



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 04:54 PM UTC

PDB ID : 5AEX / pdb_00005aex
Title : Crystal structure of *Saccharomyces cerevisiae* Mep2
Authors : Rutherford, J.C.; Chembath, A.; van den Berg, B.
Deposited on : 2015-01-12
Resolution : 3.20 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

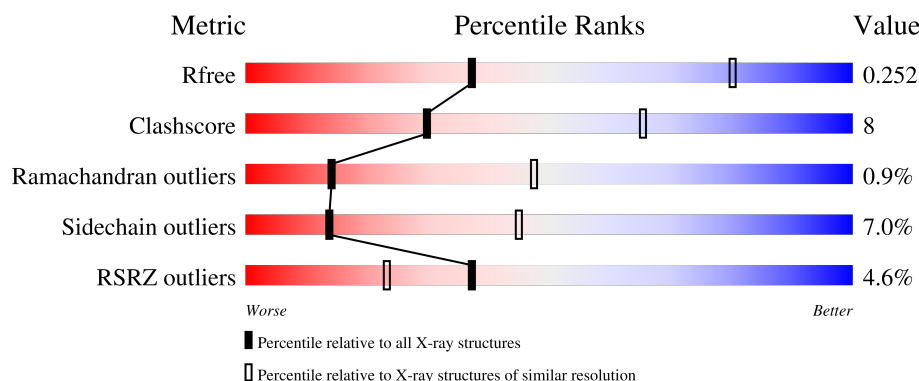
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	505	2% 72% 15% • 10%
1	B	505	2% 65% 22% • 10%
1	C	505	6% 68% 19% • 10%
1	D	505	2% 70% 17% • 10%
1	E	505	5% 66% 22% • 10%

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Mol	Chain	Length	Quality of chain
1	F	505	
1	H	505	
1	I	505	
1	J	505	

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	PO4	I	1455	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 30576 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 AMMONIUM TRANSPORTER MEP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	41	0	0
			3437	2242	561	608	26			
1	B	456	Total	C	N	O	S	65	0	0
			3437	2242	561	608	26			
1	C	456	Total	C	N	O	S	69	0	0
			3437	2242	561	608	26			
1	D	455	Total	C	N	O	S	60	0	0
			3431	2239	560	606	26			
1	E	456	Total	C	N	O	S	95	0	0
			3437	2242	561	608	26			
1	F	456	Total	C	N	O	S	57	0	0
			3437	2242	561	608	26			
1	H	440	Total	C	N	O	S	117	0	0
			3320	2175	541	578	26			
1	I	447	Total	C	N	O	S	204	0	0
			3375	2206	549	594	26			
1	J	427	Total	C	N	O	S	258	0	0
			3220	2115	519	561	25			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	500	HIS	-	expression tag	UNP P41948
A	501	HIS	-	expression tag	UNP P41948
A	502	HIS	-	expression tag	UNP P41948
A	503	HIS	-	expression tag	UNP P41948
A	504	HIS	-	expression tag	UNP P41948
A	505	HIS	-	expression tag	UNP P41948
B	500	HIS	-	expression tag	UNP P41948
B	501	HIS	-	expression tag	UNP P41948
B	502	HIS	-	expression tag	UNP P41948
B	503	HIS	-	expression tag	UNP P41948
B	504	HIS	-	expression tag	UNP P41948

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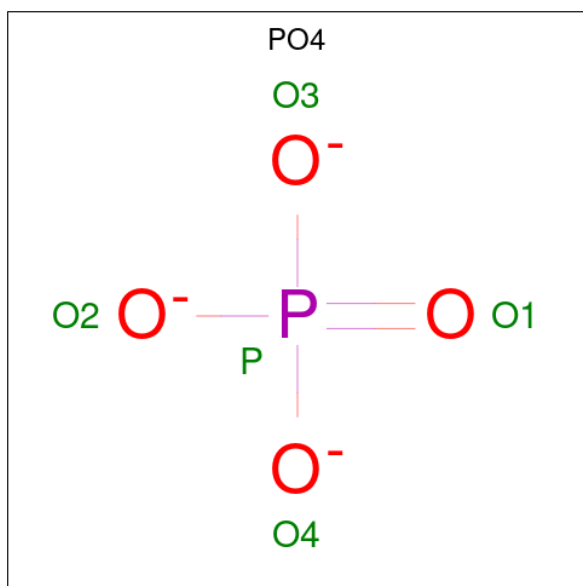
Chain	Residue	Modelled	Actual	Comment	Reference
B	505	HIS	-	expression tag	UNP P41948
C	500	HIS	-	expression tag	UNP P41948
C	501	HIS	-	expression tag	UNP P41948
C	502	HIS	-	expression tag	UNP P41948
C	503	HIS	-	expression tag	UNP P41948
C	504	HIS	-	expression tag	UNP P41948
C	505	HIS	-	expression tag	UNP P41948
D	500	HIS	-	expression tag	UNP P41948
D	501	HIS	-	expression tag	UNP P41948
D	502	HIS	-	expression tag	UNP P41948
D	503	HIS	-	expression tag	UNP P41948
D	504	HIS	-	expression tag	UNP P41948
D	505	HIS	-	expression tag	UNP P41948
E	500	HIS	-	expression tag	UNP P41948
E	501	HIS	-	expression tag	UNP P41948
E	502	HIS	-	expression tag	UNP P41948
E	503	HIS	-	expression tag	UNP P41948
E	504	HIS	-	expression tag	UNP P41948
E	505	HIS	-	expression tag	UNP P41948
F	500	HIS	-	expression tag	UNP P41948
F	501	HIS	-	expression tag	UNP P41948
F	502	HIS	-	expression tag	UNP P41948
F	503	HIS	-	expression tag	UNP P41948
F	504	HIS	-	expression tag	UNP P41948
F	505	HIS	-	expression tag	UNP P41948
H	500	HIS	-	expression tag	UNP P41948
H	501	HIS	-	expression tag	UNP P41948
H	502	HIS	-	expression tag	UNP P41948
H	503	HIS	-	expression tag	UNP P41948
H	504	HIS	-	expression tag	UNP P41948
H	505	HIS	-	expression tag	UNP P41948
I	500	HIS	-	expression tag	UNP P41948
I	501	HIS	-	expression tag	UNP P41948
I	502	HIS	-	expression tag	UNP P41948
I	503	HIS	-	expression tag	UNP P41948
I	504	HIS	-	expression tag	UNP P41948
I	505	HIS	-	expression tag	UNP P41948
J	500	HIS	-	expression tag	UNP P41948
J	501	HIS	-	expression tag	UNP P41948
J	502	HIS	-	expression tag	UNP P41948
J	503	HIS	-	expression tag	UNP P41948
J	504	HIS	-	expression tag	UNP P41948

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Chain	Residue	Modelled	Actual	Comment	Reference
J	505	HIS	-	expression tag	UNP P41948

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).

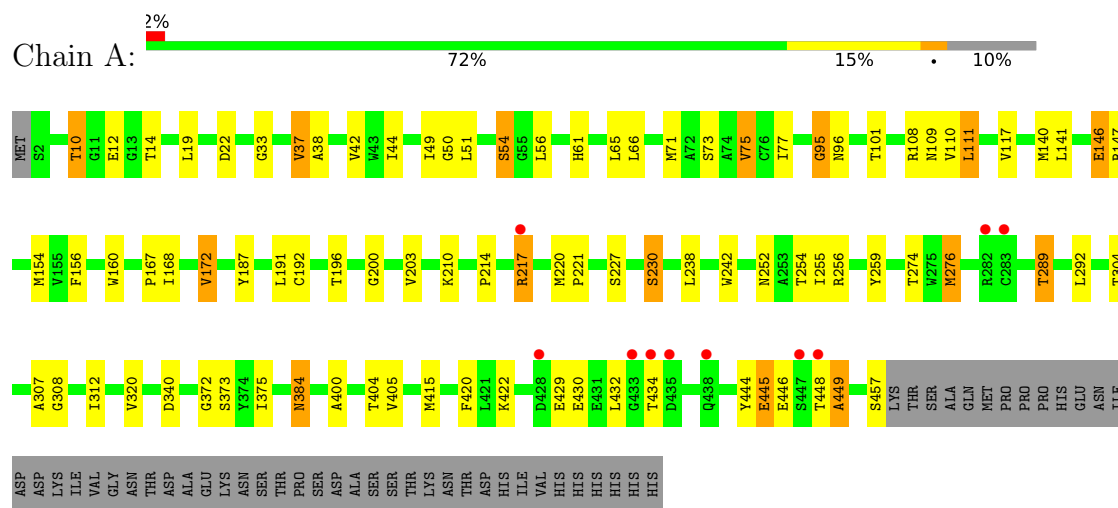


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	H	1	Total	O	P	0	0
			5	4	1		
2	I	1	Total	O	P	0	0
			5	4	1		
2	J	1	Total	O	P	0	0
			5	4	1		

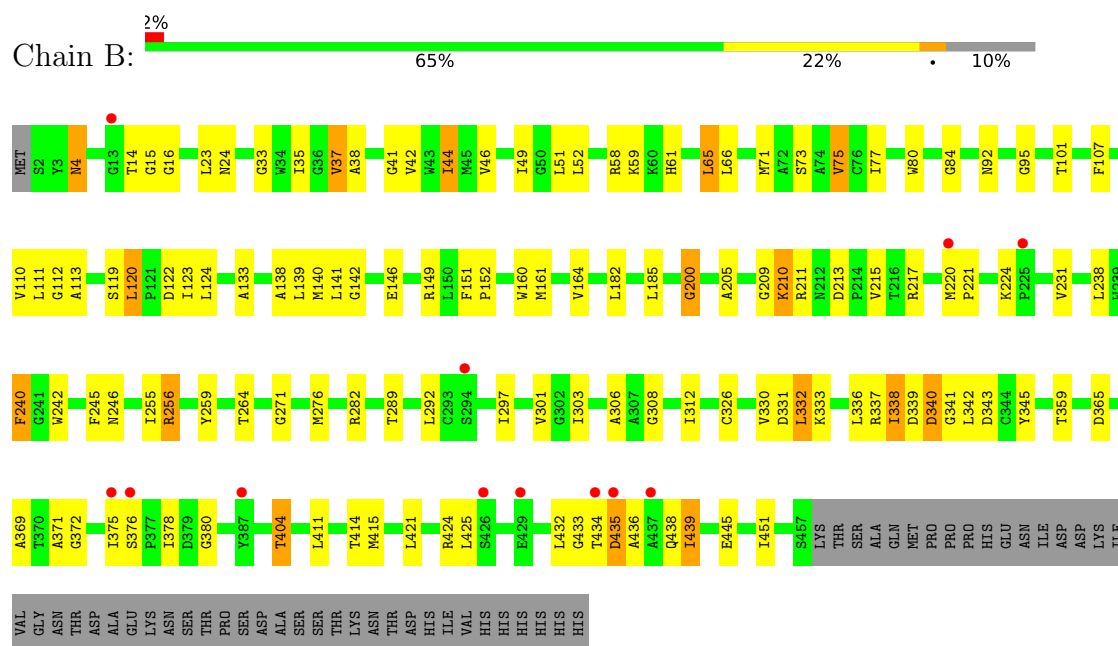
3 Residue-property plots [i](#)

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.

