	-	expression tag	UNP Q92T66
M	23	MSE	-	expression tag	UNP Q92T66

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	18	Total O 18 18	0	0

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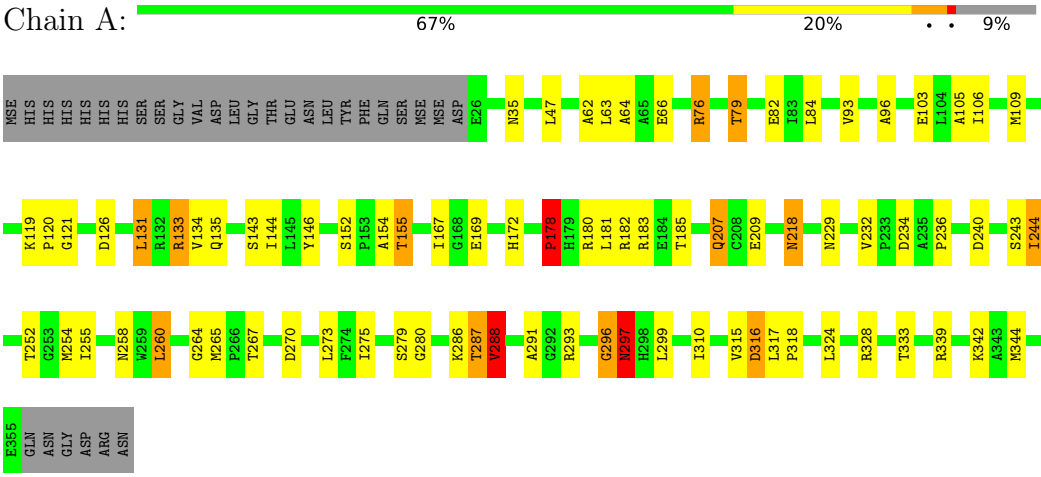
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	8	Total O 8 8	0	0
3	G	25	Total O 25 25	0	0
3	J	25	Total O 25 25	0	0
3	M	19	Total O 19 19	0	0

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.

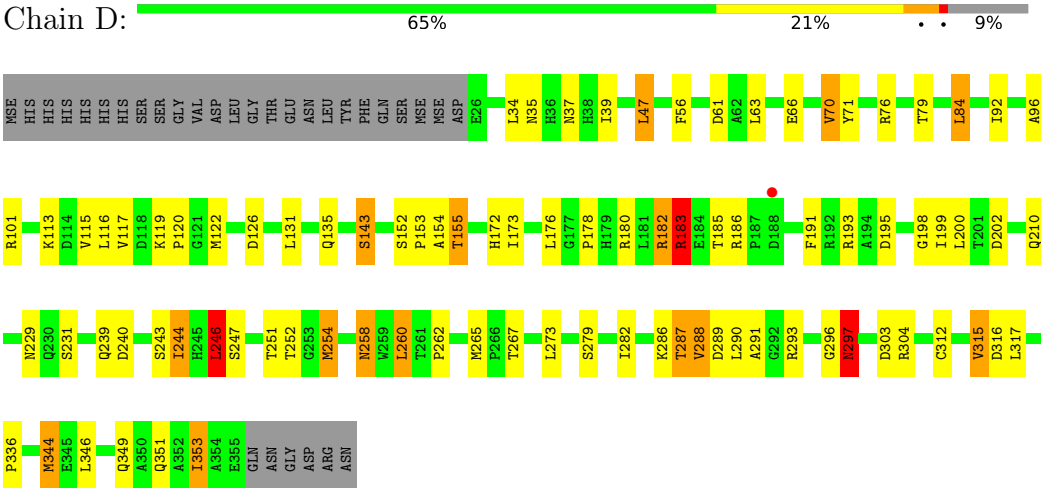
• Molecule 1: Oxidoreductase

Chain A:



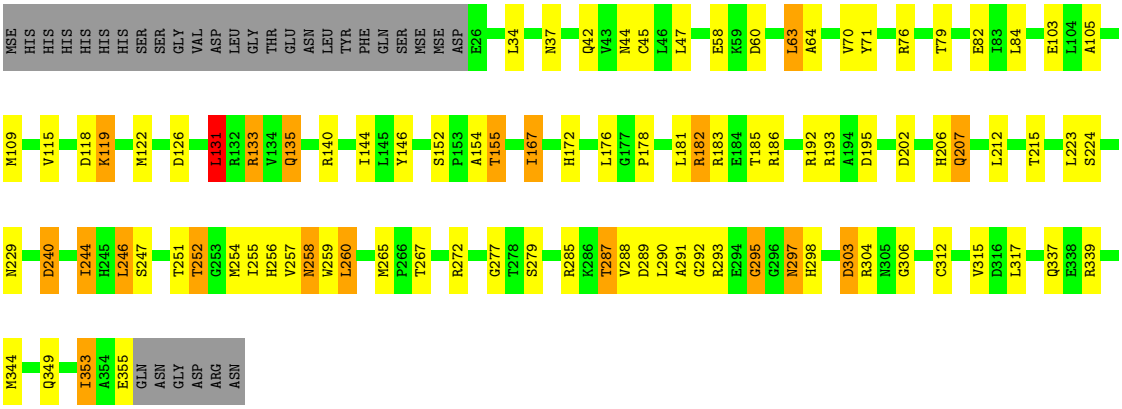
• Molecule 1: Oxidoreductase

Chain D:



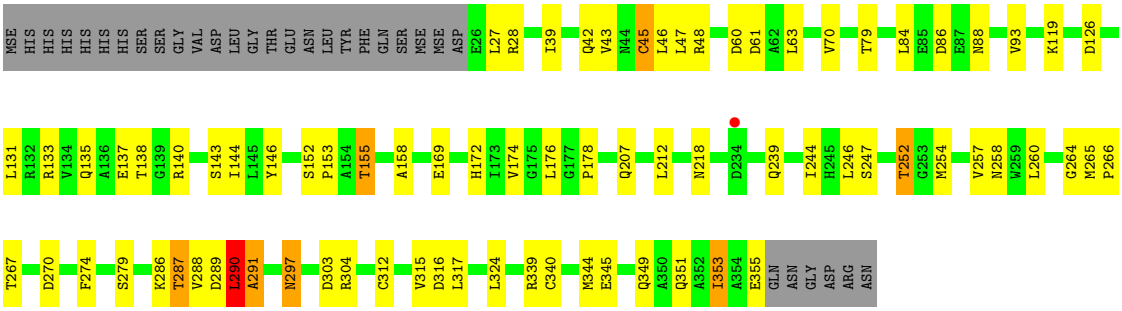
• Molecule 1: Oxidoreductase

Chain G:



