



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:54 AM UTC

PDB ID : 3N6J / pdb_00003n6j
Title : Crystal structure of Mandelate racemase/muconate lactonizing protein from *Actinobacillus succinogenes* 130Z
Authors : Malashkevich, V.N.; Toro, R.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York Structural GenomiX Research Consortium (NYSGXRC); New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2010-05-25
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

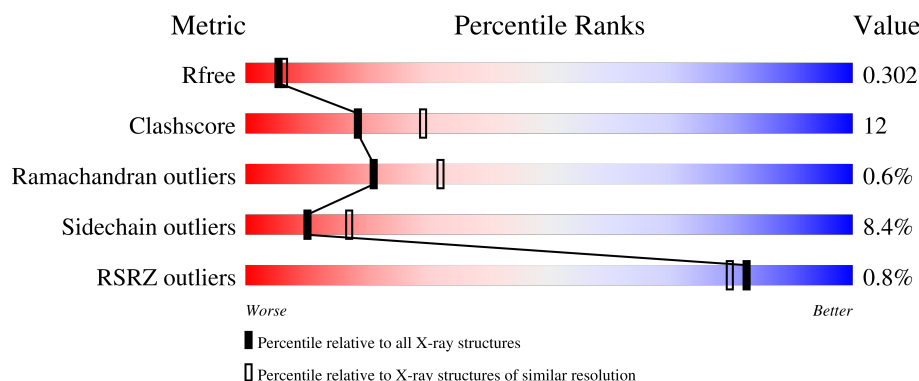
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	455	% 72% 22% • •
1	B	455	69% 22% • 5%
1	C	455	2% 65% 29% • •
1	D	455	% 67% 26% • •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14084 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 Mandelate racemase/muconate lactonizing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	Se	0	1	0
			3456	2200	596	640	6	14			
1	B	432	Total	C	N	O	S	Se	0	1	0
			3379	2150	585	624	6	14			
1	C	442	Total	C	N	O	S	Se	0	2	0
			3462	2205	597	640	6	14			
1	D	440	Total	C	N	O	S	Se	0	1	0
			3441	2192	593	636	6	14			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	expression tag	UNP A6VQF6
A	2	SER	-	expression tag	UNP A6VQF6
A	3	LEU	-	expression tag	UNP A6VQF6
A	448	GLU	-	expression tag	UNP A6VQF6
A	449	GLY	-	expression tag	UNP A6VQF6
A	450	HIS	-	expression tag	UNP A6VQF6
A	451	HIS	-	expression tag	UNP A6VQF6
A	452	HIS	-	expression tag	UNP A6VQF6
A	453	HIS	-	expression tag	UNP A6VQF6
A	454	HIS	-	expression tag	UNP A6VQF6
A	455	HIS	-	expression tag	UNP A6VQF6
B	1	MSE	-	expression tag	UNP A6VQF6
B	2	SER	-	expression tag	UNP A6VQF6
B	3	LEU	-	expression tag	UNP A6VQF6
B	448	GLU	-	expression tag	UNP A6VQF6
B	449	GLY	-	expression tag	UNP A6VQF6
B	450	HIS	-	expression tag	UNP A6VQF6
B	451	HIS	-	expression tag	UNP A6VQF6
B	452	HIS	-	expression tag	UNP A6VQF6
B	453	HIS	-	expression tag	UNP A6VQF6
B	454	HIS	-	expression tag	UNP A6VQF6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	455	HIS	-	expression tag	UNP A6VQF6
C	1	MSE	-	expression tag	UNP A6VQF6
C	2	SER	-	expression tag	UNP A6VQF6
C	3	LEU	-	expression tag	UNP A6VQF6
C	448	GLU	-	expression tag	UNP A6VQF6
C	449	GLY	-	expression tag	UNP A6VQF6
C	450	HIS	-	expression tag	UNP A6VQF6
C	451	HIS	-	expression tag	UNP A6VQF6
C	452	HIS	-	expression tag	UNP A6VQF6
C	453	HIS	-	expression tag	UNP A6VQF6
C	454	HIS	-	expression tag	UNP A6VQF6
C	455	HIS	-	expression tag	UNP A6VQF6
D	1	MSE	-	expression tag	UNP A6VQF6
D	2	SER	-	expression tag	UNP A6VQF6
D	3	LEU	-	expression tag	UNP A6VQF6
D	448	GLU	-	expression tag	UNP A6VQF6
D	449	GLY	-	expression tag	UNP A6VQF6
D	450	HIS	-	expression tag	UNP A6VQF6
D	451	HIS	-	expression tag	UNP A6VQF6
D	452	HIS	-	expression tag	UNP A6VQF6
D	453	HIS	-	expression tag	UNP A6VQF6
D	454	HIS	-	expression tag	UNP A6VQF6
D	455	HIS	-	expression tag	UNP A6VQF6

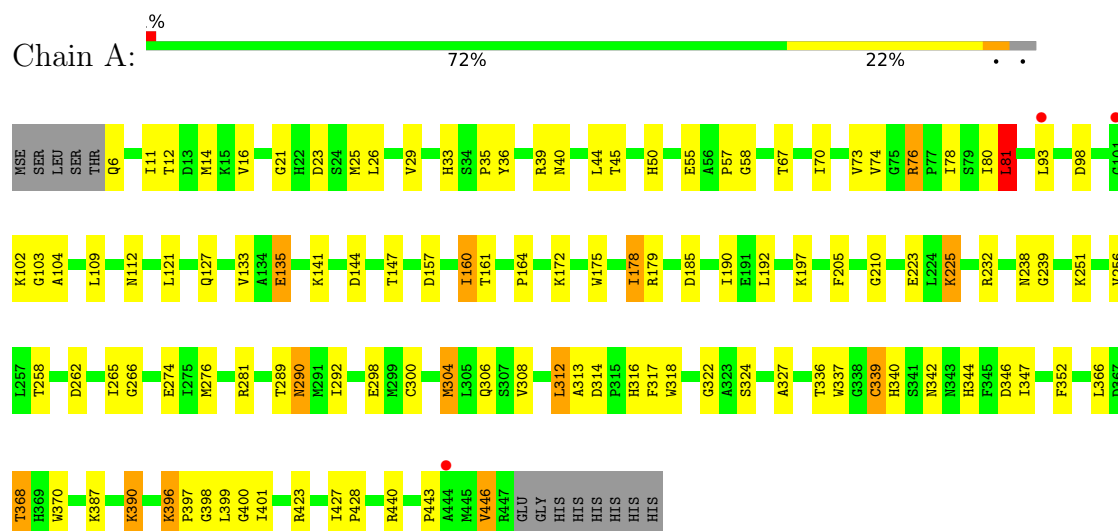
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	144	Total O 144 144	0	0
2	B	109	Total O 109 109	0	0
2	C	67	Total O 67 67	0	0
2	D	26	Total O 26 26	0	0