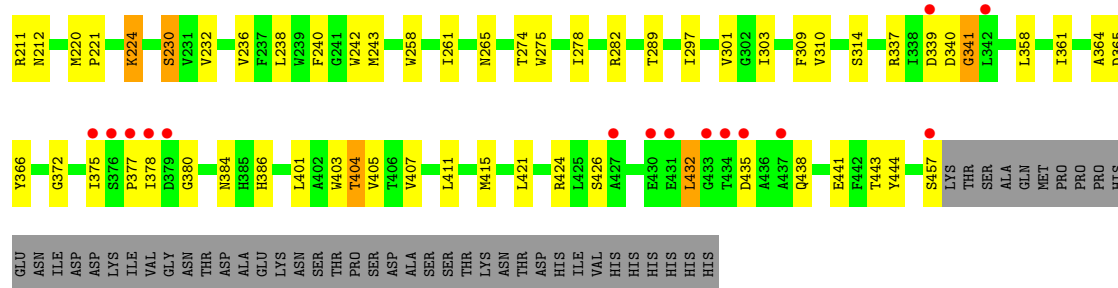
• Molecule 1: AMMONIUM TRANSPORTER MEP2



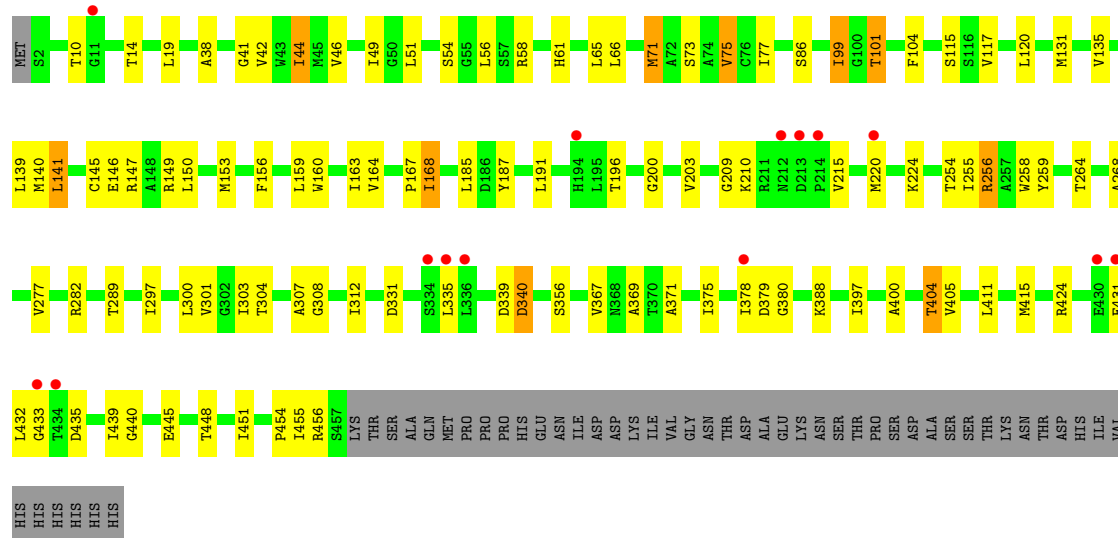
• Molecule 1: AMMONIUM TRANSPORTER MEP2



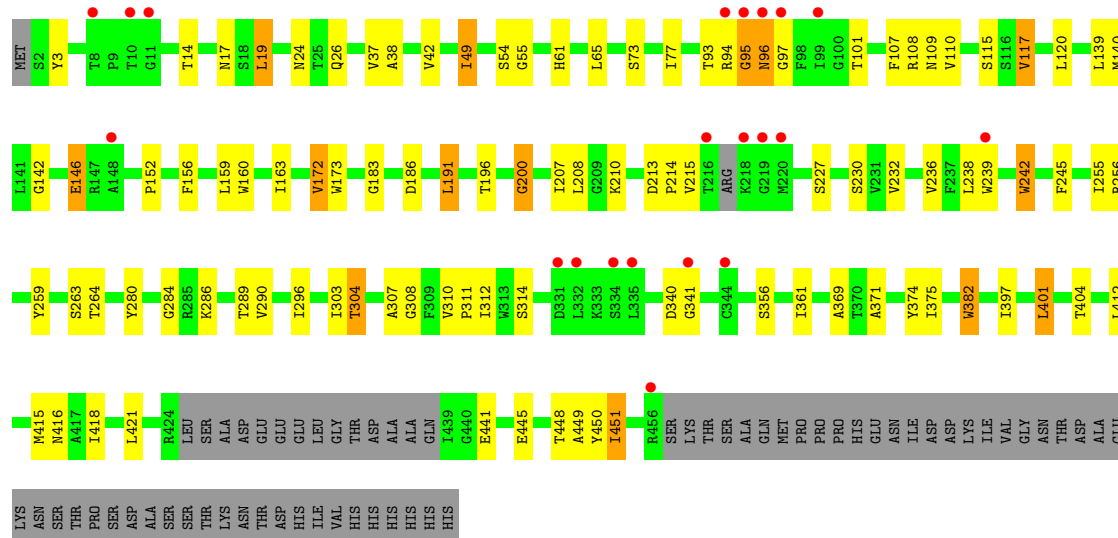
• Molecule 1: AMMONIUM TRANSPORTER MEP2



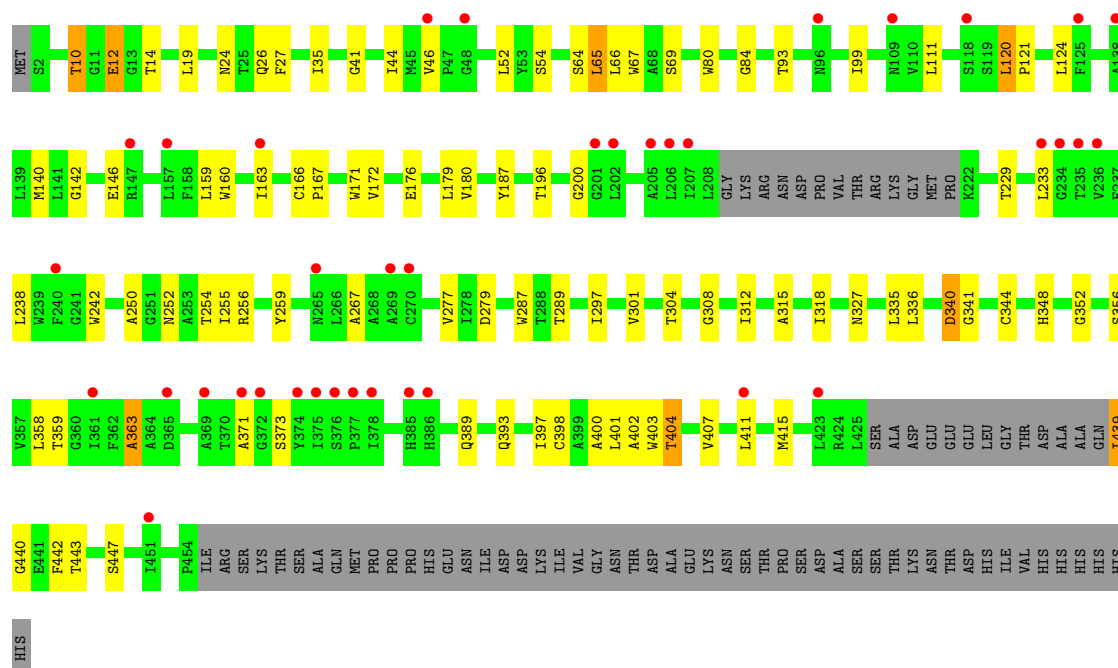
• Molecule 1: AMMONIUM TRANSPORTER MEP2



• Molecule 1: AMMONIUM TRANSPORTER MEP2



Chain I: 6% 69% 18% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	103.69Å 232.35Å 279.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.28 – 3.20 49.28 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.28-3.20) 95.6 (49.28-3.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 3.19Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.189 , 0.241 0.199 , 0.252	Depositor DCC
R_{free} test set	2453 reflections (2.19%)	wwPDB-VP
Wilson B-factor (Å ²)	85.6	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 38.3	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	0.90	EDS
Total number of atoms	30576	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.93	0/3534	0.94	3/4818 (0.1%)
1	B	0.83	0/3534	0.93	8/4818 (0.2%)
1	C	0.73	0/3534	0.89	7/4818 (0.1%)
1	D	0.85	0/3528	0.89	5/4810 (0.1%)
1	E	0.74	0/3534	0.90	2/4818 (0.0%)
1	F	0.90	0/3534	0.93	6/4818 (0.1%)
1	H	0.69	0/3415	0.86	7/4654 (0.2%)
1	I	0.56	0/3470	0.84	4/4729 (0.1%)
1	J	0.50	0/3313	0.83	5/4518 (0.1%)
All	All	0.76	0/31396	0.89	47/42801 (0.1%)

