



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:10 AM UTC

PDB ID : 1YEH / pdb_00001yeh
Title : Crystal Structure of L-fuconate Dehydratase from Xanthomonas campestris
pv. campestris str. ATCC 33913
Authors : Fedorov, A.A.; Fedorov, E.V.; Yew, W.S.; Gerlt, J.A.; Almo, S.C.; Burley,
S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2004-12-28
Resolution : 2.34 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

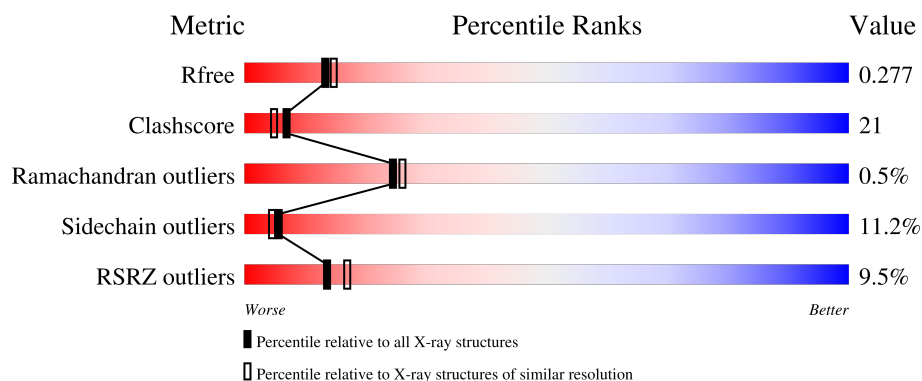
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	444	10% 58% 31% 7% .
1	B	444	9% 59% 31% 6% .
1	C	444	7% 58% 34% 6% .
1	D	444	10% 62% 30% 6% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13524 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 L-fuconate dehydratase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	Se	0	0	0
			3286	2083	587	605	2	9			
1	B	432	Total	C	N	O	S	Se	0	0	0
			3334	2112	594	617	2	9			
1	C	435	Total	C	N	O	S	Se	0	0	0
			3355	2125	597	622	2	9			
1	D	433	Total	C	N	O	S	Se	0	0	0
			3340	2116	595	618	2	9			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	cloning artifact	UNP Q8P3K2
A	-1	SER	-	cloning artifact	UNP Q8P3K2
A	0	HIS	-	cloning artifact	UNP Q8P3K2
A	1	MSE	MET	modified residue	UNP Q8P3K2
A	26	MSE	MET	modified residue	UNP Q8P3K2
A	109	MSE	MET	modified residue	UNP Q8P3K2
A	111	MSE	MET	modified residue	UNP Q8P3K2
A	245	MSE	MET	modified residue	UNP Q8P3K2
A	262	MSE	MET	modified residue	UNP Q8P3K2
A	366	MSE	MET	modified residue	UNP Q8P3K2
A	376	MSE	MET	modified residue	UNP Q8P3K2
A	414	MSE	MET	modified residue	UNP Q8P3K2
B	-2	GLY	-	cloning artifact	UNP Q8P3K2
B	-1	SER	-	cloning artifact	UNP Q8P3K2
B	0	HIS	-	cloning artifact	UNP Q8P3K2
B	1	MSE	MET	modified residue	UNP Q8P3K2
B	26	MSE	MET	modified residue	UNP Q8P3K2
B	109	MSE	MET	modified residue	UNP Q8P3K2
B	111	MSE	MET	modified residue	UNP Q8P3K2
B	245	MSE	MET	modified residue	UNP Q8P3K2
B	262	MSE	MET	modified residue	UNP Q8P3K2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	366	MSE	MET	modified residue	UNP Q8P3K2
B	376	MSE	MET	modified residue	UNP Q8P3K2
B	414	MSE	MET	modified residue	UNP Q8P3K2
C	-2	GLY	-	cloning artifact	UNP Q8P3K2
C	-1	SER	-	cloning artifact	UNP Q8P3K2
C	0	HIS	-	cloning artifact	UNP Q8P3K2
C	1	MSE	MET	modified residue	UNP Q8P3K2
C	26	MSE	MET	modified residue	UNP Q8P3K2
C	109	MSE	MET	modified residue	UNP Q8P3K2
C	111	MSE	MET	modified residue	UNP Q8P3K2
C	245	MSE	MET	modified residue	UNP Q8P3K2
C	262	MSE	MET	modified residue	UNP Q8P3K2
C	366	MSE	MET	modified residue	UNP Q8P3K2
C	376	MSE	MET	modified residue	UNP Q8P3K2
C	414	MSE	MET	modified residue	UNP Q8P3K2
D	-2	GLY	-	cloning artifact	UNP Q8P3K2
D	-1	SER	-	cloning artifact	UNP Q8P3K2
D	0	HIS	-	cloning artifact	UNP Q8P3K2
D	1	MSE	MET	modified residue	UNP Q8P3K2
D	26	MSE	MET	modified residue	UNP Q8P3K2
D	109	MSE	MET	modified residue	UNP Q8P3K2
D	111	MSE	MET	modified residue	UNP Q8P3K2
D	245	MSE	MET	modified residue	UNP Q8P3K2
D	262	MSE	MET	modified residue	UNP Q8P3K2
D	366	MSE	MET	modified residue	UNP Q8P3K2
D	376	MSE	MET	modified residue	UNP Q8P3K2
D	414	MSE	MET	modified residue	UNP Q8P3K2

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0

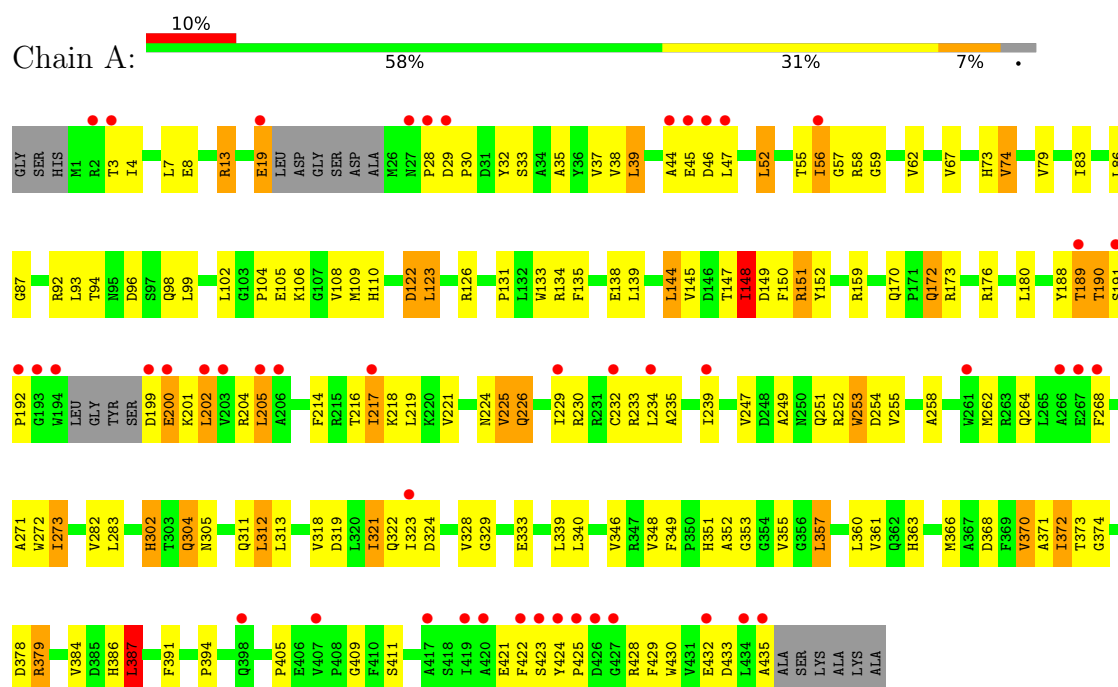
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	44	Total 44	O 44	0	0
3	B	64	Total 64	O 64	0	0
3	C	47	Total 47	O 47	0	0
3	D	50	Total 50	O 50	0	0