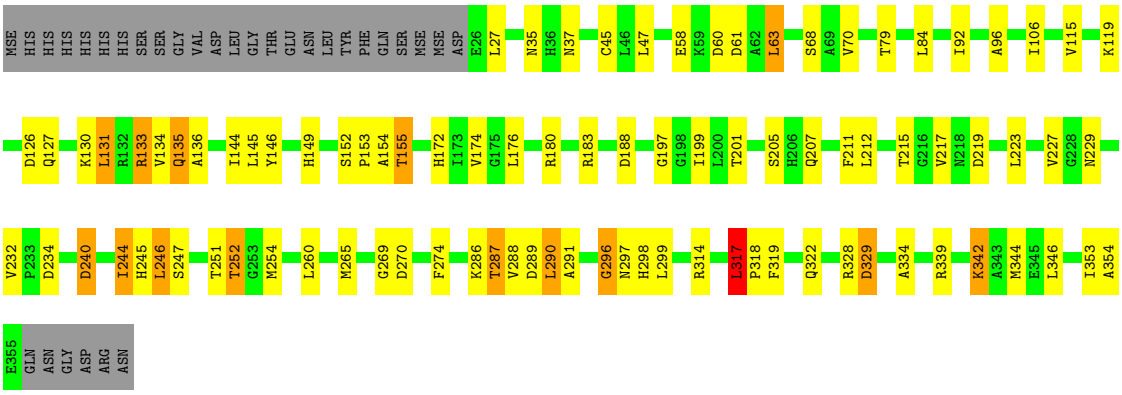
• Molecule 1: Oxidoreductase

Chain J:



• Molecule 1: Oxidoreductase

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	257.06Å 71.03Å 129.00Å 90.00° 104.68° 90.00°	Depositor
Resolution (Å)	46.78 – 2.79 46.78 – 2.79	Depositor EDS
% Data completeness (in resolution range)	98.9 (46.78-2.79) 98.9 (46.78-2.79)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.95 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.199 , 0.253 0.200 , 0.248	Depositor DCC
R_{free} test set	2837 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	42.5	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 29.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12240	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.98	2/2494 (0.1%)	0.95	6/3377 (0.2%)
1	D	0.95	2/2442 (0.1%)	0.89	6/3314 (0.2%)
1	G	1.04	2/2471 (0.1%)	0.95	8/3350 (0.2%)
1	J	0.95	4/2461 (0.2%)	0.85	3/3339 (0.1%)
1	M	0.98	1/2474 (0.0%)	0.92	4/3353 (0.1%)
All	All	0.98	11/12342 (0.1%)	0.91	27/16733 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
1	G	0	1
1	J	0	1
All	All	0	4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	257	VAL	CB-CG1	-5.92	1.40	1.52
1	G	257	VAL	CB-CG1	-5.78	1.40	1.52
1	A	66	GLU	CG-CD	5.67	1.60	1.51
1	G	355	GLU	CG-CD	5.64	1.60	1.51
1	D	288	VAL	CB-CG2	-5.61	1.41	1.52
1	J	291	ALA	CA-CB	-5.57	1.40	1.52
1	J	355	GLU	CG-CD	5.26	1.59	1.51
1	J	45	CYS	CB-SG	-5.22	1.73	1.81
1	A	288	VAL	CB-CG2	-5.11	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	45	CYS	CB-SG	-5.06	1.73	1.81
1	D	288	VAL	CB-CG1	-5.05	1.42	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	297	ASN	N-CA-C	-8.50	88.06	111.00
1	A	178	PRO	CA-N-CD	-8.21	100.00	111.50
1	G	258	ASN	CB-CA-C	-7.04	96.31	110.40
1	D	182	ARG	N-CA-C	6.30	128.01	111.00
1	G	37	ASN	CB-CA-C	-5.99	98.41	110.40
1	M	317	LEU	CA-CB-CG	5.97	129.03	115.30
1	A	296	GLY	N-CA-C	-5.95	98.23	113.10
1	A	324	LEU	CB-CG-CD1	-5.92	100.93	111.00
1	G	131	LEU	CA-CB-CG	5.90	128.87	115.30
1	M	296	GLY	N-CA-C	-5.87	98.42	113.10
1	D	84	LEU	CA-CB-CG	5.80	128.63	115.30
1	G	259	TRP	N-CA-C	-5.72	95.55	111.00
1	D	246	LEU	CA-CB-CG	5.68	128.37	115.30
1	M	188	ASP	CB-CG-OD1	5.63	123.37	118.30
1	M	291	ALA	N-CA-C	-5.63	95.81	111.00
1	D	258	ASN	CB-CA-C	-5.60	99.21	110.40
1	A	76	ARG	NE-CZ-NH1	-5.55	117.52	120.30
1	G	295	GLY	C-N-CA	5.45	133.74	122.30
1	D	183	ARG	CB-CA-C	-5.36	99.68	110.40
1	A	297	ASN	N-CA-C	-5.32	96.63	111.00
1	J	176	LEU	CB-CG-CD2	-5.17	102.21	111.00
1	G	291	ALA	N-CA-C	-5.14	97.11	111.00
1	J	290	LEU	CA-CB-CG	5.14	127.11	115.30
1	G	292	GLY	N-CA-C	5.08	125.81	113.10
1	D	297	ASN	N-CA-C	-5.08	97.30	111.00
1	J	291	ALA	N-CA-C	-5.05	97.37	111.00
1	A	76	ARG	NE-CZ-NH2	5.01	122.81	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	133	ARG	Sidechain
1	D	296	GLY	Peptide
1	G	133	ARG	Sidechain
1	J	290	LEU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2453	0	2352	78	0
1	D	2401	0	2272	82	0
1	G	2430	0	2314	69	0
1	J	2420	0	2294	53	0
1	M	2433	0	2319	71	0
2	A	4	0	3	0	0
2	G	4	0	3	2	0
3	A	18	0	0	1	0
3	D	8	0	0	0	0
3	G	25	0	0	1	0
3	J	25	0	0	0	0
3	M	19	0	0	1	0
All	All	12240	0	11557	343	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (343) 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:172:HIS:CD2	1:D:252:THR:HG23	1.56	1.38
1:M:172:HIS:HD2	1:M:252:THR:CG2	1.43	1.30
1:J:172:HIS:HD2	1:J:252:THR:CG2	1.42	1.30
1:D:349:GLN:O	1:D:353:ILE:HG23	1.37	1.20
1:M:265:MSE:CE	1:M:288:VAL:HG11	1.72	1.19
1:D:172:HIS:HD2	1:D:252:THR:CG2	1.55	1.18
1:G:265:MSE:CE	1:G:288:VAL:HG11	1.73	1.17
1:M:172:HIS:CD2	1:M:252:THR:HG22	1.79	1.17
1:M:172:HIS:CD2	1:M:252:THR:CG2	2.29	1.15
1:G:172:HIS:HD2	1:G:252:THR:HG23	1.06	1.15
1:A:172:HIS:CD2	1:A:252:THR:HG23	1.82	1.15
1:A:182:ARG:NH1	1:A:185:THR:HG21	1.60	1.14
1:J:172:HIS:HD2	1:J:252:THR:HG23	1.01	1.13
1:J:172:HIS:CD2	1:J:252:THR:HG23	1.83	1.12
1:G:172:HIS:HD2	1:G:252:THR:CG2	1.61	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:172:HIS:CD2	1:J:252:THR:CG2	2.31	1.12
1:A:182:ARG:HH11	1:A:185:THR:CG2	1.63	1.09
1:A:172:HIS:HD2	1:A:252:THR:HG23	0.98	1.09
1:G:154:ALA:HB2	1:G:297:ASN:HB3	1.20	1.08
1:D:265:MSE:CE	1:D:288:VAL:HG11	1.84	1.08
1:A:265:MSE:CE	1:A:288:VAL:HG11	1.88	1.03
1:G:172:HIS:CD2	1:G:252:THR:HG23	1.93	1.02
1:M:154:ALA:HB2	1:M:297:ASN:HB3	1.42	1.01
1:M:172:HIS:HD2	1:M:252:THR:HG22	0.87	1.00
1:A:297:ASN:N	1:A:297:ASN:HD22	1.55	0.99
1:J:265:MSE:CE	1:J:288:VAL:HG11	1.92	0.98
1:D:265:MSE:HE2	1:D:288:VAL:HG11	1.47	0.97
1:M:229:ASN:HA	1:M:240:ASP:HB2	1.47	0.96
1:A:265:MSE:HE3	1:A:288:VAL:HG11	1.45	0.96
1:D:172:HIS:CD2	1:D:252:THR:CG2	2.38	0.95
1:A:182:ARG:HH11	1:A:185:THR:HG21	0.78	0.95
1:G:186:ARG:HH11	2:G:362:ACT:H3	1.33	0.93
1:D:172:HIS:HD2	1:D:252:THR:HG23	0.76	0.93