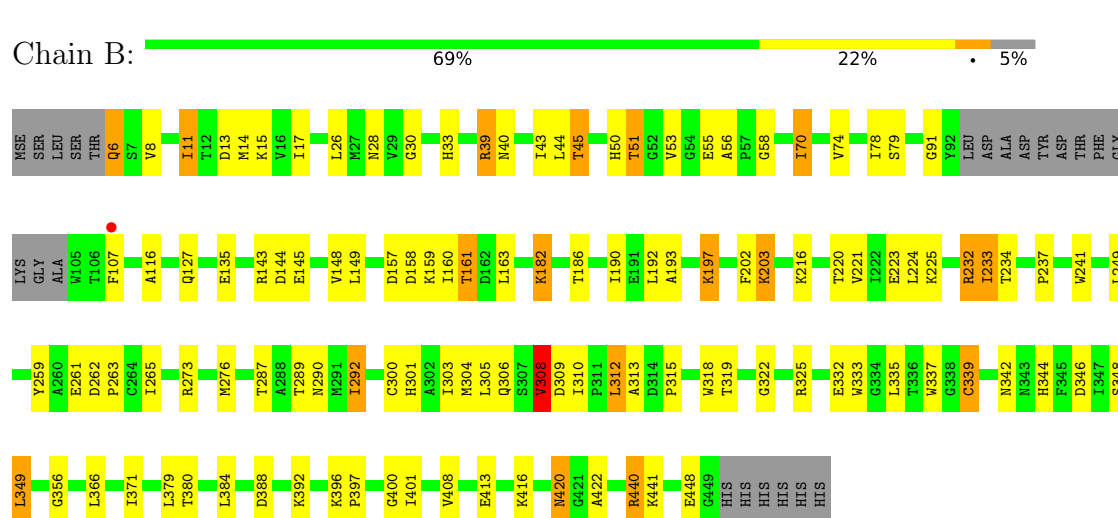
3 Residue-property plots

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: Mandelate racemase/muconate lactonizing protein