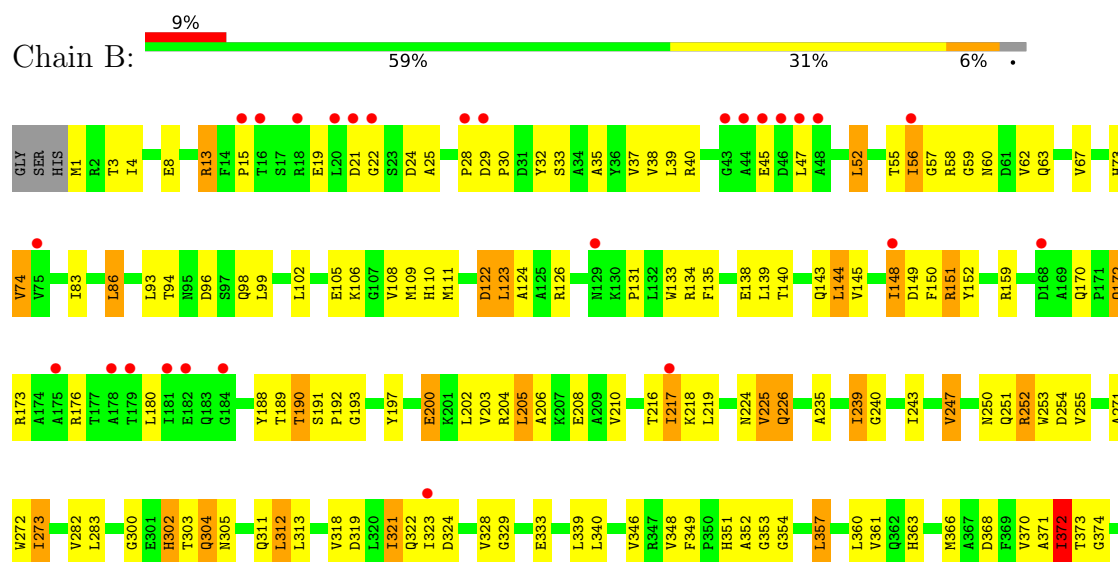
3 Residue-property plots

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: L-fuconate dehydratase

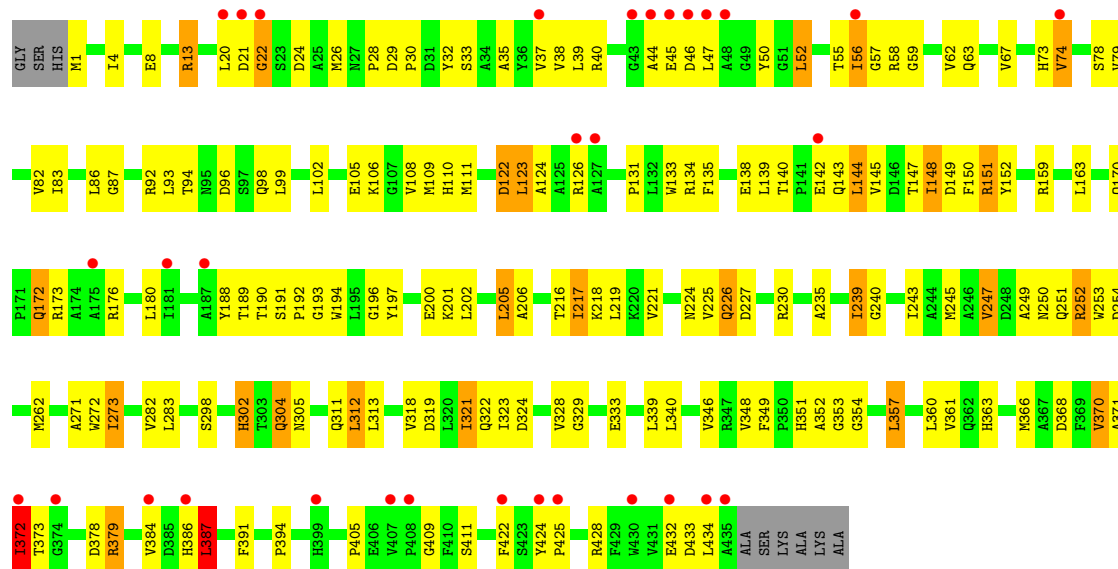


• Molecule 1: L-fuconate dehydratase

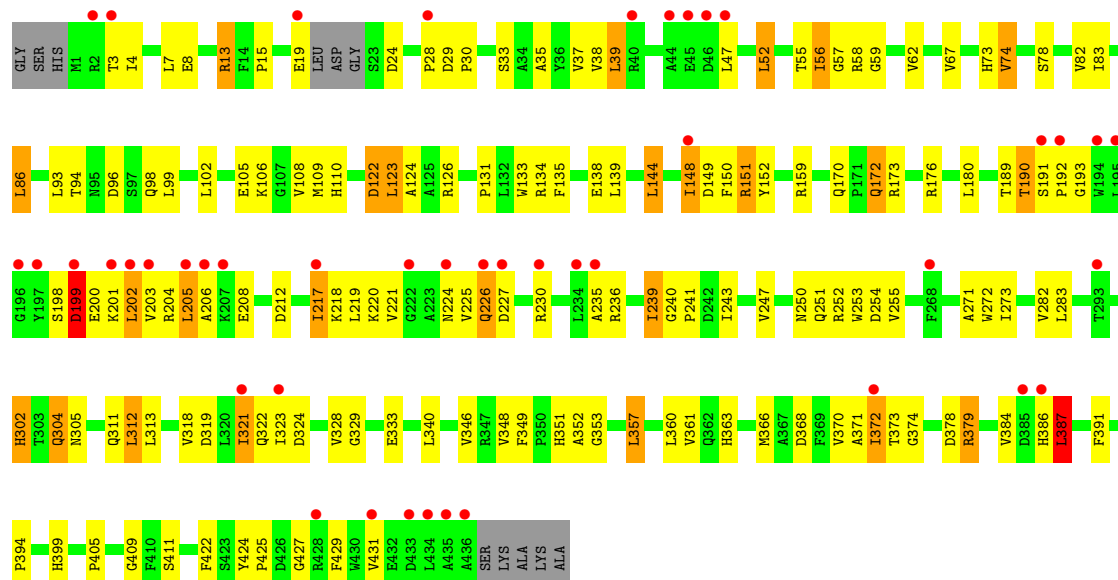




• Molecule 1: L-fuconate dehydratase



• Molecule 1: L-fuconate dehydratase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	130.53Å 130.53Å 193.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.34 25.00 – 2.34	Depositor EDS
% Data completeness (in resolution range)	96.8 (25.00-2.34) 96.7 (25.00-2.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.23 (at 2.34Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.247 , 0.272 0.251 , 0.277	Depositor DCC
R_{free} test set	4082 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13524	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% 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: MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.44	0/3349	0.98	18/4547 (0.4%)
1	B	0.47	0/3399	0.99	18/4616 (0.4%)
1	C	0.44	0/3420	0.98	17/4645 (0.4%)
1	D	0.44	0/3404	0.98	16/4622 (0.3%)
All	All	0.45	0/13572	0.98	69/18430 (0.4%)

There are no bond length outliers.

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	252	ARG	N-CA-C	11.02	124.67	111.33
1	A	74	VAL	N-CA-C	9.90	119.92	111.90
1	D	74	VAL	N-CA-C	9.67	119.73	111.90
1	D	252	ARG	N-CA-C	9.65	121.88	111.36
1	B	74	VAL	N-CA-C	9.43	119.54	111.90
1	C	74	VAL	N-CA-C	9.13	119.30	111.90
1	A	200	GLU	N-CA-C	-9.13	101.91	113.23
1	A	252	ARG	N-CA-C	9.04	121.13	111.28
1	C	252	ARG	N-CA-C	8.35	120.46	111.36
1	C	253	TRP	N-CA-C	7.80	121.08	110.55
1	D	254	ASP	N-CA-C	-7.24	100.09	110.59
1	A	253	TRP	N-CA-C	7.22	121.21	110.52
1	C	254	ASP	N-CA-C	-6.91	100.58	110.59
1	B	304	GLN	N-CA-C	6.82	119.30	111.11
1	C	304	GLN	N-CA-C	6.80	119.27	111.11
1	B	254	ASP	N-CA-C	-6.69	100.89	110.59
1	D	253	TRP	N-CA-C	6.60	120.29	110.52
1	A	254	ASP	N-CA-C	-6.54	101.10	110.59
1	A	304	GLN	N-CA-C	6.44	118.84	111.11
1	B	253	TRP	N-CA-C	6.20	119.69	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	108	VAL	N-CA-C	6.06	116.73	110.36
1	D	304	GLN	N-CA-C	6.05	118.37	111.11
1	B	108	VAL	N-CA-C	6.03	116.69	110.36
1	A	131	PRO	N-CA-C	-5.99	101.85	111.38
1	B	122	ASP	N-CA-C	-5.98	104.67	111.07
1	C	131	PRO	N-CA-C	-5.91	101.91	111.19
1	B	131	PRO	N-CA-C	-5.91	101.91	111.19
1	B	19	GLU	N-CA-C	-5.83	105.77	114.64
1	C	319	ASP	N-CA-C	-5.83	106.29	113.41
1	C	122	ASP	N-CA-C	-5.82	104.84	111.07
1	A	319	ASP	N-CA-C	-5.81	106.33	113.41
1	D	190	THR	N-CA-C	-5.80	106.05	114.12
1	C	370	VAL	N-CA-C	5.80	115.87	110.42
1	B	371	ALA	N-CA-C	5.79	120.50	113.38
1	D	422	PHE	N-CA-C	5.76	120.31	112.88
1	A	122	ASP	N-CA-C	-5.75	105.01	111.28
1	B	370	VAL	N-CA-C	5.75	115.83	110.42
1	C	35	ALA	N-CA-C	-5.75	97.87	107.99
1	D	409	GLY	N-CA-C	5.75	119.05	111.52
1	B	35	ALA	N-CA-C	-5.74	97.89	107.99
1	D	255	VAL	N-CA-C	5.72	115.91	110.42
1	A	371	ALA	N-CA-C	5.71	120.41	113.38
1	A	108	VAL	N-CA-C	5.71	116.35	110.36
1	C	108	VAL	N-CA-C	5.71	116.35	110.36
1	A	190	THR	N-CA-C	-5.68	106.22	114.12
1	C	422	PHE	N-CA-C	5.68	120.21	112.88
1	D	131	PRO	N-CA-C	-5.67	102.36	111.38
1	A	422	PHE	N-CA-C	5.67	120.19	112.88
1	C	371	ALA	N-CA-C	5.66	120.34	113.38
1	B	409	GLY	N-CA-C	5.65	118.92	111.52
1	D	122	ASP	N-CA-C	-5.64	105.03	111.07
1	D	35	ALA	N-CA-C	-5.60	98.13	107.99
1	D	370	VAL	N-CA-C	5.59	115.78	110.53
1	A	35	ALA	N-CA-C	-5.58	98.16	107.99
1	B	422	PHE	N-CA-C	5.58	120.08	112.88
1	D	371	ALA	N-CA-C	5.56	120.21	113.38
1	B	319	ASP	N-CA-C	-5.52	106.67	113.41
1	A	409	GLY	N-CA-C	5.46	118.67	111.52
1	A	370	VAL	N-CA-C	5.46	115.55	110.42
1	C	409	GLY	N-CA-C	5.38	118.56	111.52
1	A	255	VAL	N-CA-C	5.37	115.58	110.42
1	B	255	VAL	N-CA-C	5.31	115.52	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	319	ASP	N-CA-C	-5.28	106.97	113.41
1	B	190	THR	N-CA-C	-5.20	105.80	113.61
1	C	196	GLY	N-CA-C	-5.19	107.72	113.79
1	C	190	THR	N-CA-C	-5.15	105.88	113.61
1	B	372	ILE	N-CA-C	5.08	119.92	109.34
1	A	148	ILE	N-CA-C	5.07	116.57	108.87
1	C	372	ILE	N-CA-C	5.03	119.80	109.34

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	3286	0	3255	176	0
1	B	3334	0	3297	146	0
1	C	3355	0	3317	157	0
1	D	3340	0	3303	147	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	44	0	0	4	0
3	B	64	0	0	3	0
3	C	47	0	0	0	0
3	D	50	0	0	7	0
All	All	13524	0	13172	560	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 21.