1:G:265:MSE:HE1	1:G:288:VAL:HG11	1.48	0.93
1:D:183:ARG:HD2	1:D:183:ARG:O	1.72	0.89
1:M:244:ILE:HD11	1:M:246:LEU:CD1	2.03	0.89
1:G:172:HIS:CD2	1:G:252:THR:CG2	2.54	0.88
1:D:229:ASN:HA	1:D:240:ASP:HB2	1.55	0.88
1:J:287:THR:HG22	1:J:288:VAL:HG12	1.56	0.88
1:J:172:HIS:HD2	1:J:252:THR:HG22	1.39	0.86
1:M:265:MSE:HE2	1:M:288:VAL:HG11	1.58	0.86
1:G:64:ALA:CB	1:G:76:ARG:NH1	2.40	0.84
1:A:265:MSE:HE2	1:A:270:ASP:HB2	1.60	0.83
1:D:154:ALA:HB2	1:D:297:ASN:HB2	1.58	0.83
1:M:155:THR:HG21	1:M:286:LYS:HZ2	1.45	0.82
1:A:273:LEU:HD21	1:A:275:ILE:HD11	1.62	0.81
1:G:193:ARG:HG3	1:G:193:ARG:HH11	1.44	0.81
1:M:172:HIS:CD2	1:M:252:THR:HG23	2.13	0.81
1:A:182:ARG:NH1	1:A:185:THR:CG2	2.32	0.80
1:G:265:MSE:HE2	1:G:288:VAL:HG11	1.64	0.80
1:D:178:PRO:HA	1:D:258:ASN:HB2	1.63	0.80
1:A:265:MSE:HE1	1:A:288:VAL:HG11	1.63	0.79
1:A:234:ASP:O	1:A:236:PRO:HD3	1.82	0.78
1:A:297:ASN:N	1:A:297:ASN:ND2	2.28	0.78
1:D:244:ILE:HD11	1:D:246:LEU:HD13	1.66	0.77
1:A:154:ALA:HB2	1:A:297:ASN:HB2	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:212:LEU:HB3	1:J:339:ARG:HD2	1.67	0.76
1:D:155:THR:HG21	1:D:286:LYS:HZ2	1.51	0.76
1:G:146:TYR:CE1	1:G:344:MSE:HE2	2.21	0.76
1:A:265:MSE:CE	1:A:270:ASP:HB2	2.15	0.76
1:M:244:ILE:HD11	1:M:246:LEU:HD11	1.65	0.76
1:D:349:GLN:O	1:D:353:ILE:CG2	2.28	0.76
1:G:152:SER:HB3	1:G:155:THR:HG23	1.67	0.75
1:M:35:ASN:HD22	1:M:96:ALA:HA	1.52	0.74
1:D:244:ILE:HD11	1:D:246:LEU:CD1	2.17	0.74
1:M:244:ILE:HD11	1:M:246:LEU:HD13	1.70	0.74
1:J:152:SER:HB3	1:J:155:THR:HG23	1.68	0.74
1:G:64:ALA:HB2	1:G:76:ARG:NH1	2.01	0.73
1:J:172:HIS:CD2	1:J:252:THR:HG22	2.17	0.73
1:J:265:MSE:HE1	1:J:288:VAL:HG11	1.69	0.73
1:D:122:MSE:SE	1:D:344:MSE:HG3	2.40	0.72
1:D:183:ARG:O	1:D:183:ARG:CD	2.38	0.72
1:A:35:ASN:HD22	1:A:96:ALA:HA	1.54	0.72
1:M:265:MSE:HE3	1:M:288:VAL:HG11	1.67	0.72
1:A:244:ILE:HD12	1:A:350:ALA:HB2	1.72	0.71
1:D:312:CYS:O	1:D:315:VAL:HG13	1.89	0.71
1:J:288:VAL:CG2	1:J:289:ASP:N	2.54	0.71
1:J:265:MSE:HE2	1:J:288:VAL:HG11	1.70	0.70
1:J:288:VAL:HG22	1:J:289:ASP:N	2.06	0.70
1:D:215:THR:HG22	1:D:251:THR:HG21	1.72	0.69
1:A:265:MSE:CE	1:A:288:VAL:CG1	2.69	0.69
1:M:146:TYR:CE1	1:M:344:MSE:HE2	2.27	0.69
1:J:153:PRO:HD2	1:J:297:ASN:OD1	1.92	0.69
1:A:267:THR:OG1	1:A:287:THR:CG2	2.40	0.69
1:J:60:ASP:OD1	1:J:60:ASP:C	2.30	0.69
1:D:155:THR:HG21	1:D:286:LYS:NZ	2.09	0.68
1:M:318:PRO:O	1:M:322:GLN:HG3	1.94	0.67
1:A:182:ARG:O	1:A:185:THR:HB	1.95	0.67
1:G:229:ASN:HA	1:G:240:ASP:HB2	1.77	0.66
1:G:105:ALA:O	1:G:109:MSE:HG3	1.94	0.66
1:A:178:PRO:HD2	1:A:178:PRO:O	1.96	0.66
1:D:287:THR:HG22	1:D:288:VAL:HG12	1.76	0.66
1:M:183:ARG:HH22	1:M:234:ASP:HB3	1.60	0.66
1:M:265:MSE:CE	1:M:288:VAL:CG1	2.65	0.66
1:M:265:MSE:CE	1:M:270:ASP:HB2	2.26	0.65
1:M:265:MSE:HE1	1:M:288:VAL:HG11	1.77	0.65
1:J:286:LYS:O	1:J:297:ASN:HB3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:155:THR:HG21	1:M:286:LYS:NZ	2.12	0.65
1:A:64:ALA:CB	1:A:76:ARG:NH1	2.60	0.65
1:D:303:ASP:OD1	1:D:304:ARG:N	2.29	0.65
1:G:176:LEU:HD13	1:G:272:ARG:HB2	1.79	0.65
1:G:258:ASN:HB3	1:G:260:LEU:HB2	1.77	0.65
3:A:368:HOH:O	1:D:252:THR:HG21	1.97	0.65
1:M:146:TYR:HE1	1:M:344:MSE:HE2	1.63	0.64
1:G:64:ALA:HB2	1:G:76:ARG:HH12	1.62	0.64
1:J:60:ASP:OD1	1:J:61:ASP:N	2.30	0.64
1:M:154:ALA:CB	1:M:297:ASN:HB3	2.24	0.64
1:M:152:SER:OG	1:M:155:THR:CG2	2.46	0.63
1:J:146:TYR:HE1	1:J:344:MSE:HE2	1.64	0.63
1:A:144:ILE:HD13	1:A:344:MSE:HE3	1.78	0.63
1:A:105:ALA:O	1:A:109:MSE:HG3	1.99	0.63
1:G:193:ARG:HG3	1:G:193:ARG:NH1	2.10	0.63
1:J:267:THR:OG1	1:J:287:THR:CG2	2.47	0.63
1:M:154:ALA:HB2	1:M:297:ASN:CB	2.25	0.62
1:A:254:MSE:HE3	1:D:254:MSE:HB3	1.82	0.62
1:D:244:ILE:CD1	1:D:246:LEU:HD13	2.29	0.62
1:A:280:GLY:HA2	1:D:262:PRO:HB3	1.80	0.61
1:D:244:ILE:CG1	1:D:246:LEU:HD13	2.31	0.61
1:G:154:ALA:CB	1:G:297:ASN:HB3	2.13	0.61
1:G:303:ASP:OD1	1:G:304:ARG:N	2.34	0.61
1:M:152:SER:OG	1:M:155:THR:HG23	2.00	0.61
1:A:291:ALA:O	1:D:293:ARG:NH2	2.33	0.61
1:M:265:MSE:HE2	1:M:270:ASP:HB2	1.83	0.61
1:A:296:GLY:C	1:A:297:ASN:HD22	2.01	0.61
1:G:186:ARG:NH1	2:G:362:ACT:H3	2.11	0.61
1:A:244:ILE:HD11	1:A:246:LEU:CD1	2.32	0.60
1:D:231:SER:N	1:D:240:ASP:OD2	2.35	0.60
1:G:119:LYS:HE3	1:G:119:LYS:O	2.01	0.60
1:D:258:ASN:HB3	1:D:260:LEU:H	1.67	0.60
1:A:64:ALA:HB3	1:A:76:ARG:NH1	2.17	0.60
1:G:212:LEU:HB3	1:G:339:ARG:HD2	1.83	0.59
1:J:146:TYR:CE1	1:J:344:MSE:HE2	2.37	0.59
1:J:345:GLU:O	1:J:349:GLN:HG3	2.01	0.59
1:A:155:THR:HG21	1:A:286:LYS:NZ	2.17	0.59
1:J:297:ASN:N	1:J:297:ASN:HD22	2.01	0.58
1:D:99:SER:OG	1:D:195:ASP:HA	2.04	0.58
1:A:106:ILE:HG12	1:A:134:VAL:HG21	1.86	0.57
1:G:178:PRO:HA	1:G:258:ASN:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:265:MSE:HE1	1:M:290:LEU:CD2	2.34	0.57