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	B	0	1

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	340	ASP	N-CA-C	10.56	125.98	112.89
1	C	304	THR	CA-C-N	-7.90	111.66	119.87
1	C	304	THR	C-N-CA	-7.90	111.66	119.87
1	I	240	PHE	N-CA-C	7.23	118.81	111.07
1	F	367	VAL	N-CA-C	-7.01	106.22	111.90
1	J	304	THR	CA-C-N	-6.76	112.94	120.45
1	J	304	THR	C-N-CA	-6.76	112.94	120.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	304	THR	CA-C-N	-6.72	112.79	120.04
1	F	304	THR	C-N-CA	-6.72	112.79	120.04
1	C	200	GLY	N-CA-C	-6.39	106.74	114.66
1	E	240	PHE	N-CA-C	6.36	118.09	111.03
1	A	304	THR	CA-C-N	-6.11	113.44	120.04
1	A	304	THR	C-N-CA	-6.11	113.44	120.04
1	D	304	THR	CA-C-N	-6.03	114.69	120.83
1	D	304	THR	C-N-CA	-6.03	114.69	120.83
1	C	376	SER	CA-C-N	6.01	127.36	119.84
1	C	376	SER	C-N-CA	6.01	127.36	119.84
1	D	46	VAL	CA-C-N	-5.95	113.61	120.04
1	D	46	VAL	C-N-CA	-5.95	113.61	120.04
1	B	240	PHE	N-CA-C	5.89	117.39	110.97
1	B	200	GLY	N-CA-C	-5.88	107.37	114.66
1	F	46	VAL	CA-C-N	-5.88	113.76	119.87
1	F	46	VAL	C-N-CA	-5.88	113.76	119.87
1	B	151	PHE	CA-C-N	-5.80	112.90	119.28
1	B	151	PHE	C-N-CA	-5.80	112.90	119.28
1	I	304	THR	CA-C-N	-5.79	114.27	120.47
1	I	304	THR	C-N-CA	-5.79	114.27	120.47
1	A	445	GLU	N-CA-C	5.78	117.27	110.97
1	H	418	ILE	CA-C-N	5.61	125.28	119.56
1	H	418	ILE	C-N-CA	5.61	125.28	119.56
1	H	304	THR	CA-C-N	-5.31	114.56	120.45
1	H	304	THR	C-N-CA	-5.31	114.56	120.45
1	C	46	VAL	CA-C-N	-5.28	114.33	120.04
1	C	46	VAL	C-N-CA	-5.28	114.33	120.04
1	J	46	VAL	CA-C-N	-5.26	114.40	119.87
1	J	46	VAL	C-N-CA	-5.26	114.40	119.87
1	J	250	ALA	N-CA-C	-5.24	105.74	111.82
1	F	71	MET	N-CA-C	-5.20	105.79	111.82
1	H	200	GLY	N-CA-C	-5.17	106.15	112.77
1	B	376	SER	CA-C-N	-5.16	114.09	120.79
1	B	376	SER	C-N-CA	-5.16	114.09	120.79
1	H	374	TYR	CA-C-N	-5.15	115.54	122.91
1	H	374	TYR	C-N-CA	-5.15	115.54	122.91
1	B	271	GLY	N-CA-C	-5.13	106.54	112.50
1	E	164	VAL	CB-CA-C	-5.08	106.53	111.05
1	I	164	VAL	CB-CA-C	-5.07	107.41	111.71
1	D	382	TRP	N-CA-C	5.04	116.77	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	240	PHE	Peptide

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	3437	0	3401	44	0
1	B	3437	0	3401	75	0
1	C	3437	0	3401	62	1
1	D	3431	0	3396	53	0
1	E	3437	0	3401	67	0
1	F	3437	0	3401	53	0
1	H	3320	0	3295	51	0
1	I	3375	0	3337	57	1
1	J	3220	0	3188	54	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	1	0
2	F	5	0	0	0	0
2	H	5	0	0	0	0
2	I	5	0	0	2	0
2	J	5	0	0	0	0
All	All	30576	0	30221	495	1

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 8.