All (560) 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:C:239:ILE:HG23	1:C:243:ILE:HB	1.30	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:GLN:HA	1:A:173:ARG:HD3	1.40	1.02
1:C:170:GLN:HA	1:C:173:ARG:HD3	1.41	1.02
1:D:170:GLN:HA	1:D:173:ARG:HD3	1.41	1.02
1:B:170:GLN:HA	1:B:173:ARG:HD3	1.40	0.99
1:D:102:LEU:HD23	1:D:109:MSE:HE3	1.51	0.92
1:D:239:ILE:HG23	1:D:243:ILE:HB	1.51	0.92
1:B:102:LEU:HD23	1:B:109:MSE:HE3	1.51	0.91
1:C:102:LEU:HD23	1:C:109:MSE:HE3	1.52	0.90
1:A:122:ASP:O	1:A:126:ARG:HG2	1.71	0.90
1:C:109:MSE:HE1	1:D:62:VAL:HG21	1.53	0.90
1:C:235:ALA:CB	1:C:245:MSE:HE1	2.01	0.90
1:A:102:LEU:HD23	1:A:109:MSE:HE3	1.53	0.89
1:B:239:ILE:HG23	1:B:243:ILE:HB	1.53	0.89
1:C:122:ASP:O	1:C:126:ARG:HG2	1.73	0.89
1:D:122:ASP:O	1:D:126:ARG:HG2	1.73	0.87
1:B:122:ASP:O	1:B:126:ARG:HG2	1.75	0.87
1:C:235:ALA:HB1	1:C:245:MSE:HE1	1.55	0.86
1:C:239:ILE:CG2	1:C:243:ILE:HB	2.05	0.85
1:A:62:VAL:HG21	1:B:109:MSE:HE1	1.58	0.85
1:C:98:GLN:HG2	1:D:56:ILE:HG23	1.59	0.84
1:A:200:GLU:HG2	1:C:142:GLU:HB3	1.59	0.84
1:B:21:ASP:HB2	1:B:197:TYR:OH	1.79	0.83
1:A:56:ILE:HG23	1:B:98:GLN:HG2	1.57	0.83
1:C:386:HIS:HB3	1:C:387:LEU:HD22	1.61	0.82
1:A:109:MSE:HE1	1:B:62:VAL:HG21	1.60	0.82
1:C:109:MSE:CE	1:D:62:VAL:HG21	2.10	0.82
1:C:62:VAL:HG21	1:D:109:MSE:HE1	1.63	0.81
1:A:386:HIS:HB3	1:A:387:LEU:HD22	1.63	0.81
1:B:151:ARG:HD3	1:B:152:TYR:CE2	2.15	0.81
1:C:206:ALA:HB1	1:C:239:ILE:CD1	2.11	0.80
1:C:151:ARG:HD3	1:C:152:TYR:CE2	2.17	0.79
1:D:151:ARG:HD3	1:D:152:TYR:CE2	2.17	0.79
1:D:386:HIS:HB3	1:D:387:LEU:HD22	1.64	0.79
1:B:328:VAL:HG22	1:B:329:GLY:H	1.48	0.79
1:B:386:HIS:HB3	1:B:387:LEU:HD22	1.62	0.79
1:A:151:ARG:HD3	1:A:152:TYR:CE2	2.18	0.79
1:C:56:ILE:HG23	1:D:98:GLN:HG2	1.63	0.79
1:D:328:VAL:HG22	1:D:329:GLY:H	1.49	0.78
1:D:192:PRO:HB3	1:D:205:LEU:HB3	1.65	0.78
1:A:109:MSE:CE	1:B:62:VAL:HG21	2.15	0.77
1:A:37:VAL:HG22	1:A:67:VAL:HG11	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:VAL:HG22	1:B:67:VAL:HG11	1.67	0.76
1:C:62:VAL:HG21	1:D:109:MSE:CE	2.16	0.76
1:D:37:VAL:HG22	1:D:67:VAL:HG11	1.67	0.76
1:B:428:ARG:O	1:B:431:VAL:HG12	1.87	0.75
1:C:328:VAL:HG22	1:C:329:GLY:H	1.51	0.74
1:A:328:VAL:HG22	1:A:329:GLY:H	1.52	0.74
1:C:37:VAL:HG22	1:C:67:VAL:HG11	1.69	0.74
1:A:200:GLU:CG	1:C:142:GLU:HB3	2.18	0.73
1:A:282:VAL:HG22	1:A:312:LEU:HD13	1.70	0.73
1:A:98:GLN:HG2	1:B:56:ILE:HG23	1.68	0.73
1:C:52:LEU:HD21	1:C:360:LEU:HD11	1.68	0.73
1:A:201:LYS:HA	1:A:204:ARG:NH1	2.04	0.72
1:C:133:TRP:H	1:C:363:HIS:HD2	1.38	0.71
1:A:233:ARG:HB2	1:A:268:PHE:CE2	2.26	0.70
1:B:282:VAL:HG22	1:B:312:LEU:HD13	1.74	0.70
1:A:201:LYS:HG2	1:A:205:LEU:HD22	1.71	0.70
1:B:200:GLU:CD	1:B:200:GLU:H	2.00	0.70
1:A:62:VAL:HG21	1:B:109:MSE:CE	2.20	0.70
1:D:282:VAL:HG22	1:D:312:LEU:HD13	1.74	0.70
1:C:282:VAL:HG22	1:C:312:LEU:HD13	1.73	0.69
1:B:239:ILE:CG2	1:B:243:ILE:HB	2.22	0.69
1:D:83:ILE:HG13	1:D:124:ALA:HA	1.73	0.69
1:A:282:VAL:H	1:B:311:GLN:HE22	1.41	0.69
1:C:83:ILE:HD12	1:C:124:ALA:HA	1.73	0.69
1:C:52:LEU:CD2	1:C:360:LEU:HD11	2.23	0.68
1:D:198:SER:OG	1:D:200:GLU:HG3	1.94	0.68
1:C:55:THR:HG22	1:C:56:ILE:N	2.07	0.67
1:A:201:LYS:HA	1:A:204:ARG:HH12	1.56	0.67
1:D:172:GLN:H	1:D:172:GLN:NE2	1.93	0.67
1:C:59:GLY:O	1:C:62:VAL:HG22	1.96	0.66
1:C:368:ASP:HA	1:C:372:ILE:HG23	1.76	0.66
1:D:239:ILE:CG2	1:D:243:ILE:HB	2.24	0.66
1:B:59:GLY:O	1:B:62:VAL:HG22	1.95	0.66
1:A:172:GLN:H	1:A:172:GLN:NE2	1.94	0.66
1:A:200:GLU:HB2	1:C:142:GLU:HG2	1.76	0.66
1:A:133:TRP:H	1:A:363:HIS:HD2	1.44	0.66
1:B:55:THR:HG22	1:B:56:ILE:N	2.11	0.66
1:B:172:GLN:H	1:B:172:GLN:NE2	1.93	0.66
1:D:59:GLY:O	1:D:62:VAL:HG22	1.96	0.65
1:D:368:ASP:HA	1:D:372:ILE:HG23	1.78	0.65
1:A:13:ARG:HD3	1:A:424:TYR:HB3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:LEU:HD21	1:B:360:LEU:HD11	1.77	0.65
1:A:59:GLY:O	1:A:62:VAL:HG22	1.96	0.65
1:B:133:TRP:H	1:B:363:HIS:HD2	1.45	0.65
1:C:192:PRO:HB3	1:C:205:LEU:HB3	1.78	0.65
1:C:328:VAL:HG22	1:C:333:GLU:OE2	1.97	0.65
1:D:55:THR:HG22	1:D:56:ILE:N	2.12	0.65
1:A:79:VAL:O	1:A:83:ILE:HD13	1.97	0.65
1:C:235:ALA:HB1	1:C:245:MSE:CE	2.26	0.65
1:A:368:ASP:HA	1:A:372:ILE:HG23	1.79	0.64
1:D:328:VAL:HG22	1:D:333:GLU:OE2	1.97	0.64
1:A:55:THR:HG22	1:A:56:ILE:N	2.11	0.64
1:A:13:ARG:CG	1:A:424:TYR:HB2	2.27	0.64
1:B:368:ASP:HA	1:B:372:ILE:HG23	1.78	0.64
1:B:206:ALA:HB1	1:B:239:ILE:CD1	2.27	0.64
1:C:170:GLN:HA	1:C:173:ARG:CD	2.25	0.64
1:B:47:LEU:HD11	1:B:123:LEU:HD21	1.79	0.63
1:B:37:VAL:CG2	1:B:67:VAL:HG11	2.28	0.63
1:B:15:PRO:HG3	1:B:429:PHE:CZ	2.33	0.63
1:A:134:ARG:HD2	1:A:138:GLU:OE1	1.99	0.63
1:A:421:GLU:OE2	1:A:429:PHE:HB2	1.99	0.63
1:B:170:GLN:HA	1:B:173:ARG:CD	2.24	0.63
1:D:83:ILE:HD11	1:D:123:LEU:HD13	1.79	0.62
1:B:204:ARG:O	1:B:208:GLU:HG3	1.99	0.62
1:C:134:ARG:HD2	1:C:138:GLU:OE1	1.99	0.62
1:C:172:GLN:NE2	1:C:172:GLN:H	1.96	0.62
1:B:378:ASP:OD1	1:B:379:ARG:HD2	2.00	0.62
1:D:37:VAL:CG2	1:D:67:VAL:HG11	2.29	0.62
1:B:1:MSE:HE2	1:D:19:GLU:CG	2.29	0.62
1:C:37:VAL:CG2	1:C:67:VAL:HG11	2.29	0.62
1:A:37:VAL:CG2	1:A:67:VAL:HG11	2.29	0.62
1:A:201:LYS:HG3	1:A:204:ARG:HH12	1.64	0.62
1:B:52:LEU:CD2	1:B:360:LEU:HD11	2.29	0.61
1:A:8:GLU:HG3	1:A:38:VAL:HB	1.81	0.61
1:B:328:VAL:HG22	1:B:333:GLU:OE2	2.00	0.61
1:C:58:ARG:HG3	1:D:98:GLN:OE1	2.00	0.61
1:D:134:ARG:HD2	1:D:138:GLU:OE1	1.99	0.61
1:B:4:ILE:HG21	1:B:74:VAL:HG12	1.83	0.61
1:C:324:ASP:OD2	1:C:351:HIS:HD2	1.83	0.61
1:A:324:ASP:OD2	1:A:351:HIS:HD2	1.83	0.61
1:D:52:LEU:HD21	1:D:360:LEU:HD11	1.83	0.61
1:D:353:GLY:O	1:D:357:LEU:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:ILE:HG23	1:A:322:GLN:O	2.01	0.61
1:A:353:GLY:O	1:A:357:LEU:HB2	2.00	0.61
1:C:47:LEU:HD11	1:C:123:LEU:HD21	1.81	0.61
1:A:328:VAL:HG22	1:A:333:GLU:OE2	2.00	0.60
1:C:83:ILE:HD12	1:C:124:ALA:CA	2.31	0.60
1:A:311:GLN:HE22	1:B:282:VAL:H	1.48	0.60
1:D:8:GLU:HG3	1:D:38:VAL:HB	1.84	0.60
1:D:324:ASP:OD2	1:D:351:HIS:HD2	1.84	0.60
1:B:134:ARG:HD2	1:B:138:GLU:OE1	2.02	0.60
1:B:386:HIS:HB3	1:B:387:LEU:CD2	2.31	0.60
1:C:247:VAL:HG12	1:C:273:ILE:HD13	1.84	0.60
1:C:386:HIS:HB3	1:C:387:LEU:CD2	2.31	0.60
1:A:386:HIS:HB3	1:A:387:LEU:CD2	2.32	0.59
1:B:363:HIS:HE1	1:B:411:SER:OG	1.85	0.59
1:C:378:ASP:OD1	1:C:379:ARG:HD2	2.01	0.59