1:M:106:ILE:HG12	1:M:134:VAL:HG21	1.86	0.57
1:A:229:ASN:HA	1:A:240:ASP:HB2	1.86	0.57
1:D:180:ARG:NH1	1:D:267:THR:O	2.38	0.57
1:D:35:ASN:ND2	1:D:96:ALA:HA	2.19	0.56
1:G:244:ILE:HD11	1:G:246:LEU:HD13	1.86	0.56
1:M:296:GLY:HA2	1:M:298:HIS:CD2	2.41	0.56
1:G:122:MSE:HE2	1:G:131:LEU:HD23	1.87	0.56
1:G:254:MSE:HE3	1:J:254:MSE:HE3	1.87	0.56
1:D:35:ASN:HD22	1:D:96:ALA:HA	1.70	0.56
1:J:303:ASP:OD1	1:J:304:ARG:N	2.38	0.56
1:J:312:CYS:O	1:J:315:VAL:HG13	2.05	0.56
1:M:215:THR:HG22	1:M:251:THR:HG21	1.86	0.56
1:M:146:TYR:CE1	1:M:344:MSE:CE	2.88	0.56
1:A:267:THR:OG1	1:A:287:THR:HG21	2.05	0.56
1:D:153:PRO:HG2	1:D:297:ASN:OD1	2.06	0.55
1:A:244:ILE:HD12	1:A:350:ALA:CB	2.36	0.55
1:G:119:LYS:HD3	1:G:206:HIS:NE2	2.22	0.55
1:D:199:ILE:HD12	1:D:239:GLN:O	2.06	0.55
1:M:152:SER:CB	1:M:155:THR:HG23	2.37	0.55
1:A:258:ASN:HB2	1:A:260:LEU:HB2	1.89	0.55
1:A:152:SER:OG	1:A:155:THR:HG23	2.07	0.55
1:D:211:PHE:O	1:D:215:THR:HG23	2.07	0.55
1:D:297:ASN:N	1:D:297:ASN:ND2	2.55	0.55
1:A:265:MSE:HE1	1:A:288:VAL:CG1	2.34	0.54
1:D:154:ALA:CB	1:D:297:ASN:HB2	2.32	0.54
1:D:290:LEU:N	1:D:290:LEU:HD23	2.21	0.54
1:A:154:ALA:CB	1:A:297:ASN:HB2	2.36	0.54
1:M:288:VAL:HG22	1:M:289:ASP:N	2.23	0.54
1:A:62:ALA:HB2	1:G:185:THR:HG22	1.90	0.54
1:J:152:SER:CB	1:J:155:THR:HG23	2.38	0.54
3:G:363:HOH:O	1:J:252:THR:HG21	2.07	0.53
1:M:319:PHE:CD1	1:M:334:ALA:HB1	2.43	0.53
1:G:215:THR:HG22	1:G:251:THR:HG21	1.89	0.53
1:G:146:TYR:HE1	1:G:344:MSE:HE2	1.69	0.53
1:G:79:THR:HG23	1:G:82:GLU:H	1.74	0.53
1:D:265:MSE:HE1	1:D:288:VAL:HG11	1.82	0.53
1:D:297:ASN:N	1:D:297:ASN:HD22	2.07	0.53
1:A:244:ILE:HD11	1:A:246:LEU:HD13	1.91	0.52
1:D:183:ARG:HD2	1:D:183:ARG:C	2.30	0.52
1:M:244:ILE:HG13	1:M:245:HIS:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:144:ILE:HD13	1:M:344:MSE:HE3	1.91	0.52
1:M:227:VAL:HG22	1:M:354:ALA:HB1	1.91	0.52
1:A:207:GLN:HB2	1:A:255:ILE:HD13	1.90	0.52
1:A:180:ARG:NH1	1:A:267:THR:O	2.43	0.52
1:D:120:PRO:HG3	1:D:202:ASP:HA	1.91	0.52
1:J:258:ASN:OD1	1:J:258:ASN:C	2.48	0.52
1:A:234:ASP:C	1:A:236:PRO:HD3	2.30	0.52
1:M:205:SER:HB2	1:M:344:MSE:HE1	1.91	0.52
1:A:64:ALA:HB3	1:A:76:ARG:HH12	1.74	0.52
1:G:244:ILE:HD11	1:G:246:LEU:CD1	2.41	0.51
1:G:144:ILE:HD13	1:G:344:MSE:HE3	1.92	0.51
1:M:287:THR:HG22	1:M:288:VAL:HG12	1.92	0.51
1:A:265:MSE:HE3	1:A:288:VAL:CG1	2.28	0.51
1:D:92:ILE:HD11	1:D:113:LYS:HD3	1.93	0.51
1:A:79:THR:HG23	1:A:82:GLU:CB	2.41	0.51
1:D:70:VAL:HG22	1:D:71:TYR:CE2	2.45	0.51
1:A:178:PRO:O	1:A:178:PRO:CD	2.59	0.51
1:G:244:ILE:HD13	1:G:255:ILE:HD12	1.93	0.51
1:A:182:ARG:HD2	1:A:185:THR:HG21	1.93	0.51
1:D:152:SER:OG	1:D:155:THR:CG2	2.59	0.51
1:J:297:ASN:HD22	1:J:297:ASN:H	1.59	0.50
1:M:223:LEU:HD12	1:M:245:HIS:CE1	2.46	0.50
1:A:293:ARG:NH2	1:D:291:ALA:O	2.45	0.50
1:D:244:ILE:HD11	1:D:246:LEU:HD11	1.94	0.50
1:D:182:ARG:O	1:D:185:THR:N	2.41	0.50
1:M:297:ASN:N	1:M:297:ASN:HD22	2.09	0.50
1:A:120:PRO:HA	1:A:344:MSE:HE1	1.92	0.50
1:A:181:LEU:O	1:A:182:ARG:HB2	2.12	0.50
1:G:312:CYS:O	1:G:315:VAL:HG13	2.11	0.50
1:J:144:ILE:HG13	1:J:340:CYS:SG	2.51	0.50
1:A:299:LEU:HD22	1:A:310:ILE:HD12	1.93	0.50
1:J:267:THR:OG1	1:J:287:THR:HG23	2.10	0.50
1:M:153:PRO:HD3	1:M:317:LEU:HD11	1.92	0.50
1:A:316:ASP:O	1:A:318:PRO:HD3	2.11	0.49
1:D:56:PHE:CZ	1:D:76:ARG:HB2	2.47	0.49
1:J:265:MSE:HE3	1:J:266:PRO:HD2	1.94	0.49
1:M:127:GLN:O	1:M:131:LEU:HD22	2.13	0.49
1:G:349:GLN:O	1:G:353:ILE:HG23	2.13	0.49
1:M:328:ARG:HB3	1:M:329:ASP:OD1	2.12	0.49
1:D:70:VAL:HG22	1:D:71:TYR:CD2	2.48	0.49
1:D:152:SER:CB	1:D:155:THR:HG23	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:265:MSE:HE1	1:G:288:VAL:CG1	2.32	0.49
1:G:267:THR:OG1	1:G:287:THR:CG2	2.61	0.49
1:G:60:ASP:OD1	1:G:63:LEU:HB2	2.13	0.48
1:D:101:ARG:HD3	1:D:117:VAL:HG22	1.95	0.48
1:M:152:SER:HB3	1:M:155:THR:HG23	1.95	0.48
1:A:244:ILE:CD1	1:A:350:ALA:HB2	2.42	0.48
1:M:211:PHE:O	1:M:215:THR:HG23	2.14	0.48
1:G:207:GLN:HB2	1:G:255:ILE:HD13	1.95	0.48
1:G:64:ALA:CB	1:G:76:ARG:HH11	2.23	0.48
1:A:185:THR:CG2	1:A:185:THR:O	2.61	0.48
1:A:155:THR:HG21	1:A:286:LYS:HZ3	1.79	0.47
1:A:264:GLY:N	1:D:303:ASP:O	2.45	0.47
1:D:210:GLN:NE2	1:D:273:LEU:HD13	2.29	0.47
1:J:133:ARG:O	1:J:137:GLU:HG3	2.13	0.47
1:J:349:GLN:O	1:J:353:ILE:HG23	2.14	0.47
1:D:183:ARG:HB3	1:D:186:ARG:CG	2.45	0.47
1:D:212:LEU:HD21	1:D:346:LEU:HD11	1.97	0.47
1:D:66:GLU:O	1:D:70:VAL:HG12	2.14	0.47
1:G:172:HIS:CD2	1:G:252:THR:HG22	2.40	0.47
1:G:285:ARG:NH1	1:G:289:ASP:OD1	2.47	0.47
1:J:27:LEU:HD22	1:J:324:LEU:HD22	1.95	0.47
1:G:152:SER:CB	1:G:155:THR:HG23	2.38	0.47
1:J:207:GLN:H	1:J:207:GLN:HG2	1.52	0.47
1:M:92:ILE:HD13	1:M:92:ILE:HA	1.73	0.47
1:A:254:MSE:HE3	1:D:254:MSE:HE3	1.96	0.47