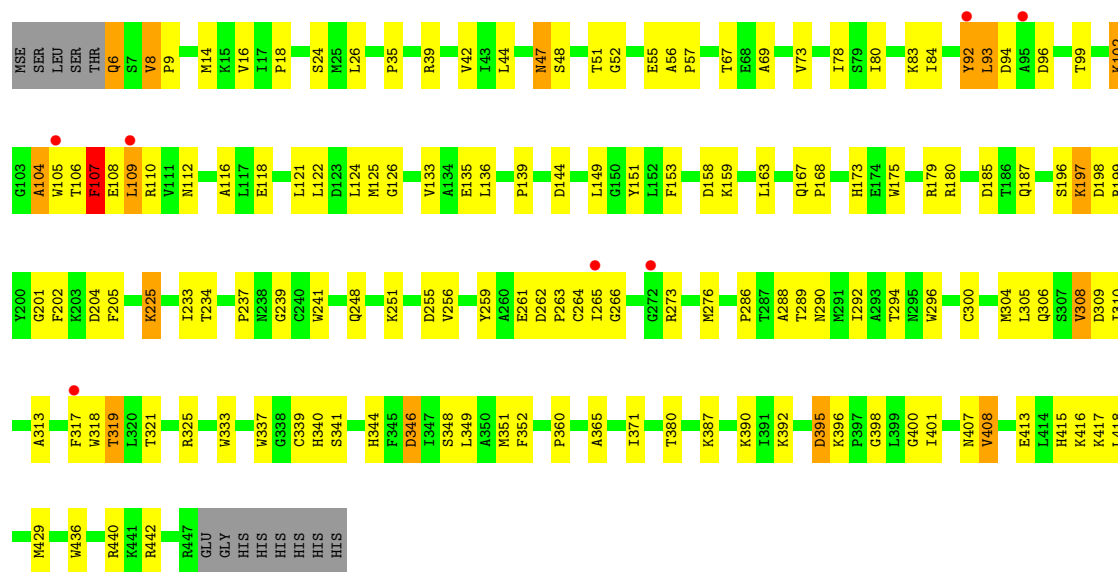


- Molecule 1: Mandelate racemase/muconate lactonizing protein

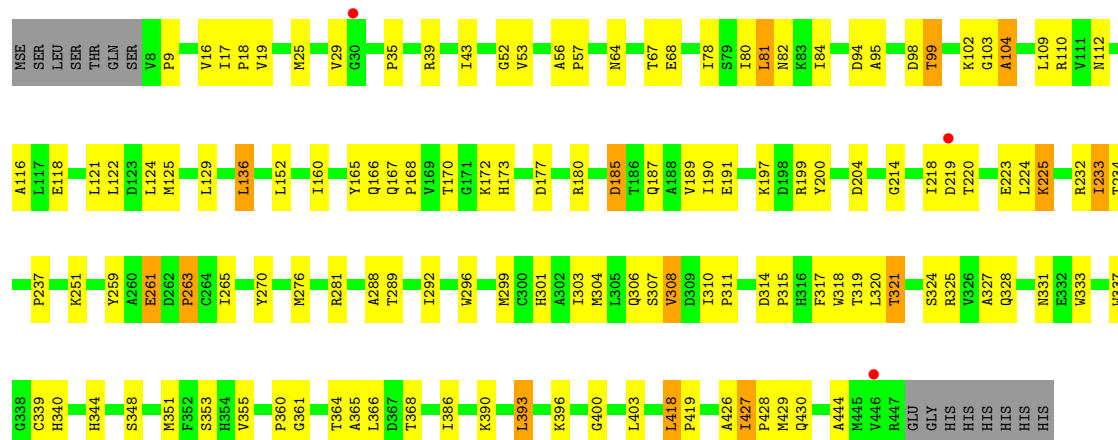


- Molecule 1: Mandelate racemase/muconate lactonizing protein





• Molecule 1: Mandelate racemase/muconate lactonizing protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.78Å 84.35Å 113.47Å 90.00° 97.92° 90.00°	Depositor
Resolution (Å)	19.95 – 2.40 19.95 – 2.40	Depositor EDS
% Data completeness (in resolution range)	68.5 (19.95-2.40) 68.3 (19.95-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.39Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.217 , 0.304 0.218 , 0.302	Depositor DCC
R_{free} test set	2313 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 25.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14084	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.66	1/3532 (0.0%)	0.95	1/4774 (0.0%)
1	B	0.63	0/3452	0.92	6/4664 (0.1%)
1	C	0.61	0/3541	0.91	4/4785 (0.1%)
1	D	0.57	1/3517 (0.0%)	0.87	1/4754 (0.0%)
All	All	0.62	2/14042 (0.0%)	0.91	12/18977 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	427	ILE	CA-CB	6.58	1.57	1.54
1	A	81	LEU	C-O	-5.71	1.17	1.24

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	107	PHE	N-CA-C	7.25	121.47	111.90
1	B	91	GLY	N-CA-C	6.77	124.12	114.64
1	D	308	VAL	N-CA-C	6.74	117.82	108.12
1	B	308	VAL	N-CA-C	6.56	117.26	108.27
1	A	251	LYS	N-CA-C	5.91	117.72	111.28
1	C	8	VAL	CA-C-N	5.73	127.00	119.84
1	C	8	VAL	C-N-CA	5.73	127.00	119.84
1	C	110	ARG	N-CA-C	5.53	118.07	111.71
1	B	70	ILE	CB-CA-C	-5.21	108.75	113.70
1	B	51	THR	CA-C-N	5.19	125.18	121.65
1	B	51	THR	C-N-CA	5.19	125.18	121.65
1	B	203	LYS	N-CA-C	-5.05	105.16	113.50

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	3456	0	3394	78	0
1	B	3379	0	3323	87	0
1	C	3462	0	3407	101	0
1	D	3441	0	3381	80	0
2	A	144	0	0	4	0
2	B	109	0	0	4	0
2	C	67	0	0	5	0
2	D	26	0	0	0	0
All	All	14084	0	13505	328	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 12.