1:C:311:GLN:HE22	1:D:282:VAL:H	1.50	0.59
1:D:133:TRP:H	1:D:363:HIS:HD2	1.47	0.59
1:D:139:LEU:HB2	1:D:144:LEU:HD22	1.83	0.59
1:B:251:GLN:HE22	1:B:302:HIS:CD2	2.20	0.59
1:A:192:PRO:HB3	1:A:205:LEU:HB3	1.84	0.59
1:A:428:ARG:HD2	1:A:428:ARG:O	2.02	0.59
1:D:170:GLN:HA	1:D:173:ARG:CD	2.26	0.59
1:D:427:GLY:O	1:D:431:VAL:HG23	2.03	0.59
1:B:139:LEU:HB2	1:B:144:LEU:HD22	1.84	0.59
1:C:368:ASP:HA	1:C:372:ILE:CG2	2.33	0.59
1:A:282:VAL:N	1:B:311:GLN:HE22	2.00	0.59
1:B:324:ASP:OD2	1:B:351:HIS:HD2	1.85	0.59
1:C:353:GLY:O	1:C:357:LEU:HB2	2.02	0.59
1:D:251:GLN:HE22	1:D:302:HIS:CD2	2.20	0.58
1:D:378:ASP:OD1	1:D:379:ARG:HD2	2.03	0.58
1:B:353:GLY:O	1:B:357:LEU:HB2	2.03	0.58
1:C:55:THR:CG2	1:C:56:ILE:N	2.67	0.58
1:C:139:LEU:HB2	1:C:144:LEU:HD22	1.86	0.58
1:D:47:LEU:HD11	1:D:123:LEU:HD21	1.84	0.58
1:A:283:LEU:H	1:B:311:GLN:HE21	1.52	0.58
1:A:311:GLN:NE2	1:B:283:LEU:H	2.02	0.58
1:D:198:SER:C	1:D:200:GLU:H	2.10	0.58
1:C:206:ALA:HB1	1:C:239:ILE:HD11	1.86	0.58
1:C:4:ILE:HG21	1:C:74:VAL:HG12	1.85	0.57
1:C:148:ILE:HD12	1:C:149:ASP:N	2.19	0.57
1:A:13:ARG:HD3	1:A:424:TYR:CB	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:LEU:HD11	1:A:235:ALA:HB2	1.86	0.57
1:A:139:LEU:HB2	1:A:144:LEU:HD22	1.85	0.57
1:A:368:ASP:HA	1:A:372:ILE:CG2	2.33	0.57
1:A:73:HIS:HE1	1:A:96:ASP:OD2	1.87	0.57
1:A:98:GLN:OE1	1:B:58:ARG:HG3	2.03	0.57
1:B:28:PRO:O	1:B:29:ASP:OD1	2.23	0.57
1:B:321:ILE:HG23	1:B:322:GLN:O	2.04	0.57
1:C:304:GLN:HG3	1:D:106:LYS:HZ2	1.69	0.57
1:A:311:GLN:HE21	1:B:283:LEU:H	1.51	0.57
1:B:73:HIS:HE1	1:B:96:ASP:OD2	1.88	0.57
1:B:192:PRO:HB3	1:B:205:LEU:HB3	1.87	0.57
1:C:247:VAL:HG12	1:C:273:ILE:CD1	2.34	0.57
1:C:47:LEU:CD1	1:C:123:LEU:HD21	2.35	0.57
1:A:104:PRO:HG2	3:A:5087:HOH:O	2.05	0.57
1:C:282:VAL:H	1:D:311:GLN:HE22	1.53	0.57
1:D:368:ASP:HA	1:D:372:ILE:CG2	2.34	0.57
1:B:368:ASP:HA	1:B:372:ILE:CG2	2.34	0.57
1:A:232:CYS:HB2	1:A:268:PHE:CD1	2.40	0.56
1:B:55:THR:HG22	1:B:57:GLY:H	1.70	0.56
1:B:56:ILE:HG23	1:B:56:ILE:O	2.04	0.56
1:C:98:GLN:HG2	1:D:56:ILE:CG2	2.33	0.56
1:D:202:LEU:HB3	3:D:5011:HOH:O	2.04	0.56
1:A:28:PRO:O	1:A:29:ASP:OD1	2.22	0.56
1:B:188:TYR:HB2	1:B:216:THR:HB	1.87	0.56
1:B:206:ALA:HB1	1:B:239:ILE:HD13	1.86	0.56
1:C:321:ILE:HG23	1:C:322:GLN:O	2.05	0.56
1:D:148:ILE:HD12	1:D:149:ASP:N	2.21	0.56
1:C:283:LEU:H	1:D:311:GLN:NE2	2.03	0.56
1:A:32:TYR:HB3	1:A:355:VAL:CG2	2.36	0.56
1:A:30:PRO:HB2	1:A:56:ILE:HG12	1.88	0.56
1:A:378:ASP:OD1	1:A:379:ARG:HD2	2.06	0.56
1:C:28:PRO:O	1:C:29:ASP:OD1	2.23	0.56
1:A:19:GLU:OE1	1:C:1:MSE:HE2	2.06	0.56
1:A:106:LYS:HZ2	1:B:304:GLN:HG3	1.71	0.56
1:C:56:ILE:HG23	1:C:56:ILE:O	2.06	0.56
1:B:30:PRO:HB2	1:B:56:ILE:HG12	1.88	0.55
1:D:200:GLU:HA	1:D:203:VAL:HG22	1.88	0.55
1:C:55:THR:HG22	1:C:57:GLY:H	1.72	0.55
1:A:56:ILE:CG2	1:B:98:GLN:HG2	2.31	0.55
1:B:176:ARG:HD3	1:B:374:GLY:HA2	1.88	0.55
1:A:55:THR:CG2	1:A:56:ILE:N	2.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ARG:HB3	1:A:92:ARG:NH2	2.21	0.55
1:D:55:THR:CG2	1:D:56:ILE:N	2.70	0.55
1:A:311:GLN:HE22	1:B:282:VAL:N	2.05	0.55
1:A:170:GLN:HA	1:A:173:ARG:CD	2.24	0.55
1:B:148:ILE:HD12	1:B:149:ASP:N	2.21	0.55
1:C:318:VAL:HG21	1:C:321:ILE:CD1	2.37	0.55
1:D:28:PRO:O	1:D:29:ASP:OD1	2.25	0.55
1:D:321:ILE:HG23	1:D:322:GLN:O	2.06	0.55
1:C:249:ALA:O	1:C:252:ARG:HG2	2.06	0.55
1:D:30:PRO:HB2	1:D:56:ILE:HG12	1.89	0.55
1:C:283:LEU:H	1:D:311:GLN:HE21	1.55	0.55
1:C:283:LEU:HG	1:D:311:GLN:HE21	1.71	0.55
1:D:386:HIS:HB3	1:D:387:LEU:CD2	2.34	0.55
1:A:55:THR:HG22	1:A:57:GLY:H	1.71	0.54
1:C:30:PRO:HB2	1:C:56:ILE:HG12	1.89	0.54
1:D:224:ASN:OD1	1:D:226:GLN:HB2	2.07	0.54
1:D:52:LEU:CD2	1:D:360:LEU:HD11	2.37	0.54
1:A:47:LEU:CD1	1:A:123:LEU:HD21	2.37	0.54
1:B:47:LEU:CD1	1:B:123:LEU:HD21	2.37	0.54
1:B:55:THR:CG2	1:B:56:ILE:N	2.70	0.54
1:C:26:MSE:HE1	3:D:5159:HOH:O	2.06	0.54
1:C:239:ILE:HG23	1:C:243:ILE:CB	2.21	0.54
1:A:224:ASN:OD1	1:A:226:GLN:HB2	2.07	0.54
1:C:239:ILE:HG22	1:C:240:GLY:O	2.07	0.54
1:C:56:ILE:CG2	1:D:98:GLN:HG2	2.36	0.54
1:C:217:ILE:HG12	1:C:218:LYS:N	2.23	0.54
1:C:92:ARG:HH21	1:C:92:ARG:HG3	1.72	0.54
1:A:56:ILE:HG23	1:A:56:ILE:O	2.06	0.54
1:A:8:GLU:CG	1:A:38:VAL:HB	2.37	0.54
1:D:55:THR:HG22	1:D:57:GLY:H	1.71	0.53
1:C:363:HIS:HE1	1:C:411:SER:OG	1.90	0.53
1:A:98:GLN:HB2	1:B:58:ARG:HH11	1.71	0.53
1:A:232:CYS:CB	1:A:268:PHE:CD1	2.91	0.53
1:A:52:LEU:HD21	1:A:360:LEU:HD11	1.90	0.53
1:D:363:HIS:HE1	1:D:411:SER:OG	1.91	0.53
1:A:387:LEU:HD22	1:A:387:LEU:N	2.24	0.53
1:B:25:ALA:HB1	1:B:252:ARG:HG3	1.90	0.53
1:C:366:MSE:SE	1:C:405:PRO:HD2	2.59	0.53
1:A:251:GLN:HE22	1:A:302:HIS:CD2	2.27	0.53
1:B:202:LEU:HD11	1:B:235:ALA:HB2	1.90	0.53
1:B:387:LEU:HD22	1:B:387:LEU:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:THR:CG2	1:C:56:ILE:H	2.21	0.53
1:D:217:ILE:HG12	1:D:218:LYS:N	2.23	0.53
1:A:92:ARG:CB	1:A:92:ARG:HH21	2.21	0.53
1:A:283:LEU:H	1:B:311:GLN:NE2	2.07	0.53
1:A:366:MSE:SE	1:A:405:PRO:HD2	2.59	0.52
1:A:105:GLU:HA	1:A:110:HIS:CG	2.44	0.52
1:C:304:GLN:CG	1:D:106:LYS:HZ2	2.23	0.52
1:A:148:ILE:HD12	1:A:149:ASP:N	2.23	0.52
1:B:8:GLU:HG3	1:B:38:VAL:HB	1.92	0.52
1:B:224:ASN:OD1	1:B:226:GLN:HB2	2.09	0.52
1:D:8:GLU:CG	1:D:38:VAL:HB	2.39	0.52
1:A:47:LEU:HD11	1:A:123:LEU:HD21	1.90	0.52
1:C:55:THR:HG22	1:C:56:ILE:H	1.73	0.52
1:C:387:LEU:HD22	1:C:387:LEU:N	2.24	0.52
1:D:239:ILE:HG22	1:D:240:GLY:O	2.10	0.52
1:B:318:VAL:HG21	1:B:321:ILE:CD1	2.40	0.51
1:C:21:ASP:HB2	1:C:197:TYR:OH	2.10	0.51
1:A:318:VAL:HG21	1:A:321:ILE:CD1	2.40	0.51
1:D:221:VAL:HG21	1:D:247:VAL:CG1	2.41	0.51
1:A:428:ARG:HD2	1:A:428:ARG:C	2.35	0.51
1:B:105:GLU:HA	1:B:110:HIS:CG	2.45	0.51
1:A:233:ARG:HA	1:A:268:PHE:CD2	2.45	0.51
1:C:282:VAL:N	1:D:311:GLN:HE22	2.08	0.51
1:A:176:ARG:HD3	1:A:374:GLY:HA2	1.91	0.51
1:A:191:SER:N	1:A:192:PRO:HD2	2.26	0.51
1:C:133:TRP:H	1:C:363:HIS:CD2	2.23	0.51
1:C:98:GLN:HB2	1:D:58:ARG:HH11	1.76	0.51
1:B:217:ILE:HG12	1:B:218:LYS:N	2.24	0.51
1:D:47:LEU:CD1	1:D:123:LEU:HD21	2.41	0.51
1:C:224:ASN:OD1	1:C:226:GLN:HB2	2.09	0.51
1:D:55:THR:CG2	1:D:56:ILE:H	2.24	0.51
1:D:56:ILE:HG23	1:D:56:ILE:O	2.09	0.51
1:D:387:LEU:HD22	1:D:387:LEU:N	2.25	0.51
1:A:363:HIS:HE1	1:A:411:SER:OG	1.93	0.51
1:C:193:GLY:HA3	1:C:219:LEU:HA	1.91	0.51