1:D:101:ARG:HD3	1:D:117:VAL:CG2	2.44	0.47
1:G:181:LEU:O	1:G:182:ARG:CB	2.63	0.47
1:G:258:ASN:HB3	1:G:260:LEU:N	2.29	0.47
1:G:181:LEU:O	1:G:182:ARG:HB2	2.14	0.47
1:A:144:ILE:HD13	1:A:344:MSE:CE	2.42	0.46
1:M:297:ASN:N	1:M:297:ASN:ND2	2.62	0.46
1:A:297:ASN:HD22	1:A:297:ASN:H	1.51	0.46
1:M:199:ILE:CG2	1:M:227:VAL:HG12	2.45	0.46
1:G:265:MSE:HE1	1:G:290:LEU:HD21	1.96	0.46
1:D:152:SER:HB3	1:D:155:THR:HG23	1.96	0.46
1:D:152:SER:OG	1:D:155:THR:HG23	2.16	0.46
1:G:42:GLN:OE1	1:G:118:ASP:HB2	2.16	0.45
1:J:152:SER:HB3	1:J:155:THR:CG2	2.41	0.45
1:G:295:GLY:O	1:G:298:HIS:NE2	2.49	0.45
1:J:178:PRO:HA	1:J:258:ASN:OD1	2.16	0.45
1:M:269:GLY:O	1:M:287:THR:HG21	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ILE:HG13	1:A:131:LEU:HD13	1.98	0.45
1:D:198:GLY:HA3	1:D:351:GLN:NE2	2.32	0.45
1:M:299:LEU:C	1:M:299:LEU:HD23	2.37	0.45
1:D:116:LEU:HA	1:D:143:SER:O	2.15	0.45
1:J:46:LEU:CD1	1:J:93:VAL:HG21	2.47	0.45
1:G:244:ILE:CG1	1:G:246:LEU:HD13	2.47	0.45
1:A:167:ILE:C	1:A:279:SER:HB2	2.37	0.45
1:J:27:LEU:HG	1:J:28:ARG:N	2.30	0.45
1:M:180:ARG:NH1	3:M:375:HOH:O	2.48	0.45
1:J:172:HIS:HA	1:J:252:THR:O	2.17	0.44
1:D:323:PHE:O	1:D:326:ASP:HB2	2.17	0.44
1:M:149:HIS:CD2	1:M:149:HIS:C	2.90	0.44
1:A:244:ILE:HD11	1:A:246:LEU:HD11	1.98	0.44
1:M:60:ASP:HB3	1:M:63:LEU:HB2	1.99	0.44
1:G:223:LEU:O	1:G:224:SER:HB3	2.17	0.44
1:M:146:TYR:HE1	1:M:344:MSE:CE	2.28	0.44
1:A:146:TYR:CE1	1:A:344:MSE:HE2	2.52	0.44
1:G:256:HIS:NE2	1:G:258:ASN:OD1	2.50	0.44
1:G:337:GLN:HA	1:G:337:GLN:NE2	2.33	0.44
1:M:197:GLY:O	1:M:201:THR:HB	2.18	0.44
1:M:130:LYS:O	1:M:133:ARG:HB2	2.18	0.43
1:J:86:ASP:OD1	1:J:88:ASN:HB2	2.18	0.43
1:M:353:ILE:HG21	1:M:353:ILE:HD13	1.65	0.43
1:A:121:GLY:H	1:A:344:MSE:HE3	1.83	0.43
1:A:146:TYR:CD2	1:A:209:GLU:HG3	2.54	0.43
1:A:218:ASN:HD21	1:A:339:ARG:HB2	1.82	0.43
1:G:135:GLN:NE2	1:G:140:ARG:O	2.52	0.43
1:G:306:GLY:N	1:J:264:GLY:HA3	2.33	0.43
1:M:265:MSE:HE1	1:M:290:LEU:HD21	1.99	0.43
1:A:207:GLN:H	1:A:207:GLN:HG2	1.41	0.43
1:D:47:LEU:HD12	1:D:47:LEU:HA	1.81	0.43
1:G:63:LEU:HD12	1:G:63:LEU:HA	1.89	0.43
1:G:172:HIS:HA	1:G:252:THR:O	2.18	0.43
1:G:119:LYS:NZ	1:G:202:ASP:OD1	2.51	0.43
1:M:58:GLU:HG2	1:M:63:LEU:HB3	2.00	0.43
1:A:155:THR:HG21	1:A:286:LYS:HZ2	1.83	0.43
1:D:251:THR:HG22	1:D:252:THR:N	2.34	0.43
1:G:192:ARG:HD2	1:G:195:ASP:OD2	2.18	0.43
1:J:174:VAL:HB	1:J:274:PHE:HB2	2.01	0.43
1:D:183:ARG:H	1:D:183:ARG:HG3	1.42	0.43
1:G:34:LEU:HG	1:G:58:GLU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:272:ARG:CD	1:G:285:ARG:HG2	2.48	0.42
1:M:135:GLN:HG3	1:M:136:ALA:N	2.33	0.42
1:A:229:ASN:C	1:A:229:ASN:OD1	2.57	0.42
1:D:98:SER:HB2	1:D:195:ASP:O	2.19	0.42
1:D:288:VAL:HG22	1:D:289:ASP:N	2.34	0.42
1:J:155:THR:O	1:J:158:ALA:HB3	2.18	0.42
1:J:297:ASN:N	1:J:297:ASN:ND2	2.66	0.42
1:M:145:LEU:HD12	1:M:145:LEU:HA	1.47	0.42
1:A:243:SER:HA	1:A:255:ILE:O	2.19	0.42
1:D:251:THR:CG2	1:D:252:THR:N	2.82	0.42
1:D:35:ASN:HD22	1:D:35:ASN:H	1.67	0.42
1:J:39:ILE:O	1:J:43:VAL:HG23	2.19	0.42
1:M:183:ARG:HH22	1:M:234:ASP:CB	2.28	0.42
1:D:289:ASP:O	1:D:290:LEU:C	2.56	0.42
1:D:193:ARG:O	1:D:193:ARG:NH1	2.52	0.42
1:M:219:ASP:HA	1:M:342:LYS:HE2	2.01	0.42
1:A:244:ILE:CG1	1:A:246:LEU:HD13	2.50	0.41
1:M:212:LEU:HB3	1:M:339:ARG:HD2	2.02	0.41
1:A:93:VAL:HA	1:A:116:LEU:O	2.20	0.41
1:M:212:LEU:HD21	1:M:346:LEU:HD11	2.02	0.41
1:A:152:SER:OG	1:A:155:THR:CG2	2.69	0.41
1:A:182:ARG:HB3	1:A:185:THR:HB	2.02	0.41
1:G:182:ARG:O	1:G:185:THR:OG1	2.36	0.41
1:D:182:ARG:HE	1:D:182:ARG:HB3	1.47	0.41
1:D:153:PRO:CD	1:D:297:ASN:OD1	2.68	0.41
1:G:167:ILE:HG13	1:G:277:GLY:HA3	2.01	0.41
1:G:293:ARG:NH2	1:J:291:ALA:O	2.53	0.41
1:J:42:GLN:O	1:J:45:CYS:HB3	2.20	0.41
1:J:138:THR:HB	1:J:140:ARG:HG2	2.02	0.41
1:G:44:ASN:ND2	1:G:71:TYR:OH	2.53	0.41
1:M:174:VAL:HB	1:M:274:PHE:HB2	2.03	0.41
1:J:239:GLN:OE1	1:J:351:GLN:NE2	2.50	0.40
1:A:120:PRO:HA	1:A:344:MSE:CE	2.51	0.40
1:D:282:ILE:HG21	1:D:282:ILE:HD13	1.84	0.40
1:M:244:ILE:CD1	1:M:246:LEU:HD13	2.47	0.40
1:D:183:ARG:CB	1:D:191:PHE:HZ	2.35	0.40
1:D:200:LEU:HB2	1:D:351:GLN:OE1	2.22	0.40
1:D:254:MSE:HE2	1:D:254:MSE:HB2	1.92	0.40
1:D:37:ASN:C	1:D:39:ILE:N	2.73	0.40
1:J:265:MSE:CE	1:J:270:ASP:HB2	2.52	0.40
1:M:265:MSE:HE1	1:M:290:LEU:HD23	2.03	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	328/361 (91%)	307 (94%)	20 (6%)	1 (0%)	41 72
1	D	328/361 (91%)	298 (91%)	30 (9%)	0	100 100
1	G	328/361 (91%)	308 (94%)	20 (6%)	0	100 100
1	J	328/361 (91%)	312 (95%)	16 (5%)	0	100 100
1	M	328/361 (91%)	313 (95%)	13 (4%)	2 (1%)	25 56
All	All	1640/1805 (91%)	1538 (94%)	99 (6%)	3 (0%)	47 78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	37	ASN
1	A	178	PRO
1	M	217	VAL