All (328) 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:306:GLN:HG3	1:C:306:GLN:HG3	1.19	1.12
1:B:232:ARG:HG3	1:B:232:ARG:HH11	1.15	1.05
1:D:103:GLY:HA3	1:D:104:ALA:HB2	1.08	1.05
1:D:103:GLY:HA3	1:D:104:ALA:CB	1.85	1.03
1:A:339:CYS:HB2	1:A:366:LEU:HD22	1.37	1.01
1:C:107:PHE:HD2	1:C:107:PHE:O	1.52	0.92
1:C:289:THR:HG22	1:C:308:VAL:HG11	1.54	0.89
1:B:339:CYS:HB2	1:B:366:LEU:HD22	1.55	0.89
1:D:263:PRO:HD2	1:D:276:MSE:SE	2.24	0.88
1:D:103:GLY:CA	1:D:104:ALA:HB2	2.02	0.85
1:A:265:ILE:CG2	1:A:266:GLY:H	1.92	0.82
1:C:35:PRO:HD3	1:C:163:LEU:HD23	1.62	0.82
1:C:263:PRO:HD2	1:C:276:MSE:SE	2.29	0.82
1:A:239:GLY:HA3	1:A:265:ILE:HD12	1.64	0.79
1:C:107:PHE:O	1:C:107:PHE:CD2	2.35	0.78
1:B:232:ARG:HG3	1:B:232:ARG:NH1	1.90	0.77
1:C:173:HIS:HE1	1:C:198:ASP:OD2	1.68	0.77
1:A:81:LEU:HD12	1:A:121:LEU:HB3	1.67	0.76
1:D:427:ILE:HB	1:D:428:PRO:HD3	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:PHE:HB3	2:A:507:HOH:O	1.84	0.75
1:D:191[A]:GLU:OE2	1:D:191[A]:GLU:HA	1.85	0.75
1:A:11:ILE:HG21	1:A:73:VAL:HG12	1.68	0.75
1:B:313:ALA:HB3	1:B:337:TRP:HE1	1.54	0.72
1:A:304:MSE:HE1	1:D:281:ARG:HH22	1.55	0.71
1:B:11:ILE:CD1	1:B:78:ILE:HG22	2.20	0.71
1:A:265:ILE:CG2	1:A:266:GLY:N	2.51	0.71
1:B:233:ILE:HG13	1:B:234:THR:N	2.06	0.71
1:A:265:ILE:HG23	1:A:266:GLY:H	1.55	0.70
1:C:69:ALA:O	1:C:73:VAL:HG23	1.92	0.69
1:A:39:ARG:HD2	1:A:344:HIS:HA	1.74	0.68
1:B:303:ILE:O	1:B:306:GLN:NE2	2.25	0.68
1:C:241:TRP:O	1:C:264:CYS:HB3	1.93	0.68
1:D:314:ASP:HB2	1:D:340:HIS:HB3	1.76	0.68
1:B:186:THR:HG23	1:B:220:THR:HA	1.76	0.67
1:C:265:ILE:CG1	1:C:266:GLY:H	2.07	0.67
1:C:139:PRO:HG3	1:C:360:PRO:HG3	1.76	0.67
1:A:103:GLY:HA3	1:A:104:ALA:HB2	1.77	0.66
1:D:168:PRO:HB3	1:D:177:ASP:O	1.94	0.66
1:A:265:ILE:HG22	1:A:266:GLY:N	2.11	0.66
1:C:107:PHE:CD2	1:C:107:PHE:C	2.74	0.66
1:A:11:ILE:HD11	1:A:121:LEU:HD21	1.77	0.66
1:D:53:VAL:HG11	1:D:403:LEU:HD13	1.78	0.66
1:B:40:ASN:ND2	1:B:58:GLY:HA2	2.11	0.65
1:A:306:GLN:CG	1:C:306:GLN:HG3	2.10	0.65
1:C:35:PRO:CD	1:C:163:LEU:HD23	2.26	0.65
1:D:81:LEU:HB2	1:D:121:LEU:HD13	1.78	0.65
1:A:135:GLU:HG3	1:A:141:LYS:H	1.62	0.64
1:B:237:PRO:HG2	1:B:263:PRO:HA	1.79	0.64
1:C:107:PHE:HD2	1:C:107:PHE:C	2.07	0.64
1:A:175:TRP:O	1:A:179:ARG:HG2	1.98	0.63
1:C:173:HIS:CD2	1:C:175:TRP:H	2.16	0.63
1:B:14:MSE:HB3	1:B:70:ILE:HG23	1.81	0.62
1:C:6:GLN:HA	1:C:6:GLN:HE21	1.64	0.62
1:B:11:ILE:HD11	1:B:78:ILE:HG22	1.79	0.62
1:B:318:TRP:O	1:B:319:THR:OG1	2.17	0.62
1:A:427:ILE:HB	1:A:428:PRO:HD3	1.82	0.62
1:C:333:TRP:CH2	1:D:303:ILE:HD12	2.33	0.62
1:A:29:VAL:HG21	1:A:238:ASN:HB2	1.82	0.62
1:D:64:ASN:O	1:D:68:GLU:HG3	2.00	0.62
1:B:17:ILE:HD12	1:B:43:ILE:HD13	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:THR:CG2	1:B:163:LEU:H	2.14	0.61
1:B:26:LEU:H	1:B:33:HIS:HB2	1.66	0.61
1:D:237:PRO:HG2	1:D:263:PRO:HA	1.83	0.61
1:C:255:ASP:HB2	2:C:606:HOH:O	2.01	0.61
1:B:344:HIS:HB2	1:B:348:SER:HB2	1.83	0.60
1:C:289:THR:CG2	1:C:308:VAL:HG11	2.29	0.60
1:B:396:LYS:HB2	1:B:400:GLY:HA2	1.84	0.60
1:D:325:ARG:HA	1:D:328:GLN:HE21	1.66	0.60
1:C:135:GLU:HG2	1:D:80:ILE:HG22	1.84	0.60
1:B:342:ASN:O	1:B:344:HIS:HD2	1.85	0.60
1:C:126:GLY:HA3	1:C:398:GLY:HA2	1.84	0.60
1:C:333:TRP:HH2	1:D:303:ILE:HD12	1.67	0.60
1:D:78:ILE:HG22	1:D:125:MSE:HE2	1.84	0.59
1:A:29:VAL:HG22	1:A:210:GLY:HA3	1.84	0.59
1:C:92:TYR:H	1:C:92:TYR:HD2	1.47	0.59
1:C:185:ASP:OD2	1:C:187:GLN:HB3	2.01	0.59
1:B:127:GLN:HA	1:B:397:PRO:HB2	1.84	0.59
1:D:52:GLY:HA3	1:D:124:LEU:HG	1.84	0.59
1:A:313:ALA:HB3	1:A:337:TRP:HE1	1.66	0.58
1:C:300:CYS:O	1:C:304:MSE:HG2	2.03	0.58
1:B:11:ILE:HD12	1:B:78:ILE:HG22	1.84	0.58
1:D:327:ALA:HA	1:D:337:TRP:CD1	2.39	0.58