All (495) 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:B:140:MET:HE1	1:B:200:GLY:HA3	1.55	0.88
1:J:10:THR:HG22	1:J:12:GLU:H	1.37	0.88
1:F:256:ARG:NH1	1:F:308:GLY:O	2.10	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:THR:HG22	1:A:12:GLU:H	1.47	0.78
1:C:400:ALA:O	1:C:404:THR:OG1	2.01	0.78
1:H:49:ILE:HG13	1:H:238:LEU:HD21	1.65	0.78
1:B:205:ALA:HB2	1:B:341:GLY:HA2	1.67	0.77
1:B:378:ILE:HG13	1:B:380:GLY:H	1.49	0.76
1:H:140:MET:HE1	1:H:200:GLY:HA3	1.65	0.76
1:I:256:ARG:NH1	1:I:308:GLY:O	2.19	0.76
1:D:342:LEU:O	1:D:346:SER:OG	2.02	0.76
1:H:95:GLY:HA3	1:H:97:GLY:N	2.02	0.75
1:E:220:MET:HG3	1:E:221:PRO:HD2	1.68	0.74
1:B:276:MET:HE3	1:B:292:LEU:HB2	1.70	0.74
1:J:400:ALA:O	1:J:404:THR:OG1	2.04	0.74
1:D:110:VAL:HG23	1:D:122:ASP:HB3	1.70	0.72
1:I:140:MET:HE1	1:I:200:GLY:HA3	1.70	0.71
1:D:447:SER:HB3	1:E:224:LYS:HG2	1.73	0.71
1:D:220:MET:HG3	1:D:221:PRO:HD2	1.73	0.70
1:A:140:MET:HE1	1:A:200:GLY:HA3	1.74	0.70
1:B:333:LYS:HG2	1:B:342:LEU:HD12	1.74	0.70
1:H:448:THR:O	1:H:450:TYR:N	2.24	0.70
1:B:256:ARG:NH1	1:B:308:GLY:O	2.24	0.69
1:I:68:ALA:O	1:I:71:MET:N	2.25	0.69
1:F:86:SER:OG	1:F:101:THR:O	2.09	0.69
1:D:369:ALA:HA	1:D:375:ILE:HG21	1.74	0.69
1:C:220:MET:HG3	1:C:221:PRO:HD2	1.75	0.69
1:E:49:ILE:HG13	1:E:238:LEU:HD21	1.74	0.69
1:F:400:ALA:O	1:F:404:THR:HG23	1.93	0.69
1:C:367:VAL:O	1:C:370:THR:OG1	2.12	0.67
1:E:372:GLY:O	1:E:375:ILE:HG13	1.93	0.67
1:H:61:HIS:CD2	1:H:146:GLU:HG2	2.30	0.67
1:J:252:ASN:OD1	1:J:254:THR:OG1	2.11	0.67
1:E:10:THR:HG22	1:E:12:GLU:H	1.59	0.66
1:H:3:TYR:OH	1:H:19:LEU:O	2.14	0.65
1:B:340:ASP:N	1:B:341:GLY:HA3	2.11	0.65
1:I:340:ASP:N	1:I:340:ASP:OD1	2.30	0.65
1:B:220:MET:HG3	1:B:221:PRO:HD2	1.79	0.64
1:F:282:ARG:NH1	1:F:331:ASP:OD2	2.27	0.64
1:H:55:GLY:HA3	1:H:230:SER:HB3	1.80	0.63
1:A:252:ASN:OD1	1:A:254:THR:OG1	2.09	0.63
1:B:58:ARG:NH2	1:B:339:ASP:OD2	2.23	0.63
1:B:65:LEU:HD21	1:B:142:GLY:HA2	1.81	0.63
1:H:451:ILE:HG12	1:I:287:TRP:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:73:SER:O	1:E:77:ILE:HG12	1.99	0.62
1:D:256:ARG:NH1	1:D:308:GLY:O	2.33	0.62
1:F:378:ILE:HG13	1:F:380:GLY:H	1.63	0.62
1:B:110:VAL:HG23	1:B:122:ASP:HB3	1.81	0.62
1:I:209:GLY:HA2	1:I:424:ARG:NH1	2.14	0.62
1:A:340:ASP:OD1	1:A:340:ASP:N	2.32	0.62
1:I:65:LEU:HA	1:I:68:ALA:HB3	1.80	0.62
1:D:340:ASP:N	1:D:340:ASP:OD1	2.33	0.61
1:B:438:GLN:O	1:B:445:GLU:N	2.29	0.61
1:F:297:ILE:O	1:F:301:VAL:HG23	2.01	0.61
1:C:49:ILE:HG13	1:C:238:LEU:HD21	1.82	0.61
2:I:1455:PO4:O4	1:J:229:THR:OG1	2.18	0.61
1:C:340:ASP:OD1	1:C:340:ASP:N	2.29	0.60
1:F:61:HIS:ND1	1:F:145:CYS:SG	2.74	0.60
1:B:49:ILE:HD13	1:B:139:LEU:HG	1.83	0.60
1:E:110:VAL:HG23	1:E:122:ASP:HB3	1.83	0.60
1:D:140:MET:HE1	1:D:200:GLY:HA3	1.82	0.60
1:J:80:TRP:HA	1:J:84:GLY:HA3	1.83	0.60
1:E:65:LEU:HD21	1:E:142:GLY:HA2	1.83	0.60
1:F:163:ILE:HD11	1:F:411:LEU:HD13	1.83	0.60
1:D:371:ALA:HB3	1:D:375:ILE:HG22	1.84	0.59
1:A:71:MET:O	1:A:75:VAL:HG13	2.02	0.59
1:C:196:THR:HA	1:C:404:THR:HG21	1.84	0.59
1:I:369:ALA:HA	1:I:375:ILE:HG21	1.83	0.59
1:E:140:MET:HE1	1:E:200:GLY:HA3	1.85	0.59
1:H:65:LEU:HD11	1:H:142:GLY:HA2	1.84	0.59
1:C:209:GLY:HA2	1:C:424:ARG:NH1	2.16	0.59
1:H:159:LEU:O	1:H:163:ILE:HG12	2.03	0.58
1:B:133:ALA:HB1	1:B:161:MET:HE1	1.83	0.58
1:J:352:GLY:O	1:J:356:SER:OG	2.20	0.58
1:B:46:VAL:HG13	1:B:138:ALA:HB2	1.86	0.58
1:D:297:ILE:O	1:D:301:VAL:HG23	2.04	0.58
1:E:196:THR:HA	1:E:404:THR:HG21	1.84	0.58
1:E:140:MET:HE3	1:E:160:TRP:CZ2	2.39	0.58
1:C:149:ARG:HG2	1:C:454:PRO:HG2	1.86	0.57
1:F:71:MET:O	1:F:75:VAL:HG13	2.03	0.57
1:H:196:THR:HA	1:H:404:THR:HG21	1.85	0.57
1:A:196:THR:HG22	1:A:404:THR:HG21	1.85	0.57
1:C:174:ASN:OD1	1:C:175:ALA:N	2.37	0.57
1:H:289:THR:HG23	1:H:290:VAL:HG13	1.86	0.57
1:J:140:MET:HE3	1:J:160:TRP:CZ2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:191:LEU:O	1:D:196:THR:HG23	2.05	0.57
1:F:149:ARG:HG2	1:F:454:PRO:HG2	1.87	0.57
1:B:111:LEU:O	1:B:113:ALA:N	2.37	0.57
1:F:140:MET:HE3	1:F:160:TRP:CZ2	2.40	0.57
1:F:369:ALA:HA	1:F:375:ILE:HG21	1.87	0.57
1:B:58:ARG:HG2	1:B:224:LYS:HB3	1.87	0.57
1:B:4:ASN:OD1	1:B:4:ASN:N	2.36	0.56
1:B:38:ALA:O	1:B:42:VAL:HG23	2.06	0.56
1:D:51:LEU:HD21	1:D:66:LEU:HD22	1.85	0.56
1:I:49:ILE:HG13	1:I:238:LEU:HD21	1.86	0.56
1:J:267:ALA:HB2	1:J:315:ALA:HB1	1.87	0.56
1:D:435:ASP:N	1:D:435:ASP:OD1	2.36	0.56
1:F:86:SER:HB2	1:F:104:PHE:HB2	1.87	0.56
1:C:282:ARG:NH2	1:C:331:ASP:OD2	2.34	0.56
1:I:194:HIS:CE1	1:I:242:TRP:HZ2	2.24	0.56
1:F:58:ARG:HG2	1:F:224:LYS:HB3	1.88	0.56
1:H:38:ALA:O	1:H:42:VAL:HG23	2.05	0.56
1:B:15:GLY:HA3	1:B:113:ALA:HB2	1.88	0.56
1:A:444:TYR:HB3	1:A:448:THR:HG21	1.86	0.55
1:E:415:MET:HG2	1:E:421:LEU:HB3	1.88	0.55
1:H:340:ASP:OD1	1:H:340:ASP:N	2.37	0.55
1:I:85:TYR:OH	1:I:122:ASP:OD1	2.21	0.55
1:J:259:TYR:CZ	1:J:312:ILE:HG12	2.42	0.55
1:E:310:VAL:HB	1:E:314:SER:OG	2.07	0.55
1:J:10:THR:HG22	1:J:12:GLU:N	2.15	0.55
1:D:49:ILE:HD13	1:D:139:LEU:HG	1.88	0.55
1:D:65:LEU:HD21	1:D:142:GLY:HA2	1.87	0.55
1:F:99:ILE:HD12	1:F:167:PRO:HG3	1.87	0.55
1:B:59:LYS:NZ	1:B:213:ASP:OD2	2.30	0.55
1:B:213:ASP:O	1:B:337:ARG:NH1	2.40	0.55
1:C:282:ARG:NH1	1:C:328:LEU:HD23	2.22	0.55
1:I:73:SER:O	1:I:77:ILE:HG12	2.07	0.55
1:I:141:LEU:HD11	1:I:157:LEU:HD11	1.89	0.55
1:E:55:GLY:HA3	1:E:230:SER:HB3	1.88	0.54
1:H:186:ASP:OD2	1:H:191:LEU:N	2.37	0.54
1:J:27:PHE:CE2	1:J:121:PRO:HB3	2.42	0.54
1:A:220:MET:HG3	1:A:221:PRO:HD2	1.89	0.54
1:C:453:GLU:HG2	1:C:454:PRO:HD2	1.89	0.54
1:H:451:ILE:HG22	1:I:289:THR:HG22	1.90	0.54
1:I:149:ARG:HB2	1:I:152:PRO:HG2	1.89	0.54
1:J:411:LEU:O	1:J:415:MET:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:MET:O	1:B:75:VAL:HG13	2.07	0.54
1:B:451:ILE:HG12	1:C:287:TRP:HB2	1.88	0.54
1:H:24:ASN:OD1	1:I:255:ILE:HG12	2.07	0.54
1:C:86:SER:OG	1:C:101:THR:O	2.25	0.54
1:C:256:ARG:NH1	1:C:308:GLY:O	2.39	0.54
1:E:209:GLY:HA2	1:E:424:ARG:NH1	2.22	0.54
1:J:41:GLY:O	1:J:44:ILE:HG22	2.07	0.54
1:I:110:VAL:HG23	1:I:122:ASP:HB3	1.90	0.53
1:C:203:VAL:HG21	1:C:405:VAL:HA	1.90	0.53
1:C:431:GLU:HB2	1:C:455:ILE:HG13	1.90	0.53
1:A:372:GLY:O	1:A:375:ILE:HG12	2.08	0.53
1:F:49:ILE:HD13	1:F:139:LEU:HG	1.90	0.53
1:I:143:GLY:HA2	1:I:341:GLY:HA3	1.90	0.53
1:D:41:GLY:O	1:D:44:ILE:HG22	2.08	0.53
1:E:168:ILE:O	1:E:172:VAL:HG23	2.09	0.53
1:H:140:MET:HE3	1:H:160:TRP:CZ2	2.44	0.53
1:I:333:LYS:HG2	1:I:342:LEU:HD12	1.91	0.53
1:I:52:LEU:O	1:I:56:LEU:HB2	2.08	0.53
1:J:340:ASP:OD1	1:J:340:ASP:N	2.41	0.53
1:B:209:GLY:HA2	1:B:424:ARG:NH1	2.24	0.53
1:H:256:ARG:NH1	1:H:308:GLY:O	2.42	0.53
1:C:95:GLY:C	1:C:97:GLY:H	2.15	0.52
1:E:51:LEU:HD21	1:E:66:LEU:HD22	1.92	0.52
1:I:333:LYS:HD3	1:I:342:LEU:HB2	1.90	0.52
1:E:111:LEU:O	1:E:113:ALA:N	2.35	0.52
1:F:73:SER:O	1:F:77:ILE:HG12	2.08	0.52
1:E:275:TRP:HD1	1:E:275:TRP:O	1.93	0.52
1:H:191:LEU:O	1:H:196:THR:HG23	2.08	0.52
1:E:10:THR:HG22	1:E:12:GLU:N	2.23	0.52
1:I:89:PHE:HA	1:I:174:ASN:HD22	1.74	0.52
1:I:240:PHE:N	1:I:241:GLY:HA3	2.24	0.52
1:D:397:ILE:O	1:D:401:LEU:HB2	2.10	0.52
1:F:187:TYR:CD2	1:F:307:ALA:HB3	2.44	0.52
1:A:140:MET:HE3	1:A:160:TRP:CZ2	2.45	0.52
1:C:86:SER:HB2	1:C:104:PHE:HB2	1.92	0.52
1:I:361:ILE:O	1:I:382:TRP:HB3	2.10	0.52
1:B:33:GLY:O	1:B:37:VAL:HG12	2.10	0.51
1:E:38:ALA:O	1:E:42:VAL:HG23	2.10	0.51
1:H:42:VAL:HG13	1:H:245:PHE:HD1	1.76	0.51