1:D:105:GLU:HA	1:D:110:HIS:CG	2.46	0.51
1:A:7:LEU:HD13	1:A:39:LEU:CD1	2.42	0.50
1:A:217:ILE:HG12	1:A:218:LYS:N	2.25	0.50
1:C:176:ARG:HD2	1:C:370:VAL:HA	1.94	0.50
1:A:233:ARG:CB	1:A:268:PHE:CE2	2.94	0.50
1:B:151:ARG:HD3	1:B:152:TYR:CZ	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:GLN:HE22	1:C:302:HIS:CD2	2.30	0.50
1:A:55:THR:CG2	1:A:56:ILE:H	2.25	0.50
1:A:202:LEU:HD21	1:A:219:LEU:HD22	1.93	0.50
1:B:191:SER:N	1:B:192:PRO:HD2	2.27	0.50
1:A:55:THR:HG23	3:B:5032:HOH:O	2.11	0.50
1:B:349:PHE:CZ	1:B:379:ARG:HA	2.47	0.50
1:C:235:ALA:HB3	1:C:245:MSE:HE1	1.90	0.50
1:A:83:ILE:HD11	1:A:123:LEU:HD13	1.94	0.50
1:B:430:TRP:C	1:B:432:GLU:H	2.20	0.50
1:A:73:HIS:HD2	3:A:5095:HOH:O	1.94	0.49
1:D:318:VAL:HG21	1:D:321:ILE:CD1	2.42	0.49
1:A:87:GLY:HA3	1:A:147:THR:HA	1.93	0.49
1:C:58:ARG:HH11	1:D:98:GLN:HB2	1.77	0.49
1:D:199:ASP:C	3:D:5011:HOH:O	2.54	0.49
1:C:188:TYR:HB2	1:C:216:THR:HB	1.94	0.49
1:C:235:ALA:CB	1:C:245:MSE:CE	2.82	0.49
1:D:206:ALA:HB1	1:D:239:ILE:CD1	2.42	0.49
1:B:172:GLN:NE2	1:B:172:GLN:N	2.60	0.49
1:B:200:GLU:CD	1:B:200:GLU:N	2.70	0.49
1:C:55:THR:HG23	3:D:5057:HOH:O	2.12	0.49
1:C:191:SER:N	1:C:192:PRO:HD2	2.27	0.49
1:A:98:GLN:HG2	1:B:56:ILE:CG2	2.40	0.49
1:B:193:GLY:HA3	1:B:219:LEU:HA	1.93	0.49
1:D:4:ILE:HG21	1:D:74:VAL:HG12	1.94	0.49
1:D:191:SER:N	1:D:192:PRO:HD2	2.26	0.49
1:A:311:GLN:HE21	1:B:283:LEU:HG	1.77	0.49
1:B:63:GLN:NE2	1:B:111:MSE:HE3	2.27	0.49
1:B:239:ILE:HG22	1:B:240:GLY:O	2.13	0.49
1:A:172:GLN:NE2	1:A:172:GLN:N	2.61	0.48
1:A:432:GLU:HG3	1:A:433:ASP:N	2.29	0.48
1:C:250:ASN:C	1:C:251:GLN:HG3	2.37	0.48
1:A:305:ASN:HA	1:A:328:VAL:HG23	1.95	0.48
1:B:55:THR:CG2	1:B:56:ILE:H	2.25	0.48
1:C:105:GLU:HA	1:C:110:HIS:CG	2.47	0.48
1:A:349:PHE:CZ	1:A:379:ARG:HA	2.47	0.48
1:A:87:GLY:CA	1:A:147:THR:HA	2.43	0.48
1:A:151:ARG:HD3	1:A:152:TYR:CZ	2.47	0.48
1:C:311:GLN:HE22	1:D:282:VAL:N	2.11	0.48
1:C:349:PHE:CZ	1:C:379:ARG:HA	2.48	0.48
1:B:366:MSE:SE	1:B:405:PRO:HD2	2.64	0.48
1:D:13:ARG:HB3	1:D:33:SER:OG	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:MSE:HE2	1:A:273:ILE:HB	1.94	0.48
1:D:366:MSE:SE	1:D:405:PRO:HD2	2.64	0.48
1:B:421:GLU:OE2	1:B:429:PHE:HB2	2.13	0.48
1:D:349:PHE:CZ	1:D:379:ARG:HA	2.49	0.48
1:A:139:LEU:HB2	1:A:144:LEU:CD2	2.44	0.47
1:C:98:GLN:OE1	1:D:58:ARG:HG3	2.14	0.47
1:C:62:VAL:HG21	1:D:109:MSE:HE3	1.96	0.47
1:A:13:ARG:HB3	1:A:33:SER:OG	2.13	0.47
1:A:106:LYS:HZ2	1:B:304:GLN:CG	2.27	0.47
1:A:192:PRO:CB	1:A:205:LEU:HB3	2.44	0.47
1:C:73:HIS:HE1	1:C:96:ASP:OD2	1.98	0.47
1:C:79:VAL:O	1:C:83:ILE:HG12	2.14	0.47
1:C:135:PHE:O	1:C:139:LEU:HG	2.15	0.47
1:A:235:ALA:O	1:A:239:ILE:HB	2.14	0.47
1:C:63:GLN:NE2	1:C:111:MSE:HE3	2.30	0.47
1:D:192:PRO:CB	1:D:205:LEU:HB3	2.38	0.47
1:A:225:VAL:HG11	1:A:264:GLN:NE2	2.30	0.47
1:C:305:ASN:HA	1:C:328:VAL:HG23	1.96	0.47
1:D:55:THR:HG22	1:D:56:ILE:H	1.79	0.47
1:D:73:HIS:HE1	1:D:96:ASP:OD2	1.98	0.47
1:D:172:GLN:NE2	1:D:172:GLN:N	2.60	0.47
1:B:225:VAL:CG2	3:B:5055:HOH:O	2.63	0.47
1:A:13:ARG:HG2	1:A:424:TYR:HB2	1.94	0.47
1:B:83:ILE:HD11	1:B:123:LEU:HD13	1.97	0.47
1:A:221:VAL:CG2	1:A:247:VAL:CG1	2.93	0.47
1:B:13:ARG:HB3	1:B:33:SER:OG	2.16	0.47
1:D:7:LEU:HD13	1:D:39:LEU:CD1	2.45	0.47
1:D:15:PRO:HG3	1:D:429:PHE:CZ	2.49	0.47
1:D:151:ARG:HD3	1:D:152:TYR:CZ	2.49	0.47
1:A:92:ARG:NH2	1:A:92:ARG:CB	2.77	0.46
1:C:151:ARG:HD3	1:C:152:TYR:CZ	2.49	0.46
1:A:339:LEU:HD23	1:A:372:ILE:HD12	1.98	0.46
1:C:352:ALA:HA	1:C:357:LEU:HB3	1.98	0.46
1:D:135:PHE:O	1:D:139:LEU:HG	2.15	0.46
1:D:271:ALA:O	1:D:272:TRP:HB3	2.15	0.46
1:D:328:VAL:HG22	1:D:333:GLU:CD	2.40	0.46
1:D:328:VAL:HG22	1:D:329:GLY:N	2.24	0.46
1:A:328:VAL:HG22	1:A:333:GLU:CD	2.39	0.46
1:C:78:SER:O	1:C:82:VAL:HG23	2.16	0.46
1:C:201:LYS:HG2	1:C:205:LEU:HD22	1.96	0.46
1:D:82:VAL:O	1:D:86:LEU:HD13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MSE:HE2	1:D:19:GLU:HG2	1.97	0.46
1:D:206:ALA:HB1	1:D:239:ILE:HD13	1.98	0.46
1:C:32:TYR:CD1	1:C:354:GLY:HA2	2.51	0.46
1:C:109:MSE:HE3	1:D:62:VAL:HG21	1.95	0.46
1:C:339:LEU:HD23	1:C:372:ILE:HD12	1.98	0.46
1:D:220:LYS:HD2	1:D:250:ASN:HD21	1.79	0.46
1:C:311:GLN:HE21	1:D:283:LEU:H	1.64	0.46
1:A:32:TYR:HB3	1:A:355:VAL:HG23	1.98	0.46
1:C:8:GLU:HG3	1:C:38:VAL:HB	1.98	0.45
1:D:83:ILE:HG13	1:D:124:ALA:CA	2.44	0.45
1:D:305:ASN:HB2	1:D:333:GLU:OE1	2.16	0.45
1:C:328:VAL:HG22	1:C:333:GLU:CD	2.41	0.45
1:D:384:VAL:HG12	1:D:386:HIS:ND1	2.32	0.45
1:A:384:VAL:HG12	1:A:386:HIS:ND1	2.31	0.45
1:B:305:ASN:HB2	1:B:333:GLU:OE1	2.16	0.45
1:C:424:TYR:HA	1:C:425:PRO:HA	1.79	0.45
1:D:139:LEU:HB2	1:D:144:LEU:CD2	2.45	0.45
1:D:221:VAL:CG2	1:D:247:VAL:HG13	2.47	0.45
1:A:52:LEU:CD2	1:A:360:LEU:HD11	2.47	0.45
1:C:200:GLU:CD	1:C:200:GLU:H	2.25	0.45
1:C:227:ASP:OD2	1:C:230:ARG:NH1	2.50	0.45
1:D:126:ARG:HG2	1:D:126:ARG:H	1.65	0.45
1:A:199:ASP:OD2	1:A:199:ASP:C	2.60	0.45
1:B:305:ASN:HA	1:B:328:VAL:HG23	1.97	0.45
1:B:431:VAL:O	1:B:431:VAL:HG13	2.16	0.45
1:B:328:VAL:HG22	1:B:329:GLY:N	2.24	0.45
1:C:172:GLN:NE2	1:C:172:GLN:N	2.63	0.45
1:D:198:SER:C	1:D:200:GLU:N	2.75	0.45
1:A:58:ARG:HH11	1:B:98:GLN:HB2	1.81	0.45
1:A:98:GLN:HB2	1:B:58:ARG:NH1	2.32	0.45
1:A:204:ARG:HH11	1:A:204:ARG:HB3	1.80	0.45
1:A:133:TRP:H	1:A:363:HIS:CD2	2.30	0.45
1:A:55:THR:HG22	1:A:56:ILE:H	1.79	0.45
1:C:139:LEU:HB2	1:C:144:LEU:CD2	2.45	0.45
1:C:433:ASP:OD1	1:C:434:LEU:HD22	2.17	0.45
1:D:324:ASP:OD2	1:D:351:HIS:CD2	2.69	0.45
1:A:230:ARG:O	1:A:234:LEU:HG	2.16	0.45
1:A:328:VAL:HG22	1:A:329:GLY:N	2.28	0.45
1:D:204:ARG:O	1:D:208:GLU:HG3	2.17	0.45
1:D:212:ASP:O	1:D:399:HIS:HA	2.17	0.45
1:A:83:ILE:HD12	1:A:83:ILE:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:ILE:HG13	1:C:150:PHE:CE1	2.52	0.44
1:C:192:PRO:CB	1:C:205:LEU:HB3	2.47	0.44
1:A:73:HIS:CE1	1:A:96:ASP:OD2	2.69	0.44
1:B:352:ALA:HA	1:B:357:LEU:HB3	1.99	0.44
1:B:384:VAL:HG12	1:B:386:HIS:ND1	2.33	0.44
1:B:139:LEU:HB2	1:B:144:LEU:CD2	2.45	0.44
1:C:24:ASP:HB2	1:C:250:ASN:ND2	2.32	0.44
1:B:32:TYR:CD1	1:B:354:GLY:HA2	2.52	0.44
1:B:140:THR:OG1	1:B:143:GLN:HG3	2.17	0.44
1:B:328:VAL:HG22	1:B:333:GLU:CD	2.41	0.44
1:C:140:THR:OG1	1:C:143:GLN:HG3	2.18	0.44
1:D:201:LYS:HG2	1:D:205:LEU:HD22	1.98	0.44
1:D:236:ARG:HG2	3:D:5198:HOH:O	2.16	0.44