1:A:57:PRO:HD2	1:A:112:ASN:HB3	1.84	0.58
1:A:314:ASP:OD1	1:A:340:HIS:ND1	2.31	0.57
1:A:127:GLN:HA	1:A:397:PRO:HB2	1.86	0.57
1:C:273:ARG:HA	1:C:292:ILE:HD12	1.87	0.57
1:B:107:PHE:HB3	2:B:498:HOH:O	2.05	0.56
1:C:237:PRO:HG2	1:C:263:PRO:HA	1.86	0.56
1:A:178:ILE:HG23	1:A:192:LEU:HD23	1.87	0.56
1:C:265:ILE:HG12	1:C:266:GLY:H	1.70	0.56
1:C:413:GLU:O	1:C:417:LYS:HG2	2.05	0.56
1:B:39:ARG:HD2	1:B:344:HIS:HA	1.86	0.56
1:D:35:PRO:HB3	1:D:165:TYR:HA	1.86	0.56
1:D:219:ASP:O	1:D:223:GLU:HG2	2.05	0.56
1:A:289:THR:OG1	1:A:292:ILE:HG12	2.06	0.55
1:A:26:LEU:H	1:A:33:HIS:HB2	1.71	0.55
1:C:99:THR:HA	1:C:102:LYS:HB2	1.88	0.55
1:B:232:ARG:HH11	1:B:232:ARG:CG	2.03	0.55
1:B:379:LEU:HD22	1:B:408:VAL:HG22	1.88	0.55
1:B:221:VAL:HG22	1:B:233:ILE:HD11	1.89	0.54
1:B:346:ASP:HA	1:B:349:LEU:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:GLY:N	1:C:262:ASP:O	2.40	0.54
1:C:52:GLY:HA3	1:C:124:LEU:HG	1.88	0.54
1:C:149:LEU:HD23	1:C:365:ALA:O	2.07	0.54
1:C:337:TRP:CH2	1:C:339:CYS:SG	3.01	0.54
1:B:440:ARG:HG2	1:B:441:LYS:HG2	1.89	0.54
1:B:233:ILE:HG13	1:B:234:THR:H	1.73	0.53
1:C:18:PRO:HB2	1:C:415:HIS:CE1	2.43	0.53
1:C:173:HIS:HD2	1:C:175:TRP:H	1.54	0.53
1:B:144:ASP:HB3	1:B:392:LYS:HE2	1.90	0.53
1:C:39:ARG:HD2	1:C:344:HIS:HA	1.88	0.53
1:A:6:GLN:HA	1:B:6:GLN:CD	2.34	0.53
1:B:28:ASN:OD1	1:B:30:GLY:N	2.33	0.53
1:C:261:GLU:HA	1:C:288:ALA:O	2.07	0.53
1:B:158:ASP:O	1:B:161:THR:HB	2.09	0.53
1:C:133:VAL:HA	1:C:136:LEU:HD12	1.91	0.53
1:A:135:GLU:HG2	2:B:491:HOH:O	2.08	0.53
1:D:17:ILE:HD12	1:D:43:ILE:HD12	1.91	0.53
1:D:95:ALA:O	1:D:99:THR:HG22	2.09	0.52
1:C:234:THR:HG21	1:C:259:TYR:CE1	2.43	0.52
1:D:396:LYS:HB3	1:D:400:GLY:HA2	1.89	0.52
1:D:261:GLU:HB3	1:D:288:ALA:HB3	1.92	0.52
1:C:396:LYS:HB3	1:C:400:GLY:HA2	1.92	0.52
1:B:203:LYS:HB3	1:B:232:ARG:HH12	1.75	0.52
1:B:448:GLU:H	1:B:448:GLU:CD	2.18	0.52
1:D:234:THR:HG21	1:D:259:TYR:CE1	2.44	0.52
1:D:315:PRO:HG3	1:D:355:VAL:HG21	1.91	0.52
1:B:335:LEU:HD23	1:D:281:ARG:HD3	1.92	0.51
1:A:147:THR:HA	1:A:390:LYS:HG3	1.92	0.51
1:A:399:LEU:HB3	1:A:401:ILE:HD12	1.91	0.51
1:B:413:GLU:HA	1:B:416:LYS:HD3	1.93	0.51
1:C:290:ASN:O	1:C:294:THR:HG22	2.11	0.51
1:D:288:ALA:HB2	1:D:310:ILE:HB	1.92	0.51
1:C:346:ASP:OD2	1:C:346:ASP:N	2.41	0.51
1:D:234:THR:HG22	1:D:259:TYR:H	1.73	0.51
1:A:29:VAL:HG23	1:A:238:ASN:HD22	1.76	0.51
1:A:112:ASN:HA	1:A:316:HIS:O	2.10	0.51
1:C:429:MSE:HG2	1:C:436:TRP:CD2	2.46	0.51
1:A:74:VAL:O	1:A:76:ARG:NH2	2.44	0.51
1:A:35:PRO:HG3	1:A:164:PRO:HD2	1.93	0.51
1:D:429:MSE:HE2	1:D:444:ALA:HB1	1.93	0.51
1:C:107:PHE:CE2	1:C:109:LEU:HD22	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:VAL:HG12	1:B:366:LEU:HB2	1.93	0.50
1:B:157:ASP:HA	1:B:182:LYS:HB3	1.94	0.50
1:D:81:LEU:HD23	1:D:82:ASN:N	2.26	0.50
1:C:276:MSE:HG3	1:C:292:ILE:HD13	1.93	0.50
1:A:265:ILE:HG22	1:A:266:GLY:H	1.70	0.50
1:B:39:ARG:HH21	1:B:55:GLU:HG2	1.76	0.50
1:A:157:ASP:HB3	1:A:160:ILE:HD12	1.94	0.50
1:A:161:THR:HG21	2:A:500:HOH:O	2.11	0.50
1:B:8:VAL:HG11	1:B:79:SER:HB2	1.94	0.50
1:B:13:ASP:HB3	1:B:45:THR:OG1	2.12	0.49
1:B:234:THR:HG21	1:B:259:TYR:CZ	2.47	0.49
1:D:166:GLN:HG2	1:D:167:GLN:N	2.27	0.49
1:D:331:ASN:ND2	1:D:360:PRO:HB2	2.27	0.49
1:B:161:THR:HG22	1:B:163:LEU:H	1.76	0.49
1:C:39:ARG:HD3	1:C:55:GLU:OE2	2.11	0.49
1:D:81:LEU:HA	1:D:84:ILE:HD12	1.95	0.49
1:B:315:PRO:HD2	1:B:339:CYS:SG	2.53	0.49
1:A:55:GLU:OE1	1:A:347:ILE:HB	2.12	0.49
1:A:232:ARG:HG2	1:A:258:THR:HG21	1.95	0.49
1:B:420:ASN:HD21	1:B:422:ALA:HB3	1.78	0.49
1:B:186:THR:HG21	1:B:223:GLU:HG3	1.94	0.48
1:A:98:ASP:O	1:A:102:LYS:HB2	2.12	0.48
1:B:55:GLU:CD	1:B:348:SER:OG	2.56	0.48
1:C:104:ALA:C	1:C:106:THR:H	2.21	0.48
1:C:348:SER:HA	1:C:351:MSE:SE	2.64	0.48