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	240/280 (86%)	208 (87%)	32 (13%)	4 12
1	D	229/280 (82%)	196 (86%)	33 (14%)	3 10
1	G	235/280 (84%)	207 (88%)	28 (12%)	5 16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	J	233/280 (83%)	207 (89%)	26 (11%)	6 18
1	M	235/280 (84%)	204 (87%)	31 (13%)	4 12
All	All	1172/1400 (84%)	1022 (87%)	150 (13%)	4 13

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LEU
1	A	63	LEU
1	A	79	THR
1	A	84	LEU
1	A	103	GLU
1	A	113	LYS
1	A	115	VAL
1	A	119	LYS
1	A	126	ASP
1	A	131	LEU
1	A	133	ARG
1	A	135	GLN
1	A	143	SER
1	A	155	THR
1	A	169	GLU
1	A	183	ARG
1	A	207	GLN
1	A	218	ASN
1	A	232	VAL
1	A	244	ILE
1	A	246	LEU
1	A	260	LEU
1	A	287	THR
1	A	288	VAL
1	A	297	ASN
1	A	315	VAL
1	A	316	ASP
1	A	317	LEU
1	A	328	ARG
1	A	333	THR
1	A	342	LYS
1	A	353	ILE
1	D	34	LEU
1	D	47	LEU