1:D:352:ALA:HA	1:D:357:LEU:HB3	1.99	0.44
1:C:221:VAL:CG2	1:C:247:VAL:HG13	2.47	0.44
1:D:305:ASN:HA	1:D:328:VAL:HG23	2.00	0.44
1:A:188:TYR:HB2	1:A:216:THR:HB	1.99	0.44
1:B:83:ILE:HG13	1:B:124:ALA:HA	1.99	0.44
1:C:372:ILE:HG12	1:C:373:THR:HG23	2.00	0.44
1:D:3:THR:HG22	1:D:4:ILE:N	2.32	0.44
1:A:83:ILE:N	1:A:83:ILE:CD1	2.81	0.44
1:A:126:ARG:HG2	1:A:126:ARG:H	1.65	0.44
1:A:352:ALA:HA	1:A:357:LEU:HB3	1.98	0.44
1:B:188:TYR:CB	1:B:216:THR:HB	2.48	0.44
1:B:391:PHE:O	1:B:394:PRO:HD3	2.18	0.44
1:A:249:ALA:HB2	1:A:253:TRP:CH2	2.53	0.44
1:D:190:THR:HG22	1:D:190:THR:O	2.18	0.44
1:A:271:ALA:O	1:A:272:TRP:HB3	2.17	0.44
1:A:324:ASP:OD2	1:A:351:HIS:CD2	2.69	0.44
1:B:135:PHE:O	1:B:139:LEU:HG	2.17	0.44
1:D:235:ALA:O	1:D:239:ILE:HB	2.18	0.44
1:A:58:ARG:NH1	1:B:98:GLN:HB2	2.32	0.43
1:A:4:ILE:HG21	1:A:74:VAL:HG12	2.00	0.43
1:A:190:THR:HG22	1:A:190:THR:O	2.18	0.43
1:A:204:ARG:NH1	1:A:204:ARG:HB3	2.34	0.43
1:A:221:VAL:HG22	1:A:247:VAL:HG13	2.00	0.43
1:A:221:VAL:HG21	1:A:247:VAL:CG1	2.48	0.43
1:C:106:LYS:HZ2	1:D:304:GLN:HG3	1.83	0.43
1:D:198:SER:O	1:D:200:GLU:N	2.51	0.43
1:B:8:GLU:CG	1:B:38:VAL:HB	2.49	0.43
1:C:56:ILE:CG2	1:D:98:GLN:HA	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:ILE:CD1	1:D:123:LEU:HD13	2.48	0.43
1:D:176:ARG:HD3	1:D:374:GLY:HA2	2.01	0.43
1:A:135:PHE:O	1:A:139:LEU:HG	2.19	0.43
1:A:328:VAL:HG13	1:A:329:GLY:N	2.33	0.43
1:A:372:ILE:HG12	1:A:373:THR:HG23	2.00	0.43
1:B:126:ARG:HG2	1:B:126:ARG:H	1.61	0.43
1:A:232:CYS:HB3	1:A:268:PHE:CD1	2.53	0.43
1:A:423:SER:O	1:A:430:TRP:HD1	2.01	0.43
1:A:432:GLU:O	1:A:435:ALA:HB3	2.19	0.43
1:B:424:TYR:HA	1:B:425:PRO:HA	1.79	0.43
1:C:305:ASN:HB2	1:C:333:GLU:OE1	2.18	0.43
1:D:200:GLU:HA	1:D:203:VAL:CG2	2.49	0.43
1:D:236:ARG:HH11	1:D:241:PRO:HA	1.83	0.43
1:C:384:VAL:HG12	1:C:386:HIS:ND1	2.34	0.43
1:C:391:PHE:O	1:C:394:PRO:HD3	2.18	0.43
1:D:328:VAL:HG13	1:D:329:GLY:N	2.33	0.43
1:A:172:GLN:H	1:A:172:GLN:HE21	1.66	0.43
1:A:423:SER:O	1:A:430:TRP:CD1	2.72	0.43
1:B:145:VAL:HG13	1:B:150:PHE:CZ	2.53	0.43
1:C:98:GLN:HA	1:D:56:ILE:CG2	2.49	0.43
1:D:55:THR:HG23	3:D:5059:HOH:O	2.18	0.43
1:A:221:VAL:CG2	1:A:247:VAL:HG13	2.49	0.43
1:D:78:SER:O	1:D:82:VAL:HG23	2.19	0.43
1:B:55:THR:HG22	1:B:56:ILE:H	1.78	0.43
1:B:225:VAL:HG23	3:B:5055:HOH:O	2.18	0.43
1:B:300:GLY:HA2	1:B:303:THR:OG1	2.19	0.43
1:C:262:MSE:HE2	1:C:273:ILE:HB	2.01	0.43
1:C:328:VAL:HG22	1:C:329:GLY:N	2.27	0.43
1:A:282:VAL:N	1:B:311:GLN:NE2	2.67	0.42
1:C:98:GLN:HB2	1:D:58:ARG:NH1	2.34	0.42
1:B:148:ILE:HG13	1:B:150:PHE:CE1	2.54	0.42
1:D:372:ILE:HG12	1:D:373:THR:HG23	2.01	0.42
1:D:424:TYR:HA	1:D:425:PRO:HA	1.80	0.42
1:A:305:ASN:HB2	1:A:333:GLU:OE1	2.20	0.42
1:B:63:GLN:HE22	1:B:111:MSE:HE3	1.85	0.42
1:A:368:ASP:CA	1:A:372:ILE:HG23	2.49	0.42
1:A:92:ARG:HH21	1:A:92:ARG:HB2	1.84	0.42
1:B:372:ILE:HG12	1:B:373:THR:HG23	2.01	0.42
1:C:145:VAL:HG13	1:C:150:PHE:CZ	2.53	0.42
1:A:148:ILE:HG13	1:A:150:PHE:CE1	2.55	0.42
1:C:368:ASP:CA	1:C:372:ILE:HG23	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:THR:HG22	1:B:4:ILE:N	2.35	0.42
1:C:271:ALA:O	1:C:272:TRP:HB3	2.20	0.42
1:D:172:GLN:O	1:D:176:ARG:HG3	2.19	0.42
1:A:189:THR:HG23	1:A:214:PHE:CE2	2.55	0.42
1:A:304:GLN:HG3	1:B:106:LYS:HZ2	1.85	0.42
1:B:190:THR:HG22	1:B:190:THR:O	2.19	0.42
1:B:429:PHE:CD1	1:B:429:PHE:C	2.97	0.42
1:C:22:GLY:HA2	1:C:194:TRP:CD2	2.54	0.42
1:B:24:ASP:HB2	1:B:250:ASN:ND2	2.34	0.42
1:D:202:LEU:N	3:D:5011:HOH:O	2.52	0.42
1:B:45:GLU:HA	1:B:45:GLU:OE2	2.20	0.42
1:C:44:ALA:C	1:C:46:ASP:N	2.77	0.42
1:A:229:ILE:HA	1:A:268:PHE:HE1	1.85	0.41
1:B:271:ALA:O	1:B:272:TRP:HB3	2.19	0.41
1:C:148:ILE:HD12	1:C:149:ASP:C	2.45	0.41
1:B:133:TRP:H	1:B:363:HIS:CD2	2.30	0.41
1:B:172:GLN:H	1:B:172:GLN:HE21	1.66	0.41
1:C:102:LEU:CD2	1:C:109:MSE:HE3	2.37	0.41
1:C:92:ARG:HG3	1:C:92:ARG:NH2	2.35	0.41
1:C:318:VAL:HG21	1:C:321:ILE:HD12	2.03	0.41
1:A:58:ARG:NH1	1:B:98:GLN:CD	2.78	0.41
1:A:98:GLN:CD	1:B:58:ARG:NH1	2.78	0.41
1:A:176:ARG:HD2	1:A:370:VAL:HA	2.02	0.41
1:B:148:ILE:HD12	1:B:149:ASP:C	2.45	0.41
1:C:87:GLY:CA	1:C:147:THR:HA	2.51	0.41
1:D:368:ASP:CA	1:D:372:ILE:HG23	2.49	0.41
1:C:56:ILE:HG22	1:D:98:GLN:HA	2.02	0.41
1:C:145:VAL:HG21	1:C:163:LEU:HG	2.02	0.41
1:D:148:ILE:HG13	1:D:150:PHE:CE1	2.56	0.41
1:B:172:GLN:O	1:B:176:ARG:HG3	2.20	0.41
1:B:210:VAL:CG2	1:B:239:ILE:HG13	2.50	0.41
1:C:40:ARG:HA	1:C:40:ARG:HD3	1.95	0.41
1:D:102:LEU:CD2	1:D:109:MSE:HE3	2.35	0.41
1:D:391:PHE:O	1:D:394:PRO:HD3	2.21	0.41
1:A:3:THR:HG22	1:A:4:ILE:N	2.35	0.41
1:C:50:TYR:HE1	1:C:126:ARG:NH1	2.19	0.41
1:C:311:GLN:NE2	1:D:283:LEU:H	2.19	0.41
1:D:221:VAL:CG2	1:D:247:VAL:CG1	2.98	0.41
1:A:172:GLN:O	1:A:176:ARG:HG3	2.21	0.41
1:A:253:TRP:HB2	1:A:258:ALA:HB2	2.02	0.41
1:B:40:ARG:HA	1:B:40:ARG:HD3	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:ASP:OD2	1:C:351:HIS:CD2	2.69	0.41
1:A:145:VAL:HG13	1:A:150:PHE:CZ	2.56	0.41
1:A:379:ARG:NH2	3:A:5110:HOH:O	2.51	0.41
1:B:86:LEU:HD12	1:B:86:LEU:HA	1.95	0.41
1:C:45:GLU:OE2	1:C:45:GLU:HA	2.21	0.41
1:C:428:ARG:HG2	1:C:428:ARG:HH11	1.86	0.41
1:C:428:ARG:HG2	1:C:428:ARG:NH1	2.36	0.41
1:D:7:LEU:HD11	1:D:37:VAL:CG1	2.51	0.41
1:A:19:GLU:CD	1:C:1:MSE:HE2	2.46	0.40
1:B:55:THR:HB	1:B:60:ASN:OD1	2.21	0.40
1:B:324:ASP:OD2	1:B:351:HIS:CD2	2.71	0.40
1:B:339:LEU:HD23	1:B:372:ILE:HD12	2.02	0.40
1:D:24:ASP:HB2	1:D:250:ASN:ND2	2.37	0.40
1:A:44:ALA:C	1:A:46:ASP:N	2.78	0.40
1:A:45:GLU:OE2	1:A:45:GLU:HA	2.20	0.40
1:A:229:ILE:O	1:A:268:PHE:CE1	2.75	0.40
1:C:13:ARG:HB3	1:C:33:SER:OG	2.21	0.40
1:B:247:VAL:CG1	1:B:273:ILE:HD13	2.51	0.40
1:D:193:GLY:HA3	1:D:219:LEU:HA	2.02	0.40
1:D:227:ASP:OD2	1:D:230:ARG:NH1	2.55	0.40
1:A:98:GLN:HA	1:B:56:ILE:CG2	2.52	0.40
1:A:191:SER:N	1:A:192:PRO:CD	2.84	0.40
1:A:391:PHE:O	1:A:394:PRO:HD3	2.21	0.40
3:A:5012:HOH:O	1:B:56:ILE:HG22	2.21	0.40
1:A:424:TYR:HA	1:A:425:PRO:HA	1.79	0.40
1:C:235:ALA:C	1:C:245:MSE:HE1	2.47	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	419/444 (94%)	401 (96%)	17 (4%)	1 (0%)	43	50
1	B	430/444 (97%)	410 (95%)	17 (4%)	3 (1%)	18	18
1	C	433/444 (98%)	415 (96%)	16 (4%)	2 (0%)	24	26
1	D	429/444 (97%)	412 (96%)	15 (4%)	2 (0%)	24	26
All	All	1711/1776 (96%)	1638 (96%)	65 (4%)	8 (0%)	24	26