1:J:65:LEU:HD21	1:J:142:GLY:HA2	1.93	0.51
1:J:66:LEU:O	1:J:69:SER:OG	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:393:GLN:O	1:J:397:ILE:HG13	2.10	0.51
1:C:14:THR:HG23	1:C:16:GLY:H	1.75	0.51
1:A:33:GLY:O	1:A:37:VAL:HG12	2.11	0.51
1:A:187:TYR:CD2	1:A:307:ALA:HB3	2.46	0.51
1:A:289:THR:HG21	1:C:448:THR:O	2.10	0.51
1:F:378:ILE:HD12	1:F:379:ASP:H	1.75	0.51
1:H:361:ILE:HA	1:H:382:TRP:HB2	1.93	0.51
1:H:369:ALA:HA	1:H:375:ILE:HG21	1.92	0.51
1:J:159:LEU:O	1:J:163:ILE:HG12	2.11	0.51
1:A:422:LYS:HE2	1:A:429:GLU:OE2	2.11	0.51
1:B:369:ALA:HA	1:B:375:ILE:HG21	1.93	0.51
1:C:187:TYR:CD2	1:C:307:ALA:HB3	2.45	0.51
1:I:49:ILE:HD11	1:I:135:VAL:HG13	1.93	0.51
1:H:397:ILE:O	1:H:401:LEU:HB2	2.11	0.50
1:B:326:CYS:O	1:B:330:VAL:HG23	2.12	0.50
1:F:115:SER:OG	1:F:117:VAL:O	2.26	0.50
1:H:156:PHE:HA	1:H:415:MET:HE1	1.94	0.50
1:I:111:LEU:O	1:I:113:ALA:N	2.44	0.50
1:J:318:ILE:HA	1:J:358:LEU:HD13	1.93	0.50
1:B:52:LEU:HD12	1:B:231:VAL:HG13	1.92	0.50
1:C:140:MET:HE3	1:C:160:TRP:CZ2	2.47	0.50
1:F:38:ALA:O	1:F:42:VAL:HG23	2.11	0.50
1:J:163:ILE:HD11	1:J:411:LEU:HD22	1.94	0.50
1:C:41:GLY:O	1:C:44:ILE:HG22	2.11	0.50
1:E:191:LEU:O	1:E:196:THR:HG23	2.12	0.50
1:A:154:MET:HE1	1:B:276:MET:SD	2.51	0.50
1:J:256:ARG:HB3	1:J:371:ALA:HB2	1.93	0.50
1:E:384:ASN:O	1:E:386:HIS:ND1	2.44	0.49
1:A:217:ARG:HG2	1:A:220:MET:HE2	1.92	0.49
1:E:36:GLY:HA3	1:F:258:TRP:CZ3	2.47	0.49
1:E:258:TRP:HE3	1:E:261:ILE:HD12	1.78	0.49
1:A:449:ALA:O	1:B:289:THR:N	2.45	0.49
1:C:35:ILE:HG21	1:C:120:LEU:HD21	1.94	0.49
1:D:62:ALA:HA	1:D:439:ILE:HD11	1.94	0.49
1:H:108:ARG:O	1:H:109:ASN:HB2	2.12	0.49
1:B:80:TRP:HA	1:B:84:GLY:HA3	1.94	0.49
1:C:333:LYS:HE3	1:C:339:ASP:OD1	2.11	0.49
1:D:361:ILE:HA	1:D:382:TRP:HB2	1.94	0.49
1:J:93:THR:OG1	1:J:176:GLU:OE1	2.30	0.49
1:C:73:SER:O	1:C:77:ILE:HG12	2.13	0.49
1:D:187:TYR:CD2	1:D:307:ALA:HB3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:54:SER:HB2	1:J:65:LEU:HB2	1.94	0.49
1:C:115:SER:OG	1:C:117:VAL:O	2.28	0.49
1:F:131:MET:O	1:F:135:VAL:HG23	2.12	0.49
1:H:95:GLY:HA3	1:H:96:ASN:C	2.38	0.49
1:A:73:SER:O	1:A:77:ILE:HG12	2.13	0.48
1:I:185:LEU:HD11	1:I:378:ILE:HG12	1.95	0.48
1:I:140:MET:HE3	1:I:160:TRP:CE2	2.48	0.48
1:J:403:TRP:CE2	1:J:407:VAL:HG21	2.49	0.48
1:B:338:ILE:HG22	1:B:339:ASP:H	1.79	0.48
1:B:49:ILE:HG13	1:B:238:LEU:HD21	1.95	0.48
1:B:336:LEU:HB3	1:B:338:ILE:HG13	1.95	0.48
1:D:136:THR:OG1	1:D:193:VAL:HG13	2.14	0.48
1:H:371:ALA:HB3	1:H:375:ILE:HG22	1.96	0.48
1:J:187:TYR:CE1	1:J:308:GLY:HA3	2.49	0.48
1:B:140:MET:HE3	1:B:160:TRP:CE2	2.48	0.48
1:I:340:ASP:HA	1:I:341:GLY:HA2	1.59	0.48
1:F:141:LEU:HD12	1:F:153:MET:SD	2.53	0.48
1:A:256:ARG:NH1	1:A:308:GLY:O	2.47	0.48
1:B:73:SER:O	1:B:77:ILE:HG12	2.14	0.48
1:F:58:ARG:NH2	1:F:339:ASP:OD2	2.38	0.48
1:I:33:GLY:O	1:I:37:VAL:HG12	2.14	0.48
1:A:400:ALA:O	1:A:404:THR:HG23	2.13	0.48
1:I:90:SER:OG	1:I:92:ASN:O	2.32	0.48
1:D:95:GLY:HA2	1:D:96:ASN:HA	1.54	0.47
1:C:110:VAL:HG13	1:C:122:ASP:HB3	1.95	0.47
1:E:243:MET:HE2	1:E:265:ASN:OD1	2.14	0.47
1:E:403:TRP:CE2	1:E:407:VAL:HG21	2.49	0.47
1:C:213:ASP:OD1	1:C:215:VAL:HG23	2.15	0.47
1:C:214:PRO:O	1:C:220:MET:HE3	2.13	0.47
1:D:73:SER:O	1:D:77:ILE:HG12	2.15	0.47
1:E:93:THR:HA	1:E:100:GLY:HA2	1.95	0.47
1:F:140:MET:HE1	1:F:200:GLY:HA3	1.96	0.47
1:B:164:VAL:CG1	1:B:404:THR:HG22	2.44	0.47
1:B:297:ILE:O	1:B:301:VAL:HG23	2.14	0.47
1:E:380:GLY:HA3	1:E:384:ASN:HD22	1.79	0.47
1:H:259:TYR:CZ	1:H:312:ILE:HG12	2.49	0.47
1:I:35:ILE:HG13	1:I:120:LEU:HD21	1.95	0.47
1:C:49:ILE:HD13	1:C:139:LEU:HG	1.96	0.47
1:C:202:LEU:HB2	1:C:345:TYR:CD1	2.49	0.47
1:A:276:MET:HE3	1:A:292:LEU:HB2	1.95	0.47
1:J:196:THR:HA	1:J:404:THR:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:LEU:HD21	1:A:66:LEU:HD22	1.97	0.47
1:B:342:LEU:HA	1:B:345:TYR:HB3	1.96	0.47
1:H:49:ILE:HD13	1:H:139:LEU:HG	1.95	0.47
1:I:276:MET:HE3	1:I:292:LEU:HD22	1.96	0.47
1:I:358:LEU:HD23	1:I:361:ILE:HD12	1.97	0.47
1:B:42:VAL:HG13	1:B:245:PHE:HD1	1.80	0.47
1:E:24:ASN:OD1	1:F:255:ILE:HG13	2.15	0.47
1:B:16:GLY:HA3	1:B:23:LEU:HD21	1.97	0.47
1:B:35:ILE:HG21	1:B:120:LEU:HD21	1.97	0.47
1:D:49:ILE:HG13	1:D:238:LEU:HD21	1.95	0.47
1:D:214:PRO:O	1:D:220:MET:HE3	2.14	0.47
1:E:51:LEU:HG	1:E:66:LEU:HD13	1.97	0.47
1:E:71:MET:HG3	1:E:154:MET:HE2	1.96	0.47
1:E:358:LEU:HD23	1:E:361:ILE:HD12	1.97	0.47
1:A:147:ARG:NH2	1:A:430:GLU:OE2	2.41	0.47
1:D:140:MET:HE3	1:D:160:TRP:CZ2	2.50	0.47
1:F:264:THR:HA	1:F:303:ILE:HG21	1.97	0.47
1:B:246:ASN:ND2	1:B:264:THR:OG1	2.25	0.46
1:B:365:ASP:N	1:B:365:ASP:OD1	2.48	0.46
1:C:434:THR:O	1:C:436:ALA:N	2.45	0.46
1:F:150:LEU:HD22	1:F:451:ILE:HD11	1.96	0.46
1:I:256:ARG:HD3	1:I:371:ALA:HB2	1.95	0.46
1:E:441:GLU:N	2:E:1458:PO4:O1	2.48	0.46
1:A:168:ILE:O	1:A:172:VAL:HG12	2.15	0.46
1:E:58:ARG:NH1	1:E:221:PRO:O	2.49	0.46
1:F:146:GLU:HG3	1:F:147:ARG:HG2	1.96	0.46
1:D:187:TYR:CE2	1:D:307:ALA:HB3	2.51	0.46
1:D:434:THR:O	1:D:436:ALA:N	2.48	0.46
1:H:94:ARG:HD3	1:H:101:THR:HG22	1.97	0.46
1:H:238:LEU:O	1:H:242:TRP:HB2	2.16	0.46
1:B:436:ALA:C	1:B:438:GLN:H	2.23	0.46
1:C:51:LEU:HD21	1:C:66:LEU:HD22	1.97	0.46
1:E:194:HIS:CG	1:E:301:VAL:HG13	2.50	0.46
1:F:164:VAL:O	1:F:168:ILE:HG13	2.15	0.46
1:J:279:ASP:OD1	1:J:327:ASN:ND2	2.36	0.46
1:A:255:ILE:HG13	1:C:24:ASN:OD1	2.16	0.46
1:A:259:TYR:CZ	1:A:312:ILE:HG12	2.50	0.46
1:D:61:HIS:CE1	1:D:146:GLU:HG2	2.51	0.46
1:F:71:MET:HE3	1:F:71:MET:HB3	1.83	0.46
1:F:209:GLY:HA2	1:F:424:ARG:NH1	2.31	0.46
1:H:340:ASP:HA	1:H:341:GLY:HA2	1.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:LEU:HD12	1:B:65:LEU:HA	1.71	0.46
1:J:146:GLU:HG2	1:J:340:ASP:OD2	2.16	0.46
1:B:333:LYS:NZ	1:B:343:ASP:OD1	2.41	0.46
1:D:166:CYS:HB2	1:D:167:PRO:HD3	1.98	0.46
1:C:140:MET:HE1	1:C:200:GLY:HA3	1.97	0.46
1:E:232:VAL:O	1:E:236:VAL:HG23	2.16	0.46
1:J:64:SER:OG	1:J:443:THR:HA	2.15	0.46
1:A:61:HIS:ND1	1:A:146:GLU:HG2	2.30	0.46
1:B:438:GLN:HA	1:B:445:GLU:HB2	1.98	0.46
1:D:174:ASN:OD1	1:D:175:ALA:N	2.49	0.46
1:H:77:ILE:HG21	1:I:265:ASN:O	2.16	0.46
1:H:232:VAL:O	1:H:236:VAL:HG23	2.16	0.46
1:J:52:LEU:HD21	1:J:297:ILE:HG13	1.98	0.46
1:A:61:HIS:CE1	1:A:146:GLU:HG2	2.52	0.45
1:F:71:MET:HE1	1:F:141:LEU:HD13	1.98	0.45
1:A:49:ILE:HG13	1:A:238:LEU:HD21	1.98	0.45
1:B:282:ARG:NH2	1:B:331:ASP:OD2	2.41	0.45
1:D:164:VAL:CG1	1:D:404:THR:HG22	2.46	0.45
1:D:217:ARG:HB2	1:D:337:ARG:HH22	1.82	0.45
1:E:172:VAL:HG22	1:E:179:LEU:HD12	1.98	0.45
1:E:303:ILE:O	1:E:303:ILE:HG13	2.17	0.45
1:F:203:VAL:HG21	1:F:405:VAL:HA	1.98	0.45
1:J:238:LEU:O	1:J:242:TRP:HB2	2.16	0.45
1:A:227:SER:HB3	1:A:230:SER:HB2	1.98	0.45
1:B:24:ASN:OD1	1:C:255:ILE:HG12	2.16	0.45
1:D:211:ARG:HE	1:D:211:ARG:HB3	1.65	0.45
1:J:335:LEU:O	1:J:336:LEU:HD12	2.16	0.45
1:D:16:GLY:HA3	1:D:23:LEU:HD21	1.99	0.45
1:E:136:THR:OG1	1:E:193:VAL:HG13	2.16	0.45
1:B:51:LEU:HD21	1:B:66:LEU:HD22	1.98	0.45
1:B:92:ASN:O	1:B:101:THR:HG23	2.17	0.45
1:D:282:ARG:NH2	1:D:331:ASP:OD2	2.34	0.45
1:F:156:PHE:HB2	1:F:415:MET:HE1	1.99	0.45
1:H:412:LEU:O	1:H:416:ASN:HB2	2.17	0.45
1:I:441:GLU:N	2:I:1455:PO4:O1	2.50	0.45
1:J:35:ILE:HG13	1:J:120:LEU:HD21	1.99	0.45
1:F:340:ASP:OD1	1:F:340:ASP:N	2.49	0.45
1:J:397:ILE:O	1:J:401:LEU:HB2	2.17	0.45
1:E:61:HIS:CE1	1:E:146:GLU:HG2	2.52	0.44
1:F:159:LEU:O	1:F:163:ILE:HG12	2.17	0.44