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Mol	Chain	Res	Type
1	D	61	ASP
1	D	63	LEU
1	D	70	VAL
1	D	79	THR
1	D	84	LEU
1	D	99	SER
1	D	115	VAL
1	D	119	LYS
1	D	126	ASP
1	D	131	LEU
1	D	135	GLN
1	D	143	SER
1	D	155	THR
1	D	173	ILE
1	D	176	LEU
1	D	183	ARG
1	D	243	SER
1	D	244	ILE
1	D	246	LEU
1	D	247	SER
1	D	254	MSE
1	D	260	LEU
1	D	279	SER
1	D	287	THR
1	D	297	ASN
1	D	315	VAL
1	D	316	ASP
1	D	317	LEU
1	D	336	PRO
1	D	344	MSE
1	D	353	ILE
1	G	45	CYS
1	G	47	LEU
1	G	63	LEU
1	G	70	VAL
1	G	84	LEU
1	G	103	GLU
1	G	115	VAL
1	G	119	LYS
1	G	126	ASP
1	G	131	LEU
1	G	133	ARG

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Mol	Chain	Res	Type
1	G	135	GLN
1	G	155	THR
1	G	167	ILE
1	G	182	ARG
1	G	183	ARG
1	G	207	GLN
1	G	240	ASP
1	G	244	ILE
1	G	246	LEU
1	G	247	SER
1	G	252	THR
1	G	260	LEU
1	G	279	SER
1	G	287	THR
1	G	303	ASP
1	G	317	LEU
1	G	353	ILE
1	J	47	LEU
1	J	48	ARG
1	J	63	LEU
1	J	70	VAL
1	J	79	THR
1	J	84	LEU
1	J	119	LYS
1	J	126	ASP
1	J	131	LEU
1	J	135	GLN
1	J	143	SER
1	J	155	THR
1	J	169	GLU
1	J	218	ASN
1	J	244	ILE
1	J	246	LEU
1	J	247	SER
1	J	252	THR
1	J	260	LEU
1	J	279	SER
1	J	287	THR
1	J	290	LEU
1	J	297	ASN
1	J	316	ASP
1	J	317	LEU

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Mol	Chain	Res	Type
1	J	353	ILE
1	M	27	LEU
1	M	47	LEU
1	M	61	ASP
1	M	63	LEU
1	M	68	SER
1	M	70	VAL
1	M	79	THR
1	M	84	LEU
1	M	115	VAL
1	M	119	LYS
1	M	126	ASP
1	M	131	LEU
1	M	133	ARG
1	M	135	GLN
1	M	155	THR
1	M	176	LEU
1	M	207	GLN
1	M	232	VAL
1	M	240	ASP
1	M	244	ILE
1	M	246	LEU
1	M	247	SER
1	M	252	THR
1	M	254	MSE
1	M	260	LEU
1	M	287	THR
1	M	290	LEU
1	M	314	ARG
1	M	317	LEU
1	M	329	ASP
1	M	342	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	44	ASN
1	A	172	HIS
1	A	218	ASN
1	A	297	ASN
1	D	35	ASN

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Mol	Chain	Res	Type
1	D	44	ASN
1	D	172	HIS
1	D	210	GLN
1	D	349	GLN
1	G	35	ASN
1	G	44	ASN
1	G	135	GLN
1	G	172	HIS
1	G	210	GLN
1	J	35	ASN
1	J	44	ASN
1	J	172	HIS
1	M	35	ASN
1	M	44	ASN
1	M	172	HIS
1	M	210	GLN
1	M	297	ASN
1	M	322	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)

2 ligands 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	$\#\|Z\| > 2$
2	ACT	G	362	-	3,3,3	1.62	1 (33%)	3,3,3	0.82	0
2	ACT	A	362	-	3,3,3	1.74	1 (33%)	3,3,3	0.54	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	362	ACT	CH3-C	2.60	1.60	1.49
2	G	362	ACT	CH3-C	2.36	1.59	1.49

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	362	ACT	2	0

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, 95^{th} 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	324/361 (89%)	-0.49	1 (0%) 94 93	15, 31, 46, 60	0
1	D	324/361 (89%)	-0.19	1 (0%) 94 93	26, 45, 60, 66	0
1	G	324/361 (89%)	-0.53	0 100 100	17, 29, 43, 48	0
1	J	324/361 (89%)	-0.50	1 (0%) 94 93	18, 33, 48, 53	0
1	M	324/361 (89%)	-0.39	0 100 100	18, 32, 48, 58	0
All	All	1620/1805 (89%)	-0.42	3 (0%) 95 94	15, 33, 52, 66	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	188	ASP	2.5
1	A	249	GLY	2.3
1	J	234	ASP	2.3

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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, 95^{th} 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
2	ACT	A	362	4/4	0.87	0.22	31,34,38,38	0
2	ACT	G	362	4/4	0.89	0.20	34,39,40,41	0

6.5 Other polymers (i)

There are no such residues in this entry.