1:D:57:PRO:HD2	1:D:112:ASN:HB3	1.94	0.48
1:A:133:VAL:HG23	1:A:398:GLY:C	2.39	0.48
1:C:237:PRO:HD2	1:C:261:GLU:O	2.13	0.48
1:A:290:ASN:HB3	1:A:312:LEU:HD12	1.95	0.48
1:D:118:GLU:HG2	1:D:122:LEU:HD12	1.96	0.48
1:C:296:TRP:O	1:D:333:TRP:NE1	2.46	0.47
1:C:395:ASP:OD2	1:C:395:ASP:N	2.42	0.47
1:A:81:LEU:HB2	1:A:121:LEU:HD13	1.95	0.47
1:C:96:ASP:HB3	1:C:108:GLU:HB2	1.96	0.47
1:A:344:HIS:NE2	1:A:368:THR:HG22	2.28	0.47
1:B:202:PHE:CZ	1:B:371:ILE:HG21	2.48	0.47
1:D:39:ARG:HD2	1:D:344:HIS:HA	1.96	0.47
1:A:428:PRO:HB3	2:A:500:HOH:O	2.13	0.47
1:C:133:VAL:HG23	1:C:398:GLY:C	2.39	0.47
1:D:314:ASP:HB3	1:D:317:PHE:CE2	2.50	0.47
1:B:11:ILE:HG22	1:B:74:VAL:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:HIS:HD2	1:C:175:TRP:HB3	1.80	0.47
1:A:274:GLU:HG2	1:D:301:HIS:CD2	2.49	0.47
1:B:289:THR:HG22	1:B:308:VAL:HG11	1.96	0.47
1:B:289:THR:O	1:B:312:LEU:HB2	2.15	0.47
1:C:196:SER:HB2	1:C:202:PHE:HE2	1.80	0.47
1:D:426:ALA:O	1:D:430:GLN:HG2	2.15	0.47
1:A:178:ILE:CG2	1:A:192:LEU:HD23	2.44	0.46
1:D:173:HIS:CE1	1:D:199:ARG:HB2	2.50	0.46
1:B:161:THR:HG23	1:B:163:LEU:H	1.79	0.46
1:B:273:ARG:HB3	1:B:305:LEU:HD12	1.97	0.46
1:D:418:LEU:HD23	1:D:419:PRO:HD2	1.98	0.46
1:B:157:ASP:HB2	1:B:182:LYS:HD3	1.97	0.46
1:C:56:ALA:HB2	1:C:116:ALA:HB2	1.96	0.46
1:A:11:ILE:HG22	1:A:74:VAL:HA	1.97	0.46
1:C:325:ARG:NH1	2:C:569:HOH:O	2.49	0.46
1:A:80:ILE:HG22	1:B:135:GLU:HG2	1.98	0.46
1:A:23:ASP:OD2	1:A:33:HIS:HD2	1.99	0.46
1:C:122:LEU:O	1:C:126:GLY:N	2.49	0.46
1:B:193:ALA:O	1:B:197:LYS:HB2	2.16	0.46
1:C:118:GLU:HA	1:C:121:LEU:HD12	1.98	0.46
1:C:197:LYS:HB2	1:C:205:PHE:HZ	1.80	0.46
1:C:265:ILE:CG1	1:C:266:GLY:N	2.75	0.46
1:C:313:ALA:HB3	1:C:337:TRP:HE1	1.81	0.46
1:B:233:ILE:CG1	1:B:234:THR:N	2.77	0.46
1:B:17:ILE:HD12	1:B:43:ILE:CD1	2.46	0.45
1:C:44:LEU:HB2	1:C:124:LEU:HD11	1.97	0.45
1:C:241:TRP:O	1:C:264:CYS:CB	2.63	0.45
1:A:14:MSE:SE	1:A:70:ILE:HA	2.66	0.45
1:A:225:LYS:HG3	1:A:256:VAL:HA	1.99	0.45
1:A:298:GLU:HG2	1:D:270:TYR:CE1	2.52	0.45
1:B:202:PHE:HZ	1:B:371:ILE:HG21	1.80	0.45
1:B:380:THR:HG22	1:B:401:ILE:HG23	1.97	0.45
1:C:173:HIS:HD2	1:C:175:TRP:CB	2.30	0.45
1:A:21:GLY:O	1:A:36:TYR:HA	2.16	0.45
1:A:304:MSE:HE1	1:D:281:ARG:NH2	2.26	0.45
1:B:234:THR:HG21	1:B:259:TYR:CE1	2.52	0.45
1:C:80:ILE:O	1:C:84:ILE:HD12	2.16	0.45
1:A:396:LYS:HB3	1:A:400:GLY:HA2	1.97	0.45
1:B:39:ARG:CD	1:B:55:GLU:OE2	2.64	0.45
1:D:351:MSE:O	1:D:355:VAL:HG23	2.17	0.45
1:D:261:GLU:HA	1:D:288:ALA:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:339:CYS:HB2	1:D:366:LEU:HG	1.98	0.45
1:A:239:GLY:N	1:A:262:ASP:O	2.50	0.44
1:B:44:LEU:O	1:B:51:THR:HA	2.16	0.44
1:C:93:LEU:HD13	1:C:94:ASP:N	2.32	0.44
1:C:288:ALA:HA	1:C:310:ILE:O	2.18	0.44
1:C:407:ASN:O	1:C:408:VAL:C	2.61	0.44
1:D:17:ILE:HA	1:D:18:PRO:HD2	1.82	0.44
1:D:168:PRO:HG3	1:D:180:ARG:HB2	1.99	0.44
1:D:348:SER:HA	1:D:351:MSE:SE	2.67	0.44
1:A:262:ASP:OD1	1:A:289:THR:OG1	2.23	0.44
1:B:304:MSE:HE2	1:B:304:MSE:HA	1.98	0.44
1:D:56:ALA:HB2	1:D:116:ALA:HB2	1.98	0.44
1:C:18:PRO:HB2	1:C:415:HIS:NE2	2.33	0.44
1:C:442:ARG:HD3	2:C:575:HOH:O	2.17	0.44
1:D:320:LEU:HD12	1:D:320:LEU:H	1.83	0.44
1:A:368:THR:HG21	1:A:370:TRP:HB2	1.99	0.44
1:A:443:PRO:HB2	1:A:446:VAL:HG23	1.99	0.44
1:D:152:LEU:HD22	1:D:189:VAL:HG13	1.99	0.44
1:D:364:THR:HG23	1:D:365:ALA:O	2.17	0.44
1:B:241:TRP:HB2	1:B:263:PRO:O	2.17	0.43
1:C:144:ASP:O	1:C:392:LYS:HA	2.18	0.43
1:C:318:TRP:O	1:C:319:THR:OG1	2.31	0.43
1:B:305:LEU:HD21	1:C:305:LEU:HG	2.00	0.43
1:C:80:ILE:HG22	1:C:83:LYS:HB3	1.99	0.43
1:D:225:LYS:HG2	1:D:233:ILE:HD13	1.99	0.43
1:D:299:MSE:HE1	1:D:311:PRO:HB3	1.99	0.43
1:A:352:PHE:CE2	1:A:368:THR:HG23	2.53	0.43