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	199	ASP
1	D	387	LEU
1	A	387	LEU
1	B	387	LEU
1	C	387	LEU
1	C	22	GLY
1	B	22	GLY
1	B	431	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	333/336 (99%)	297 (89%)	36 (11%)	6	5
1	B	338/336 (101%)	300 (89%)	38 (11%)	6	4
1	C	340/336 (101%)	300 (88%)	40 (12%)	5	4
1	D	338/336 (101%)	301 (89%)	37 (11%)	6	5
All	All	1349/1344 (100%)	1198 (89%)	151 (11%)	6	4

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	19	GLU
1	A	39	LEU

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Mol	Chain	Res	Type
1	A	52	LEU
1	A	56	ILE
1	A	86	LEU
1	A	93	LEU
1	A	94	THR
1	A	99	LEU
1	A	123	LEU
1	A	144	LEU
1	A	148	ILE
1	A	151	ARG
1	A	159	ARG
1	A	172	GLN
1	A	180	LEU
1	A	189	THR
1	A	202	LEU
1	A	205	LEU
1	A	217	ILE
1	A	225	VAL
1	A	226	GLN
1	A	273	ILE
1	A	302	HIS
1	A	312	LEU
1	A	313	LEU
1	A	321	ILE
1	A	323	ILE
1	A	340	LEU
1	A	346	VAL
1	A	348	VAL
1	A	357	LEU
1	A	361	VAL
1	A	372	ILE
1	A	379	ARG
1	A	387	LEU
1	B	13	ARG
1	B	39	LEU
1	B	52	LEU
1	B	56	ILE
1	B	86	LEU
1	B	93	LEU
1	B	94	THR
1	B	99	LEU
1	B	123	LEU