1:I:238:LEU:O	1:I:242:TRP:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:ASN:O	1:D:180:VAL:HG21	2.18	0.44
1:J:140:MET:HE1	1:J:200:GLY:HA3	1.98	0.44
1:J:340:ASP:HA	1:J:341:GLY:HA2	1.62	0.44
1:C:191:LEU:O	1:C:196:THR:HG23	2.17	0.44
1:D:228:VAL:O	1:D:232:VAL:HG23	2.17	0.44
1:C:210:LYS:O	1:C:338:ILE:HG23	2.18	0.44
1:E:35:ILE:HG21	1:E:120:LEU:HD21	2.00	0.44
1:F:445:GLU:O	1:F:448:THR:OG1	2.24	0.44
1:H:115:SER:OG	1:H:117:VAL:O	2.32	0.44
1:F:185:LEU:HD11	1:F:378:ILE:HG12	1.99	0.44
1:F:196:THR:HG22	1:F:404:THR:HG21	2.00	0.44
1:I:293:CYS:O	1:I:297:ILE:HG12	2.18	0.44
1:J:389:GLN:O	1:J:393:GLN:HG2	2.18	0.44
1:A:156:PHE:HD1	1:A:415:MET:HE1	1.82	0.44
1:A:276:MET:SD	1:C:154:MET:HE1	2.58	0.44
1:B:161:MET:HB3	1:B:161:MET:HE3	1.65	0.44
1:C:163:ILE:HD11	1:C:411:LEU:HD13	2.00	0.44
1:C:340:ASP:HA	1:C:341:GLY:HA2	1.78	0.44
1:E:150:LEU:HG	1:E:154:MET:HE3	2.00	0.44
1:F:371:ALA:HB3	1:F:375:ILE:CG2	2.48	0.44
1:A:140:MET:HE3	1:A:160:TRP:CE2	2.53	0.44
1:H:17:ASN:C	1:H:19:LEU:H	2.26	0.44
1:A:95:GLY:HA2	1:A:96:ASN:HA	1.47	0.44
1:A:156:PHE:HA	1:A:415:MET:HE1	1.98	0.43
1:B:371:ALA:HB3	1:B:375:ILE:HG22	2.00	0.43
1:C:150:LEU:HD22	1:C:451:ILE:HD11	2.00	0.43
1:I:187:TYR:CD2	1:I:307:ALA:HB3	2.53	0.43
1:I:297:ILE:O	1:I:301:VAL:HG23	2.18	0.43
1:B:210:LYS:N	1:B:340:ASP:OD2	2.51	0.43
1:B:433:GLY:HA3	1:B:434:THR:HA	1.74	0.43
1:C:439:ILE:HA	1:C:440:GLY:HA3	1.76	0.43
1:D:37:VAL:HG21	1:E:37:VAL:HG21	1.99	0.43
1:D:326:CYS:O	1:D:330:VAL:HG23	2.17	0.43
1:J:439:ILE:HA	1:J:440:GLY:HA3	1.64	0.43
1:B:71:MET:HE1	1:B:141:LEU:HD11	1.99	0.43
1:C:136:THR:OG1	1:C:193:VAL:HG13	2.19	0.43
1:D:188:ALA:HB3	1:D:304:THR:HG23	2.00	0.43
1:E:274:THR:O	1:E:278:ILE:HG13	2.19	0.43
1:E:411:LEU:O	1:E:415:MET:HB2	2.17	0.43
1:F:51:LEU:HD21	1:F:66:LEU:HD22	2.00	0.43
1:I:164:VAL:HA	1:I:403:TRP:HE1	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:LEU:HD11	1:B:378:ILE:HG12	2.01	0.43
1:I:68:ALA:O	1:I:70:MET:N	2.51	0.43
1:E:156:PHE:HD1	1:E:415:MET:HE1	1.84	0.43
1:I:194:HIS:CE1	1:I:301:VAL:HG22	2.53	0.43
1:D:65:LEU:HA	1:D:65:LEU:HD12	1.65	0.43
1:C:133:ALA:HB1	1:C:161:MET:HE2	2.00	0.43
1:C:238:LEU:O	1:C:242:TRP:HB2	2.18	0.43
1:J:233:LEU:HD23	1:J:233:LEU:HA	1.76	0.43
1:B:152:PRO:HB3	1:B:421:LEU:O	2.19	0.43
1:C:185:LEU:N	1:C:393:GLN:OE1	2.45	0.43
1:E:401:LEU:O	1:E:405:VAL:HG23	2.19	0.43
1:J:64:SER:OG	1:J:442:PHE:O	2.37	0.43
1:B:107:PHE:CD2	1:B:110:VAL:HG11	2.54	0.43
1:B:411:LEU:O	1:B:415:MET:HE3	2.18	0.43
1:D:57:SER:OG	1:D:59:LYS:O	2.36	0.43
1:I:56:LEU:HD12	1:I:56:LEU:HA	1.82	0.43
1:D:400:ALA:O	1:D:404:THR:OG1	2.20	0.43
1:E:278:ILE:O	1:E:282:ARG:HB2	2.18	0.43
1:E:365:ASP:H	1:E:384:ASN:HD21	1.67	0.43
1:H:172:VAL:HG22	1:H:173:TRP:CD1	2.54	0.43
1:I:141:LEU:HD12	1:I:153:MET:HE2	2.00	0.43
1:I:387:TYR:C	1:I:389:GLN:H	2.26	0.43
1:B:123:ILE:HG12	1:C:259:TYR:HA	2.00	0.42
1:C:35:ILE:HG13	1:C:120:LEU:HD21	2.00	0.42
1:C:213:ASP:HA	1:C:214:PRO:HD2	1.80	0.42
1:E:212:ASN:HA	1:E:337:ARG:HB3	2.02	0.42
1:F:433:GLY:C	1:F:435:ASP:H	2.27	0.42
1:I:194:HIS:CG	1:I:301:VAL:HG13	2.54	0.42
1:A:38:ALA:O	1:A:42:VAL:HG23	2.19	0.42
1:I:151:PHE:HB2	1:J:287:TRP:HZ2	1.84	0.42
1:J:166:CYS:HB2	1:J:167:PRO:HD3	2.02	0.42
1:D:340:ASP:HA	1:D:341:GLY:HA2	1.60	0.42
1:J:171:TRP:O	1:J:180:VAL:HG23	2.20	0.42
1:J:179:LEU:HD23	1:J:179:LEU:HA	1.83	0.42
1:D:87:LEU:HD22	1:D:99:ILE:HD11	2.01	0.42
1:E:339:ASP:O	1:E:341:GLY:N	2.52	0.42
1:A:203:VAL:HG21	1:A:405:VAL:HA	2.02	0.42
1:B:306:ALA:HB2	1:B:359:THR:OG1	2.20	0.42
1:C:365:ASP:H	1:C:384:ASN:HD21	1.68	0.42
1:C:415:MET:HE3	1:C:415:MET:HB2	1.93	0.42
1:D:50:GLY:O	1:D:54:SER:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:412:LEU:HD23	1:I:412:LEU:HA	1.84	0.42
1:A:384:ASN:HD22	1:A:384:ASN:HA	1.70	0.42
1:B:61:HIS:O	1:B:439:ILE:HD13	2.20	0.42
1:E:95:GLY:HA2	1:E:96:ASN:HA	1.53	0.42
1:B:259:TYR:CZ	1:B:312:ILE:HG12	2.55	0.42
1:B:434:THR:C	1:B:436:ALA:H	2.28	0.42
1:C:43:TRP:HB2	1:C:131:MET:SD	2.59	0.42
1:C:192:CYS:O	1:C:196:THR:OG1	2.25	0.42
1:C:202:LEU:HD22	1:C:345:TYR:CE1	2.55	0.42
1:E:49:ILE:HD11	1:E:135:VAL:HG13	2.02	0.42
1:F:56:LEU:HD12	1:F:56:LEU:HA	1.83	0.41
1:H:310:VAL:HB	1:H:314:SER:OG	2.20	0.41
1:I:15:GLY:HA3	1:I:113:ALA:HB2	2.02	0.41
1:A:274:THR:OG1	1:A:320:VAL:HG22	2.21	0.41
1:B:149:ARG:HD2	1:B:425:LEU:HG	2.02	0.41
1:E:186:ASP:HB2	1:E:191:LEU:HD13	2.02	0.41
1:F:439:ILE:HA	1:F:440:GLY:HA3	1.83	0.41
1:E:185:LEU:HD22	1:E:309:PHE:CZ	2.56	0.41
1:H:280:TYR:HA	1:H:286:LYS:O	2.20	0.41
1:J:120:LEU:HG	1:J:124:LEU:HD23	2.02	0.41
1:A:22:ASP:OD1	1:B:372:GLY:HA3	2.19	0.41
1:C:276:MET:HE2	1:C:276:MET:HB3	1.67	0.41
1:E:23:LEU:HD13	1:E:112:GLY:HA3	2.03	0.41
1:F:41:GLY:O	1:F:44:ILE:HG22	2.21	0.41
1:H:264:THR:HA	1:H:303:ILE:HG21	2.02	0.41
1:I:328:LEU:O	1:I:331:ASP:N	2.51	0.41
1:J:359:THR:O	1:J:363:ALA:HB2	2.19	0.41
1:A:50:GLY:O	1:A:54:SER:HB3	2.20	0.41
1:E:297:ILE:O	1:E:301:VAL:HG23	2.19	0.41
1:F:153:MET:CE	1:F:156:PHE:HD2	2.32	0.41
1:F:259:TYR:CZ	1:F:312:ILE:HG12	2.55	0.41
1:F:371:ALA:HB3	1:F:375:ILE:HG22	2.03	0.41
1:I:27:PHE:CE2	1:I:121:PRO:HB3	2.55	0.41
1:J:24:ASN:C	1:J:26:GLN:H	2.28	0.41
1:J:65:LEU:HD12	1:J:65:LEU:HA	1.78	0.41
1:D:56:LEU:HD12	1:D:56:LEU:HA	1.88	0.41
1:E:208:LEU:HD13	1:E:424:ARG:HB3	2.02	0.41
1:H:140:MET:HE3	1:H:160:TRP:CE2	2.56	0.41
1:H:152:PRO:HB3	1:H:421:LEU:O	2.19	0.41
1:J:398:CYS:O	1:J:402:ALA:N	2.46	0.41
1:E:159:LEU:O	1:E:163:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:443:THR:OG1	1:E:444:TYR:N	2.51	0.41
1:H:289:THR:O	1:J:67:TRP:NE1	2.38	0.41
1:B:332:LEU:HD23	1:B:342:LEU:HD13	2.03	0.41
1:H:263:SER:OG	1:H:312:ILE:HD13	2.20	0.41
1:I:42:VAL:HG13	1:I:245:PHE:HD1	1.86	0.41
1:A:71:MET:SD	1:A:154:MET:HG2	2.61	0.41
1:D:71:MET:O	1:D:75:VAL:HG13	2.21	0.41
1:D:289:THR:HG21	1:F:448:THR:O	2.21	0.41
1:D:328:LEU:O	1:D:330:VAL:N	2.54	0.41
1:D:425:LEU:HB2	1:D:430:GLU:HG2	2.02	0.41
1:D:453:GLU:HG2	1:D:454:PRO:HD2	2.02	0.41
1:E:375:ILE:HG22	1:E:377:PRO:HD3	2.03	0.41
1:J:99:ILE:HG13	1:J:167:PRO:HA	2.03	0.41
1:B:264:THR:HA	1:B:303:ILE:HG21	2.02	0.41
1:I:51:LEU:O	1:I:230:SER:OG	2.32	0.41
1:I:361:ILE:HA	1:I:382:TRP:HB2	2.02	0.41
1:C:188:ALA:HB3	1:C:304:THR:HG23	2.02	0.40
1:E:43:TRP:NE1	1:E:73:SER:OG	2.40	0.40
1:E:52:LEU:O	1:E:56:LEU:HB2	2.21	0.40
1:F:356:SER:HB2	1:F:397:ILE:HD11	2.04	0.40
1:H:356:SER:HB2	1:H:397:ILE:HD11	2.03	0.40
1:I:156:PHE:CD1	1:I:411:LEU:HD11	2.56	0.40
1:J:35:ILE:HB	1:J:124:LEU:HD21	2.02	0.40
1:B:220:MET:CG	1:B:221:PRO:HD2	2.49	0.40
1:E:378:ILE:HD12	1:E:378:ILE:HA	1.91	0.40
1:H:239:TRP:CZ3	1:H:296:ILE:HD13	2.56	0.40
1:B:41:GLY:O	1:B:44:ILE:HG22	2.22	0.40
1:B:124:LEU:HD13	1:C:258:TRP:CG	2.56	0.40
1:E:435:ASP:HB3	1:E:438:GLN:OE1	2.21	0.40
1:H:310:VAL:HA	1:H:311:PRO:HD3	1.89	0.40
1:J:344:CYS:O	1:J:348:HIS:HB2	2.21	0.40
1:A:214:PRO:O	1:A:220:MET:HE3	2.22	0.40
1:C:64:SER:OG	1:C:443:THR:HA	2.21	0.40
1:C:318:ILE:O	1:C:322:THR:OG1	2.36	0.40
1:A:108:ARG:O	1:A:109:ASN:HB2	2.21	0.40
1:B:107:PHE:O	1:B:110:VAL:HG12	2.21	0.40
1:E:364:ALA:HB1	1:E:366:TYR:CE1	2.57	0.40
1:F:268:ALA:HB2	1:F:300:LEU:HG	2.03	0.40
1:H:207:ILE:O	1:H:208:LEU:HD23	2.20	0.40
1:H:227:SER:HB2	1:H:441:GLU:HG2	2.04	0.40
1:J:297:ILE:O	1:J:301:VAL:HG23	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:GLU:OE2	1:I:387:TYR:OH[4_545]	2.19	0.01