1:A:427:ILE:CB	1:A:428:PRO:HD3	2.49	0.43
1:C:57:PRO:HD2	1:C:112:ASN:HB3	2.00	0.43
1:C:204:ASP:OD2	1:C:365:ALA:HB2	2.18	0.43
1:C:225:LYS:HB2	1:C:256:VAL:HG13	2.01	0.43
1:D:237:PRO:CG	1:D:263:PRO:HA	2.46	0.43
1:D:289:THR:OG1	1:D:292:ILE:HG12	2.19	0.43
1:B:149:LEU:C	1:B:149:LEU:HD12	2.44	0.43
1:C:197:LYS:O	1:C:201:GLY:N	2.47	0.43
1:D:353:SER:HB3	1:D:393:LEU:HD22	2.00	0.43
1:A:25:MSE:HE3	2:A:500:HOH:O	2.17	0.43
1:D:331:ASN:OD1	1:D:361:GLY:HA3	2.19	0.43
1:A:197:LYS:HB2	1:A:205:PHE:HZ	1.84	0.43
1:A:318:TRP:O	1:A:322:GLY:HA3	2.19	0.43
1:C:14:MSE:HE3	1:C:42:VAL:HG13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:PRO:HB2	1:D:78:ILE:HD12	2.01	0.43
1:D:25:MSE:HB2	1:D:165:TYR:CE2	2.53	0.43
1:A:265:ILE:HG22	1:A:440:ARG:NH2	2.34	0.42
1:B:318:TRP:O	1:B:322:GLY:HA3	2.18	0.42
1:D:185:ASP:OD2	1:D:187:GLN:HG3	2.19	0.42
1:A:39:ARG:HD3	1:A:55:GLU:OE2	2.19	0.42
1:A:40:ASN:ND2	1:A:58:GLY:HA2	2.34	0.42
1:D:204:ASP:OD1	1:D:232:ARG:HB2	2.18	0.42
1:B:313:ALA:HB3	1:B:337:TRP:NE1	2.26	0.42
1:B:440:ARG:HD2	2:B:512:HOH:O	2.18	0.42
1:C:14:MSE:SE	1:C:73:VAL:HG21	2.69	0.42
1:B:261:GLU:O	1:B:262:ASP:C	2.62	0.42
1:C:167:GLN:HB3	1:C:168:PRO:CD	2.49	0.42
1:D:118:GLU:OE1	1:D:321:THR:HB	2.20	0.42
1:B:344:HIS:HB2	1:B:348:SER:CB	2.48	0.42
1:C:26:LEU:HB3	1:C:153:PHE:CD1	2.54	0.42
1:A:14:MSE:HG3	1:A:44:LEU:CD2	2.50	0.42
1:B:342:ASN:O	1:B:344:HIS:CD2	2.70	0.42
1:D:296:TRP:CE2	1:D:318:TRP:HZ3	2.38	0.42
1:B:384:LEU:HA	2:B:472:HOH:O	2.20	0.42
1:D:81:LEU:HD23	1:D:82:ASN:H	1.85	0.42
1:D:259:TYR:CD1	1:D:310:ILE:HD13	2.55	0.42
1:B:143:ARG:NH2	1:B:356:GLY:O	2.50	0.42
1:B:309:ASP:C	1:B:310:ILE:HG13	2.45	0.42
1:C:416:LYS:C	1:C:418:LEU:H	2.28	0.42
1:B:273:ARG:HD2	1:B:301:HIS:HB2	2.02	0.41
1:D:214:GLY:O	1:D:218:ILE:HG12	2.19	0.41
1:A:324:SER:O	1:A:327:ALA:HB3	2.19	0.41
1:C:173:HIS:CE1	1:C:198:ASP:OD2	2.59	0.41
1:C:265:ILE:HG13	1:C:266:GLY:H	1.84	0.41
1:D:261:GLU:CB	1:D:288:ALA:HB3	2.50	0.41
1:C:309:ASP:HA	2:C:470:HOH:O	2.21	0.41
1:D:200:TYR:HB3	1:D:386:ILE:CG2	2.50	0.41
1:A:190:ILE:HD11	1:A:223:GLU:HB3	2.00	0.41
1:A:276:MSE:HG3	1:A:292:ILE:HG21	2.02	0.41
1:B:39:ARG:HD3	1:B:55:GLU:OE2	2.20	0.41
1:B:300:CYS:O	1:B:304:MSE:HG2	2.21	0.41
1:C:80:ILE:O	1:C:80:ILE:HG22	2.20	0.41
1:D:324:SER:O	1:D:328:GLN:HG3	2.20	0.41
1:B:304:MSE:HG3	2:C:479:HOH:O	2.19	0.41
1:C:380:THR:CG2	1:C:401:ILE:HG23	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:THR:HA	1:B:50:HIS:O	2.21	0.41
1:C:179:ARG:NH1	1:C:371:ILE:O	2.47	0.41
1:A:29:VAL:CG2	1:A:238:ASN:HB2	2.49	0.41
1:A:45:THR:HA	1:A:50:HIS:O	2.21	0.41
1:A:300:CYS:HB2	1:B:333:TRP:CD1	2.56	0.41
1:B:159:LYS:C	1:B:161:THR:H	2.29	0.41
1:B:276:MSE:HG3	1:B:292:ILE:HD13	2.02	0.41
1:B:346:ASP:OD2	1:B:346:ASP:N	2.47	0.41
1:C:9:PRO:HA	1:C:47:ASN:OD1	2.20	0.41
1:C:333:TRP:HH2	1:D:303:ILE:CD1	2.33	0.41
1:A:342:ASN:O	1:A:344:HIS:HD2	2.04	0.41
1:C:8:VAL:HG21	1:D:129:LEU:HA	2.03	0.41
1:C:24:SER:OG	1:C:180:ARG:HD3	2.20	0.41
1:C:340:HIS:CG	1:C:341:SER:N	2.89	0.41
1:A:11:ILE:HD13	1:A:73:VAL:HG13	2.03	0.40
1:C:122:LEU:HA	1:C:125:MSE:HB3	2.03	0.40
1:D:81:LEU:HD12	1:D:121:LEU:HB3	2.03	0.40
1:B:56:ALA:HB2	1:B:116:ALA:HB2	2.02	0.40
1:C:8:VAL:HG21	1:D:129:LEU:O	2.22	0.40
1:C:286:PRO:HA	1:C:309:ASP:OD1	2.21	0.40
1:C:349:LEU:HA	1:C:352:PHE:CE2	2.57	0.40
1:D:129:LEU:HD12	1:D:136:LEU:HD21	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	441/455 (97%)	420 (95%)	21 (5%)	0	100	100
1	B	429/455 (94%)	404 (94%)	25 (6%)	0	100	100
1	C	442/455 (97%)	407 (92%)	29 (7%)	6 (1%)	9	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	439/455 (96%)	409 (93%)	26 (6%)	4 (1%)	14	22
All	All	1751/1820 (96%)	1640 (94%)	101 (6%)	10 (1%)	21	32

