



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:41 PM UTC

PDB ID : 3RBZ / pdb_00003rbz
Title : MthK channel, Ca²⁺-bound
Authors : Taylor, A.B.; Parfenova, L.V.; Rothberg, B.S.
Deposited on : 2011-03-30
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
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

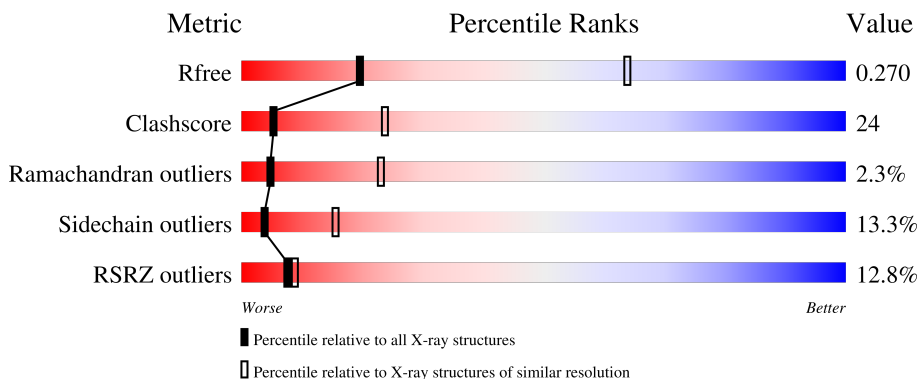
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	340	13% 47% 31% 7% 15%
1	B	340	12% 49% 28% 6% 17%
1	C	340	10% 51% 27% 6% 16%
1	D	340	8% 51% 26% 6% 16%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8153 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 Calcium-gated potassium channel mthK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	0
			2082	1300	366	408	8			
1	B	281	Total	C	N	O	S	0	0	0
			2012	1249	357	399	7			
1	C	286	Total	C	N	O	S	0	0	0
			2028	1258	360	403	7			
1	D	285	Total	C	N	O	S	0	0	0
			2019	1255	359	398	7			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	85	ALA	GLY	engineered mutation	UNP O27564
A	92	ALA	GLU	engineered mutation	UNP O27564
A	96	THR	GLU	engineered mutation	UNP O27564
A	107	ILE	MET	engineered mutation	UNP O27564
A	337	LEU	-	expression tag	UNP O27564
A	338	VAL	-	expression tag	UNP O27564
A	339	PRO	-	expression tag	UNP O27564
A	340	ARG	-	expression tag	UNP O27564
B	85	ALA	GLY	engineered mutation	UNP O27564
B	92	ALA	GLU	engineered mutation	UNP O27564
B	96	THR	GLU	engineered mutation	UNP O27564
B	107	ILE	MET	engineered mutation	UNP O27564
B	337	LEU	-	expression tag	UNP O27564
B	338	VAL	-	expression tag	UNP O27564
B	339	PRO	-	expression tag	UNP O27564
B	340	ARG	-	expression tag	UNP O27564
C	85	ALA	GLY	engineered mutation	UNP O27564
C	92	ALA	GLU	engineered mutation	UNP O27564
C	96	THR	GLU	engineered mutation	UNP O27564
C	107	ILE	MET	engineered mutation	UNP O27564
C	337	LEU	-	expression tag	UNP O27564

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Chain	Residue	Modelled	Actual	Comment	Reference
C	338	VAL	-	expression tag	UNP O27564
C	339	PRO	-	expression tag	UNP O27564
C	340	ARG	-	expression tag	UNP O27564
D	85	ALA	GLY	engineered mutation	UNP O27564
D	92	ALA	GLU	engineered mutation	UNP O27564
D	96	THR	GLU	engineered mutation	UNP O27564
D	107	ILE	MET	engineered mutation	UNP O27564
D	337	LEU	-	expression tag	UNP O27564
D	338	VAL	-	expression tag	UNP O27564
D	339	PRO	-	expression tag	UNP O27564
D	340	ARG	-	expression tag	UNP O27564