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	454/505 (90%)	429 (94%)	21 (5%)	4 (1%)	14	47
1	B	454/505 (90%)	422 (93%)	29 (6%)	3 (1%)	18	52
1	C	454/505 (90%)	421 (93%)	29 (6%)	4 (1%)	14	47
1	D	453/505 (90%)	419 (92%)	29 (6%)	5 (1%)	11	43
1	E	454/505 (90%)	421 (93%)	28 (6%)	5 (1%)	11	43
1	F	454/505 (90%)	429 (94%)	24 (5%)	1 (0%)	43	73
1	H	434/505 (86%)	406 (94%)	20 (5%)	8 (2%)	6	34
1	I	441/505 (87%)	402 (91%)	34 (8%)	5 (1%)	11	43
1	J	421/505 (83%)	387 (92%)	32 (8%)	2 (0%)	24	59
All	All	4019/4545 (88%)	3736 (93%)	246 (6%)	37 (1%)	14	47

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	112	GLY
1	D	435	ASP
1	I	112	GLY
1	A	95	GLY
1	B	95	GLY
1	C	372	GLY
1	C	433	GLY
1	D	95	GLY

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Mol	Chain	Res	Type
1	E	95	GLY
1	E	112	GLY
1	E	340	ASP
1	H	445	GLU
1	H	449	ALA
1	I	69	SER
1	J	363	ALA
1	A	111	LEU
1	A	449	ALA
1	C	435	ASP
1	D	329	ALA
1	C	447	SER
1	D	445	GLU
1	H	307	ALA
1	I	115	SER
1	J	111	LEU
1	A	446	GLU
1	B	435	ASP
1	D	111	LEU
1	E	341	GLY
1	E	432	LEU
1	F	254	THR
1	H	95	GLY
1	H	96	ASN
1	H	284	GLY
1	H	214	PRO
1	H	183	GLY
1	I	95	GLY
1	I	207	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	353/398 (89%)	321 (91%)	32 (9%)	9 34
1	B	353/398 (89%)	329 (93%)	24 (7%)	14 46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	353/398 (89%)	327 (93%)	26 (7%)	13	43
1	D	352/398 (88%)	324 (92%)	28 (8%)	11	40
1	E	353/398 (89%)	328 (93%)	25 (7%)	13	44
1	F	353/398 (89%)	326 (92%)	27 (8%)	12	42
1	H	341/398 (86%)	317 (93%)	24 (7%)	14	45
1	I	346/398 (87%)	327 (94%)	19 (6%)	19	52
1	J	330/398 (83%)	315 (96%)	15 (4%)	24	58
All	All	3134/3582 (88%)	2914 (93%)	220 (7%)	14	45

All (220) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	THR
1	A	14	THR
1	A	19	LEU
1	A	37	VAL
1	A	44	ILE
1	A	54	SER
1	A	56	LEU
1	A	65	LEU
1	A	75	VAL
1	A	101	THR
1	A	110	VAL
1	A	111	LEU
1	A	117	VAL
1	A	141	LEU
1	A	146	GLU
1	A	167	PRO
1	A	172	VAL
1	A	191	LEU
1	A	192	CYS
1	A	210	LYS
1	A	217	ARG
1	A	230	SER
1	A	242	TRP
1	A	276	MET
1	A	289	THR
1	A	373	SER
1	A	384	ASN
1	A	420	PHE

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Mol	Chain	Res	Type
1	A	432	LEU
1	A	434	THR
1	A	445	GLU
1	A	457	SER
1	B	4	ASN
1	B	14	THR
1	B	37	VAL
1	B	44	ILE
1	B	65	LEU
1	B	75	VAL
1	B	119	SER
1	B	120	LEU
1	B	146	GLU
1	B	182	LEU
1	B	210	LYS
1	B	211	ARG
1	B	215	VAL
1	B	217	ARG
1	B	242	TRP
1	B	255	ILE
1	B	256	ARG
1	B	332	LEU
1	B	338	ILE
1	B	404	THR
1	B	414	THR
1	B	432	LEU
1	B	435	ASP
1	B	439	ILE
1	C	12	GLU
1	C	19	LEU
1	C	44	ILE
1	C	54	SER
1	C	73	SER
1	C	75	VAL
1	C	90	SER
1	C	120	LEU
1	C	182	LEU
1	C	191	LEU
1	C	215	VAL
1	C	256	ARG
1	C	276	MET
1	C	288	THR

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Mol	Chain	Res	Type
1	C	289	THR
1	C	340	ASP
1	C	373	SER
1	C	388	LYS
1	C	390	VAL
1	C	404	THR
1	C	431	GLU
1	C	434	THR
1	C	435	ASP
1	C	439	ILE
1	C	447	SER
1	C	455	ILE
1	D	6	THR
1	D	12	GLU
1	D	14	THR
1	D	19	LEU
1	D	54	SER
1	D	65	LEU
1	D	73	SER
1	D	75	VAL
1	D	90	SER
1	D	111	LEU
1	D	146	GLU
1	D	172	VAL
1	D	211	ARG
1	D	215	VAL
1	D	217	ARG
1	D	274	THR
1	D	277	VAL
1	D	286	LYS
1	D	289	THR
1	D	332	LEU
1	D	346	SER
1	D	382	TRP
1	D	401	LEU
1	D	404	THR
1	D	435	ASP
1	D	438	GLN
1	D	453	GLU
1	D	455	ILE
1	E	8	THR
1	E	18	SER

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Mol	Chain	Res	Type
1	E	37	VAL
1	E	44	ILE
1	E	65	LEU
1	E	73	SER
1	E	75	VAL
1	E	111	LEU
1	E	116	SER
1	E	117	VAL
1	E	118	SER
1	E	120	LEU
1	E	146	GLU
1	E	172	VAL
1	E	182	LEU
1	E	210	LYS
1	E	211	ARG
1	E	224	LYS
1	E	230	SER
1	E	242	TRP
1	E	289	THR
1	E	404	THR
1	E	426	SER
1	E	432	LEU
1	E	457	SER
1	F	10	THR
1	F	14	THR
1	F	19	LEU
1	F	44	ILE
1	F	54	SER
1	F	65	LEU
1	F	75	VAL
1	F	99	ILE
1	F	101	THR
1	F	120	LEU
1	F	141	LEU
1	F	168	ILE
1	F	191	LEU
1	F	210	LYS
1	F	215	VAL
1	F	220	MET
1	F	256	ARG
1	F	277	VAL
1	F	289	THR

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Mol	Chain	Res	Type
1	F	335	LEU
1	F	340	ASP
1	F	388	LYS
1	F	404	THR
1	F	431	GLU
1	F	432	LEU
1	F	455	ILE
1	F	456	ARG
1	H	14	THR
1	H	19	LEU
1	H	26	GLN
1	H	37	VAL
1	H	49	ILE
1	H	54	SER
1	H	73	SER
1	H	93	THR
1	H	107	PHE
1	H	110	VAL
1	H	117	VAL
1	H	120	LEU
1	H	146	GLU
1	H	172	VAL
1	H	191	LEU
1	H	210	LYS
1	H	213	ASP
1	H	215	VAL
1	H	242	TRP
1	H	255	ILE
1	H	304	THR
1	H	382	TRP
1	H	401	LEU
1	H	451	ILE
1	I	6	THR
1	I	37	VAL
1	I	44	ILE
1	I	65	LEU
1	I	93	THR
1	I	107	PHE
1	I	111	LEU
1	I	117	VAL
1	I	120	LEU
1	I	211	ARG