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Mol	Chain	Res	Type
1	B	144	LEU
1	B	148	ILE
1	B	151	ARG
1	B	159	ARG
1	B	172	GLN
1	B	180	LEU
1	B	189	THR
1	B	200	GLU
1	B	203	VAL
1	B	205	LEU
1	B	217	ILE
1	B	225	VAL
1	B	226	GLN
1	B	239	ILE
1	B	247	VAL
1	B	273	ILE
1	B	302	HIS
1	B	312	LEU
1	B	313	LEU
1	B	321	ILE
1	B	323	ILE
1	B	340	LEU
1	B	346	VAL
1	B	348	VAL
1	B	357	LEU
1	B	361	VAL
1	B	372	ILE
1	B	379	ARG
1	B	387	LEU
1	C	13	ARG
1	C	20	LEU
1	C	39	LEU
1	C	52	LEU
1	C	56	ILE
1	C	86	LEU
1	C	93	LEU
1	C	94	THR
1	C	99	LEU
1	C	123	LEU
1	C	144	LEU
1	C	148	ILE
1	C	151	ARG

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Mol	Chain	Res	Type
1	C	159	ARG
1	C	172	GLN
1	C	180	LEU
1	C	189	THR
1	C	202	LEU
1	C	205	LEU
1	C	217	ILE
1	C	225	VAL
1	C	226	GLN
1	C	239	ILE
1	C	247	VAL
1	C	273	ILE
1	C	298	SER
1	C	302	HIS
1	C	312	LEU
1	C	313	LEU
1	C	321	ILE
1	C	323	ILE
1	C	340	LEU
1	C	346	VAL
1	C	348	VAL
1	C	357	LEU
1	C	361	VAL
1	C	372	ILE
1	C	379	ARG
1	C	387	LEU
1	C	432	GLU
1	D	13	ARG
1	D	39	LEU
1	D	52	LEU
1	D	56	ILE
1	D	86	LEU
1	D	93	LEU
1	D	94	THR
1	D	99	LEU
1	D	123	LEU
1	D	144	LEU
1	D	148	ILE
1	D	151	ARG
1	D	159	ARG
1	D	172	GLN
1	D	180	LEU

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Mol	Chain	Res	Type
1	D	189	THR
1	D	199	ASP
1	D	202	LEU
1	D	205	LEU
1	D	217	ILE
1	D	225	VAL
1	D	226	GLN
1	D	239	ILE
1	D	273	ILE
1	D	302	HIS
1	D	312	LEU
1	D	313	LEU
1	D	321	ILE
1	D	323	ILE
1	D	340	LEU
1	D	346	VAL
1	D	348	VAL
1	D	357	LEU
1	D	361	VAL
1	D	372	ILE
1	D	379	ARG
1	D	387	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	73	HIS
1	A	129	ASN
1	A	170	GLN
1	A	172	GLN
1	A	183	GLN
1	A	250	ASN
1	A	285	HIS
1	A	302	HIS
1	A	304	GLN
1	A	311	GLN
1	A	314	GLN
1	A	351	HIS
1	A	362	GLN
1	A	363	HIS
1	A	390	HIS

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Mol	Chain	Res	Type
1	B	63	GLN
1	B	73	HIS
1	B	170	GLN
1	B	172	GLN
1	B	183	GLN
1	B	250	ASN
1	B	285	HIS
1	B	302	HIS
1	B	304	GLN
1	B	311	GLN
1	B	314	GLN
1	B	351	HIS
1	B	362	GLN
1	B	363	HIS
1	B	390	HIS
1	C	63	GLN
1	C	73	HIS
1	C	170	GLN
1	C	172	GLN
1	C	183	GLN
1	C	250	ASN
1	C	285	HIS
1	C	302	HIS
1	C	304	GLN
1	C	311	GLN
1	C	314	GLN
1	C	351	HIS
1	C	362	GLN
1	C	363	HIS
1	C	390	HIS
1	D	63	GLN
1	D	73	HIS
1	D	170	GLN
1	D	172	GLN
1	D	183	GLN
1	D	250	ASN
1	D	285	HIS
1	D	302	HIS
1	D	304	GLN
1	D	311	GLN
1	D	314	GLN
1	D	351	HIS

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Mol	Chain	Res	Type
1	D	362	GLN
1	D	363	HIS
1	D	390	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 ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	416/444 (93%)	0.71	46 (11%)	10 12	19, 34, 58, 80	0
1	B	423/444 (95%)	0.53	38 (8%)	15 18	15, 31, 57, 83	0
1	C	426/444 (95%)	0.73	32 (7%)	20 24	17, 36, 61, 84	0
1	D	424/444 (95%)	0.59	44 (10%)	11 14	19, 34, 56, 82	0
All	All	1689/1776 (95%)	0.64	160 (9%)	14 17	15, 33, 58, 84	0

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	20	LEU	6.8
1	A	46	ASP	6.5
1	C	46	ASP	6.4
1	A	435	ALA	6.2
1	D	202	LEU	6.1
1	D	436	ALA	5.9
1	A	434	LEU	5.6
1	A	191	SER	5.3
1	B	20	LEU	4.9
1	C	434	LEU	4.7
1	A	424	TYR	4.7
1	A	427	GLY	4.5
1	A	44	ALA	4.5
1	B	46	ASP	4.4
1	A	425	PRO	4.4
1	B	426	ASP	4.3
1	B	44	ALA	4.2
1	A	423	SER	4.2
1	A	419	ILE	4.0
1	B	424	TYR	3.9
1	C	386	HIS	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	426	ASP	3.9
1	B	431	VAL	3.9
1	C	44	ALA	3.8
1	A	268	PHE	3.7
1	C	47	LEU	3.7
1	A	217	ILE	3.7
1	B	45	GLU	3.7
1	A	194	TRP	3.6
1	D	434	LEU	3.6
1	B	432	GLU	3.5
1	C	435	ALA	3.5
1	A	47	LEU	3.5
1	D	234	LEU	3.5
1	B	407	VAL	3.4
1	C	37	VAL	3.4
1	A	199	ASP	3.4
1	D	45	GLU	3.4
1	D	203	VAL	3.4
1	D	194	TRP	3.3
1	D	2	ARG	3.2
1	B	387	LEU	3.2
1	C	372	ILE	3.2
1	B	129	ASN	3.2
1	A	193	GLY	3.1
1	B	386	HIS	3.1
1	C	181	ILE	3.1
1	C	22	GLY	3.1
1	D	19	GLU	3.1
1	D	196	GLY	3.1
1	B	28	PRO	3.1
1	C	43	GLY	3.1
1	D	207	LYS	3.1
1	D	199	ASP	3.0
1	A	192	PRO	3.0
1	C	142	GLU	3.0
1	D	46	ASP	3.0
1	B	178	ALA	3.0
1	A	203	VAL	3.0
1	B	47	LEU	2.9
1	B	48	ALA	2.9
1	D	235	ALA	2.9
1	A	28	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	197	TYR	2.8
1	B	15	PRO	2.8
1	A	422	PHE	2.8
1	A	200	GLU	2.8
1	B	425	PRO	2.8
1	D	44	ALA	2.8
1	C	424	TYR	2.8
1	C	422	PHE	2.7
1	C	384	VAL	2.7
1	A	45	GLU	2.7
1	B	175	ALA	2.7
1	D	28	PRO	2.7
1	D	293	THR	2.7
1	A	229	ILE	2.7
1	A	202	LEU	2.6
1	B	168	ASP	2.6
1	D	227	ASP	2.6
1	D	386	HIS	2.6
1	A	261	TRP	2.6
1	C	45	GLU	2.6
1	D	433	ASP	2.6
1	A	267	GLU	2.6
1	B	179	THR	2.6
1	D	40	ARG	2.5
1	C	21	ASP	2.5
1	D	3	THR	2.5
1	A	420	ALA	2.5
1	B	184	GLY	2.5
1	C	430	TRP	2.5
1	D	431	VAL	2.5
1	A	205	LEU	2.5
1	D	205	LEU	2.5
1	A	266	ALA	2.5
1	A	27	ASN	2.4
1	C	187	ALA	2.4
1	A	19	GLU	2.4
1	D	230	ARG	2.4
1	B	16	THR	2.4
1	A	56	ILE	2.4
1	B	429	PHE	2.4
1	C	399	HIS	2.4
1	A	398	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	29	ASP	2.4
1	D	47	LEU	2.4
1	D	222	GLY	2.3
1	B	56	ILE	2.3
1	B	182	GLU	2.3
1	B	43	GLY	2.3
1	D	268	PHE	2.3
1	D	195	LEU	2.3
1	A	206	ALA	2.3
1	A	189	THR	2.3
1	A	432	GLU	2.3
1	B	217	ILE	2.3
1	A	234	LEU	2.2
1	D	435	ALA	2.2
1	C	74	VAL	2.2
1	D	191	SER	2.2
1	D	148	ILE	2.2
1	D	224	ASN	2.2
1	A	3	THR	2.2
1	A	239	ILE	2.2
1	C	56	ILE	2.2
1	D	323	ILE	2.2
1	B	21	ASP	2.2
1	C	408	PRO	2.2
1	B	427	GLY	2.2
1	D	372	ILE	2.1
1	D	385	ASP	2.1
1	D	192	PRO	2.1
1	B	399	HIS	2.1
1	B	22	GLY	2.1
1	C	127	ALA	2.1
1	C	126	ARG	2.1
1	B	148	ILE	2.1
1	A	407	VAL	2.1
1	B	75	VAL	2.1
1	C	48	ALA	2.1
1	D	217	ILE	2.1
1	C	407	VAL	2.1
1	C	425	PRO	2.1
1	B	29	ASP	2.1
1	B	323	ILE	2.1
1	C	374	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	18	ARG	2.1
1	C	432	GLU	2.0
1	D	226	GLN	2.0
1	B	181	ILE	2.0
1	D	321	ILE	2.0
1	A	2	ARG	2.0
1	A	417	ALA	2.0
1	C	175	ALA	2.0
1	D	206	ALA	2.0
1	A	232	CYS	2.0
1	A	323	ILE	2.0
1	D	428	ARG	2.0
1	D	201	LYS	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($\text{\AA}^2$)	Q<0.9
2	MG	B	6002	1/1	0.73	0.18	33,33,33,33	0
2	MG	D	6004	1/1	0.79	0.21	43,43,43,43	0
2	MG	A	6001	1/1	0.80	0.25	61,61,61,61	0
2	MG	C	6003	1/1	0.82	0.16	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.