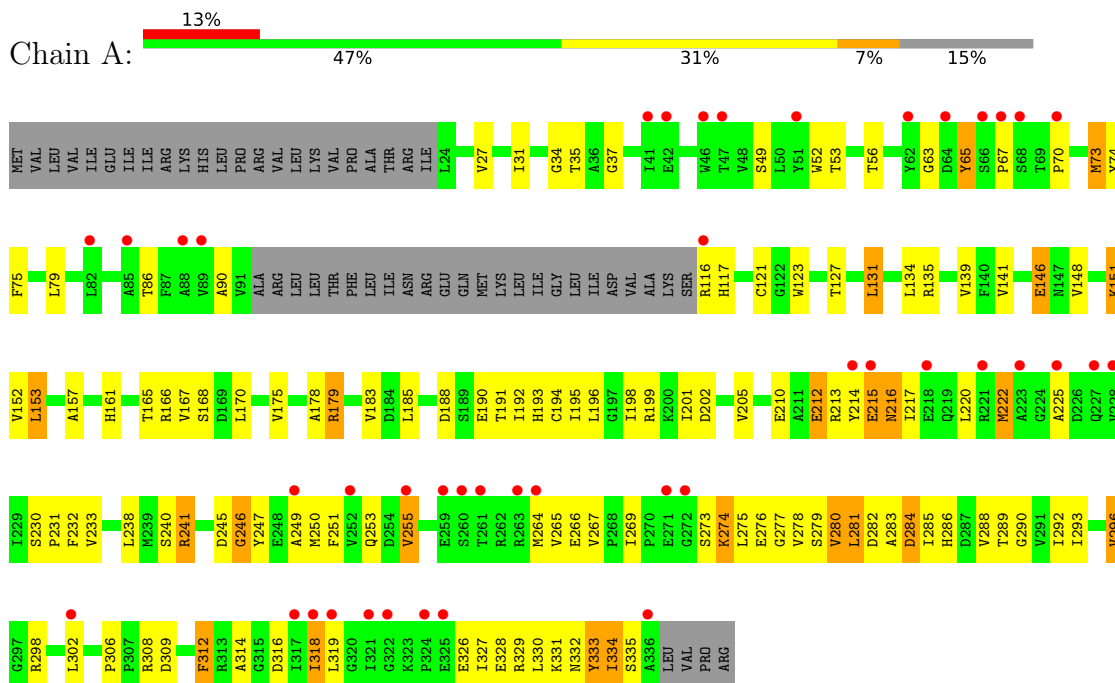
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total 3	Ca 3	0	0
2	B	3	Total 3	Ca 3	0	0
2	C	3	Total 3	Ca 3	0	0
2	D	3	Total 3	Ca 3	0	0

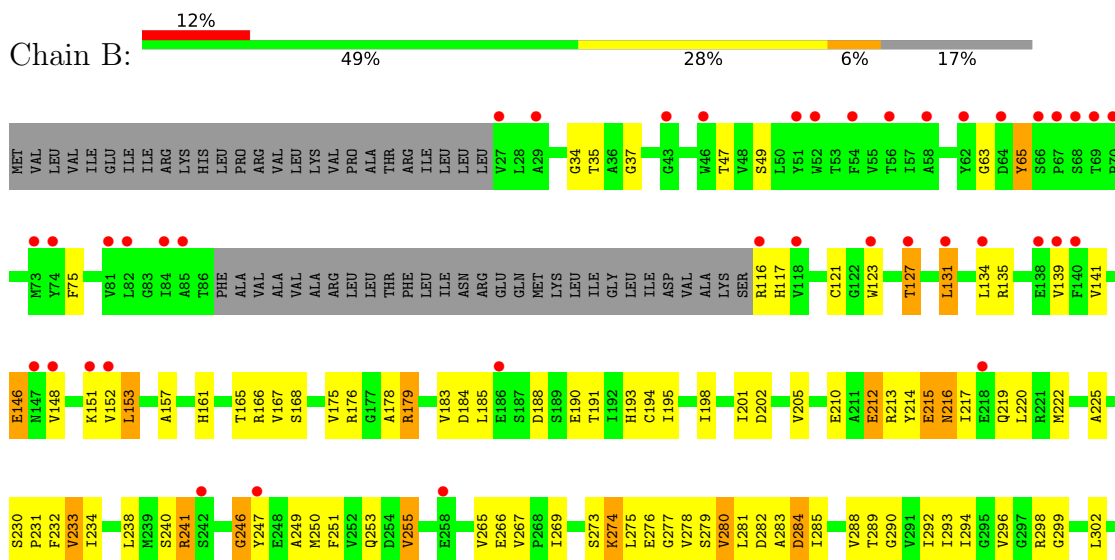
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Calcium-gated potassium channel mthK