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Mol	Chain	Res	Type
1	I	215	VAL
1	I	217	ARG
1	I	229	THR
1	I	242	TRP
1	I	276	MET
1	I	340	ASP
1	I	379	ASP
1	I	404	THR
1	I	411	LEU
1	J	10	THR
1	J	12	GLU
1	J	14	THR
1	J	19	LEU
1	J	65	LEU
1	J	120	LEU
1	J	172	VAL
1	J	255	ILE
1	J	277	VAL
1	J	289	THR
1	J	340	ASP
1	J	373	SER
1	J	404	THR
1	J	439	ILE
1	J	447	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	226	HIS
1	B	26	GLN
1	B	212	ASN
1	B	386	HIS
1	C	92	ASN
1	C	129	GLN
1	C	199	HIS
1	C	438	GLN
1	D	26	GLN
1	D	61	HIS
1	D	226	HIS
1	E	129	GLN
1	E	384	ASN
1	E	389	GLN

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Mol	Chain	Res	Type
1	E	416	ASN
1	F	26	GLN
1	F	265	ASN
1	H	246	ASN
1	H	386	HIS
1	I	226	HIS
1	I	386	HIS
1	J	17	ASN
1	J	246	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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	PO4	A	1458	-	4,4,4	1.24	0	6,6,6	0.60	0
2	PO4	C	1458	-	4,4,4	1.12	0	6,6,6	0.46	0
2	PO4	J	1455	-	4,4,4	0.99	0	6,6,6	0.51	0
2	PO4	B	1458	-	4,4,4	1.06	0	6,6,6	0.53	0
2	PO4	F	1458	-	4,4,4	1.20	0	6,6,6	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	H	1457	-	4,4,4	1.00	0	6,6,6	0.42	0
2	PO4	I	1455	-	4,4,4	1.00	0	6,6,6	0.43	0
2	PO4	E	1458	-	4,4,4	1.17	0	6,6,6	0.42	0
2	PO4	D	1458	-	4,4,4	1.09	0	6,6,6	0.49	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	1455	PO4	2	0
2	E	1458	PO4	1	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, 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	456/505 (90%)	-0.27	10 (2%)	62	42	27, 62, 90, 173	11 (2%)
1	B	456/505 (90%)	-0.09	12 (2%)	57	37	38, 71, 102, 170	18 (3%)
1	C	456/505 (90%)	0.07	29 (6%)	25	16	32, 79, 119, 155	19 (4%)
1	D	455/505 (90%)	-0.17	8 (1%)	67	48	33, 69, 102, 158	16 (3%)
1	E	456/505 (90%)	0.04	26 (5%)	29	19	36, 74, 107, 207	25 (5%)
1	F	456/505 (90%)	-0.14	14 (3%)	51	32	31, 63, 93, 158	15 (3%)
1	H	440/505 (87%)	0.14	21 (4%)	35	22	36, 81, 130, 160	31 (7%)
1	I	447/505 (88%)	0.24	28 (6%)	26	17	54, 98, 142, 188	55 (12%)
1	J	426/505 (84%)	0.42	38 (8%)	15	10	42, 110, 150, 167	71 (16%)
All	All	4048/4545 (89%)	0.02	186 (4%)	37	23	27, 75, 130, 207	261 (6%)

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	334	SER	10.7
1	E	376	SER	7.1
1	C	368	ASN	6.2
1	E	377	PRO	6.1
1	A	447	SER	6.1
1	C	219	GLY	6.0
1	C	378	ILE	6.0
1	E	430	GLU	5.8
1	C	377	PRO	5.6
1	A	434	THR	5.6
1	C	381	GLY	5.5
1	F	335	LEU	5.5
1	H	332	LEU	5.5
1	B	437	ALA	5.3
1	C	375	ILE	4.7

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Mol	Chain	Res	Type	RSRZ
1	E	434	THR	4.7
1	H	10	THR	4.7
1	H	97	GLY	4.6
1	E	103	GLU	4.6
1	J	109	ASN	4.5
1	F	433	GLY	4.4
1	I	19	LEU	4.4
1	C	364	ALA	4.3
1	J	235	THR	4.3
1	C	435	ASP	4.3
1	J	206	LEU	4.2
1	H	148	ALA	4.1
1	C	382	TRP	4.1
1	J	423	LEU	4.0
1	H	335	LEU	4.0
1	H	219	GLY	4.0
1	E	207	ILE	3.9
1	C	376	SER	3.9
1	J	233	LEU	3.9
1	C	109	ASN	3.8
1	F	212	ASN	3.8
1	C	363	ALA	3.8
1	J	202	LEU	3.8
1	A	283	CYS	3.8
1	J	236	VAL	3.7
1	H	456	ARG	3.7
1	E	109	ASN	3.7
1	F	430	GLU	3.7
1	H	11	GLY	3.6
1	E	437	ALA	3.6
1	J	372	GLY	3.6
1	C	373	SER	3.6
1	I	18	SER	3.6
1	H	216	THR	3.5
1	J	234	GLY	3.5
1	E	375	ILE	3.5
1	C	96	ASN	3.4
1	I	71	MET	3.4
1	H	331	ASP	3.4
1	E	163	ILE	3.4
1	I	431	GLU	3.3
1	I	17	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	I	150	LEU	3.3
1	I	219	GLY	3.3
1	J	201	GLY	3.3
1	A	435	ASP	3.2
1	H	99	ILE	3.2
1	H	95	GLY	3.2
1	D	428	ASP	3.2
1	A	433	GLY	3.1
1	J	48	GLY	3.1
1	J	207	ILE	3.1
1	C	379	ASP	3.1
1	E	431	GLU	3.1
1	J	46	VAL	3.1
1	D	4	ASN	3.0
1	F	336	LEU	3.0
1	B	435	ASP	3.0
1	B	13	GLY	3.0
1	H	218	LYS	3.0
1	D	117	VAL	3.0
1	I	442	PHE	3.0
1	E	206	LEU	3.0
1	H	344	CYS	3.0
1	H	94	ARG	2.9
1	I	47	PRO	2.9
1	J	269	ALA	2.9
1	C	365	ASP	2.9
1	J	365	ASP	2.9
1	F	214	PRO	2.9
1	J	371	ALA	2.9
1	E	339	ASP	2.9
1	J	205	ALA	2.9
1	C	384	ASN	2.9
1	D	118	SER	2.8
1	H	8	THR	2.8
1	B	376	SER	2.8
1	C	380	GLY	2.8
1	I	54	SER	2.8
1	F	434	THR	2.7
1	I	64	SER	2.7
1	F	11	GLY	2.7
1	I	441	GLU	2.7
1	J	147	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	118	SER	2.7
1	C	361	ILE	2.6
1	J	411	LEU	2.6
1	A	282	ARG	2.6
1	J	374	TYR	2.6
1	C	308	GLY	2.6
1	J	96	ASN	2.6
1	F	378	ILE	2.5
1	J	163	ILE	2.5
1	E	92	ASN	2.5
1	J	369	ALA	2.5
1	I	430	GLU	2.5
1	E	435	ASP	2.5
1	F	220	MET	2.5
1	E	105	PHE	2.5
1	J	157	LEU	2.5
1	C	427	ALA	2.4
1	I	69	SER	2.4
1	F	431	GLU	2.4
1	H	239	TRP	2.4
1	E	379	ASP	2.4
1	J	451	ILE	2.4
1	E	342	LEU	2.4
1	C	389	GLN	2.4
1	C	390	VAL	2.4
1	E	378	ILE	2.4
1	J	375	ILE	2.4
1	B	220	MET	2.3
1	I	65	LEU	2.3
1	B	225	PRO	2.3
1	B	426	SER	2.3
1	C	360	GLY	2.3
1	E	427	ALA	2.3
1	J	125	PHE	2.3
1	E	2	SER	2.3
1	D	96	ASN	2.3
1	I	391	GLY	2.3
1	J	378	ILE	2.3
1	E	159	LEU	2.3
1	J	265	ASN	2.3
1	B	387	TYR	2.3
1	J	361	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	217	ARG	2.2
1	J	270	CYS	2.2
1	I	439	ILE	2.2
1	I	108	ARG	2.2
1	J	376	SER	2.2
1	F	194	HIS	2.2
1	C	220	MET	2.2
1	I	220	MET	2.2
1	J	138	ALA	2.2
1	C	218	LYS	2.2
1	I	46	VAL	2.2
1	D	119	SER	2.2
1	A	428	ASP	2.2
1	F	213	ASP	2.2
1	J	385	HIS	2.2
1	C	236	VAL	2.1
1	I	216	THR	2.1
1	I	230	SER	2.1
1	B	429	GLU	2.1
1	E	433	GLY	2.1
1	I	13	GLY	2.1
1	H	341	GLY	2.1
1	B	434	THR	2.1
1	E	202	LEU	2.1
1	B	294	SER	2.1
1	J	240	PHE	2.1
1	J	386	HIS	2.1
1	H	220	MET	2.1
1	I	387	TYR	2.1
1	D	219	GLY	2.1
1	F	334	SER	2.1
1	J	118	SER	2.1
1	C	103	GLU	2.1
1	E	457	SER	2.0
1	H	96	ASN	2.0
1	I	51	LEU	2.0
1	A	448	THR	2.0
1	I	344	CYS	2.0
1	D	125	PHE	2.0
1	J	377	PRO	2.0
1	I	343	ASP	2.0
1	I	78	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	438	GLN	2.0
1	B	375	ILE	2.0
1	C	383	ILE	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](#)

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
2	PO4	H	1457	5/5	0.70	0.10	200,202,202,204	0
2	PO4	I	1455	5/5	0.76	0.10	178,181,181,182	0
2	PO4	J	1455	5/5	0.84	0.07	163,163,163,163	0
2	PO4	A	1458	5/5	0.91	0.09	98,101,104,105	0
2	PO4	D	1458	5/5	0.92	0.12	142,143,144,147	0
2	PO4	B	1458	5/5	0.92	0.09	99,100,101,102	0
2	PO4	F	1458	5/5	0.94	0.10	97,97,100,104	0
2	PO4	C	1458	5/5	0.96	0.06	110,110,111,112	0
2	PO4	E	1458	5/5	0.96	0.08	113,113,114,114	0

6.5 Other polymers [i](#)

There are no such residues in this entry.