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	104	ALA
1	D	251	LYS
1	C	47	ASN
1	C	104	ALA
1	C	251	LYS
1	D	319	THR
1	C	105	TRP
1	C	319	THR
1	D	263	PRO
1	C	408	VAL

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	365/361 (101%)	336 (92%)	29 (8%)	11	19
1	B	358/361 (99%)	326 (91%)	32 (9%)	9	15
1	C	366/361 (101%)	338 (92%)	28 (8%)	12	20
1	D	363/361 (101%)	330 (91%)	33 (9%)	9	14
All	All	1452/1444 (101%)	1330 (92%)	122 (8%)	10	17

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	THR
1	A	16	VAL
1	A	67	THR
1	A	76	ARG

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Mol	Chain	Res	Type
1	A	78	ILE
1	A	81	LEU
1	A	93	LEU
1	A	109	LEU
1	A	135	GLU
1	A	144	ASP
1	A	160	ILE
1	A	172	LYS
1	A	178	ILE
1	A	185	ASP
1	A	225	LYS
1	A	281	ARG
1	A	290	ASN
1	A	304	MSE
1	A	308	VAL
1	A	312	LEU
1	A	336	THR
1	A	339	CYS
1	A	346	ASP
1	A	368	THR
1	A	387	LYS
1	A	390	LYS
1	A	396	LYS
1	A	423	ARG
1	A	446	VAL
1	B	6	GLN
1	B	11	ILE
1	B	15	LYS
1	B	39	ARG
1	B	45	THR
1	B	53	VAL
1	B	145	GLU
1	B	160	ILE
1	B	161	THR
1	B	182	LYS
1	B	190	ILE
1	B	192	LEU
1	B	197	LYS
1	B	216	LYS
1	B	224	LEU
1	B	225	LYS
1	B	232	ARG

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Mol	Chain	Res	Type
1	B	233	ILE
1	B	249	LEU
1	B	265	ILE
1	B	287	THR
1	B	290	ASN
1	B	292	ILE
1	B	308	VAL
1	B	312	LEU
1	B	325	ARG
1	B	332	GLU
1	B	339	CYS
1	B	349	LEU
1	B	388	ASP
1	B	420	ASN
1	B	440	ARG
1	C	6	GLN
1	C	16	VAL
1	C	48	SER
1	C	51	THR
1	C	67	THR
1	C	78	ILE
1	C	92	TYR
1	C	93	LEU
1	C	102	LYS
1	C	107	PHE
1	C	109	LEU
1	C	151	TYR
1	C	158	ASP
1	C	159[A]	LYS
1	C	159[B]	LYS
1	C	197	LYS
1	C	199	ARG
1	C	225	LYS
1	C	233	ILE
1	C	248	GLN
1	C	308	VAL
1	C	317	PHE
1	C	321	THR
1	C	346	ASP
1	C	387	LYS
1	C	390	LYS
1	C	395	ASP

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Mol	Chain	Res	Type
1	C	440	ARG
1	D	16	VAL
1	D	19	VAL
1	D	29	VAL
1	D	67	THR
1	D	81	LEU
1	D	94	ASP
1	D	98	ASP
1	D	99	THR
1	D	102	LYS
1	D	109	LEU
1	D	110	ARG
1	D	136	LEU
1	D	160	ILE
1	D	170	THR
1	D	172	LYS
1	D	185	ASP
1	D	190	ILE
1	D	197	LYS
1	D	220	THR
1	D	224	LEU
1	D	225	LYS
1	D	233	ILE
1	D	261	GLU
1	D	265	ILE
1	D	304	MSE
1	D	306	GLN
1	D	307	SER
1	D	308	VAL
1	D	321	THR
1	D	368	THR
1	D	390	LYS
1	D	393	LEU
1	D	418	LEU

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	33	HIS
1	A	86	ASN
1	A	238	ASN
1	B	6	GLN

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Mol	Chain	Res	Type
1	B	40	ASN
1	B	86	ASN
1	B	142	GLN
1	B	254	ASN
1	B	268	ASN
1	B	344	HIS
1	B	415	HIS
1	C	6	GLN
1	C	50	HIS
1	C	64	ASN
1	C	127	GLN
1	C	173	HIS
1	C	342	ASN
1	D	254	ASN
1	D	268	ASN
1	D	290	ASN
1	D	328	GLN
1	D	342	ASN
1	D	407	ASN
1	D	412	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	428/455 (94%)	-0.14	3 (0%) 84 81	7, 23, 53, 71	1 (0%)
1	B	418/455 (91%)	-0.09	1 (0%) 91 89	8, 26, 49, 60	1 (0%)
1	C	428/455 (94%)	0.20	7 (1%) 70 66	20, 36, 65, 76	2 (0%)
1	D	426/455 (93%)	0.39	3 (0%) 84 81	23, 47, 66, 80	1 (0%)
All	All	1700/1820 (93%)	0.09	14 (0%) 82 80	7, 34, 63, 80	5 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	265	ILE	3.2
1	B	107	PHE	2.8
1	C	105	TRP	2.6
1	D	446	VAL	2.3
1	C	109	LEU	2.2
1	A	101	GLY	2.2
1	C	272	GLY	2.2
1	A	93	LEU	2.2
1	D	30	GLY	2.2
1	C	92	TYR	2.2
1	A	444	ALA	2.1
1	C	95	ALA	2.1
1	C	317	PHE	2.0
1	D	219	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.