- Molecule 1: Calcium-gated potassium channel mthK



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	138.56Å 138.56Å 371.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.50 – 3.40 48.50 – 3.40	Depositor EDS
% Data completeness (in resolution range)	86.9 (48.50-3.40) 85.2 (48.50-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.60 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.257 , 0.288 0.242 , 0.270	Depositor DCC
R_{free} test set	2000 reflections (7.14%)	wwPDB-VP
Wilson B-factor (Å ²)	75.7	Xtriage
Anisotropy	0.508	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 112.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	8153	wwPDB-VP
Average B, all atoms (Å ²)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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: CA

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	0.67	0/2110	0.99	3/2868 (0.1%)
1	B	0.67	0/2037	0.99	3/2766 (0.1%)
1	C	0.72	1/2052 (0.0%)	1.00	2/2790 (0.1%)
1	D	0.79	1/2043 (0.0%)	1.06	9/2775 (0.3%)
All	All	0.72	2/8242 (0.0%)	1.01	17/11199 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	193	HIS	CE1-NE2	7.58	1.40	1.32
1	D	202	ASP	CA-CB	6.17	1.60	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	TYR	N-CA-C	7.14	119.97	111.33
1	C	247	TYR	N-CA-C	6.99	118.90	111.28
1	B	247	TYR	N-CA-C	6.84	118.73	111.28
1	D	299	GLY	N-CA-C	6.62	117.77	111.67
1	D	247	TYR	N-CA-C	6.43	118.28	111.28
1	D	246	GLY	N-CA-C	6.09	121.16	114.40
1	C	246	GLY	N-CA-C	5.72	120.96	114.67
1	D	202	ASP	N-CA-C	-5.70	97.15	107.75
1	B	246	GLY	N-CA-C	5.66	121.23	113.99
1	A	246	GLY	N-CA-C	5.31	120.59	114.16
1	D	233	VAL	N-CA-C	-5.27	105.71	110.82
1	D	288	VAL	CB-CA-C	-5.17	105.26	111.88
1	D	221	ARG	N-CA-C	-5.08	105.83	111.36
1	D	163	ASP	CA-C-N	5.07	126.17	119.84
1	D	163	ASP	C-N-CA	5.07	126.17	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	LEU	N-CA-C	-5.05	105.67	111.07
1	B	299	GLY	N-CA-C	5.02	116.29	111.67

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	2082	0	1948	106	0
1	B	2012	0	1870	93	0
1	C	2028	0	1869	102	0
1	D	2019	0	1862	91	1
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
All	All	8153	0	7549	381	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 24.

All (381) 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:165:THR:HB	1:C:193:HIS:CD2	1.68	1.28
1:C:241:ARG:HG2	1:C:241:ARG:HH11	1.13	1.13
1:C:165:THR:HB	1:C:193:HIS:HD2	0.93	1.10
1:B:241:ARG:HG2	1:B:241:ARG:HH11	1.12	1.09
1:D:241:ARG:HH11	1:D:241:ARG:HG2	1.12	1.09
1:A:241:ARG:HG2	1:A:241:ARG:HH11	1.14	1.08
1:C:165:THR:CB	1:C:193:HIS:HD2	1.67	1.06
1:B:179:ARG:HG3	1:B:179:ARG:HH11	1.25	1.02
1:A:179:ARG:HG3	1:A:179:ARG:HH11	1.27	0.98
1:C:179:ARG:HG3	1:C:179:ARG:HH11	1.27	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:ARG:HG3	1:D:179:ARG:HH11	1.29	0.95
1:A:241:ARG:HH11	1:A:241:ARG:CG	1.92	0.82
1:D:251:PHE:O	1:D:255:VAL:HG22	1.80	0.81
1:B:213:ARG:HH11	1:B:213:ARG:HG3	1.44	0.80
1:B:165:THR:HB	1:B:193:HIS:CD2	2.16	0.80
1:C:213:ARG:HG3	1:C:213:ARG:HH11	1.45	0.80
1:B:284:ASP:O	1:B:288:VAL:HG23	1.81	0.80
1:D:284:ASP:O	1:D:288:VAL:HG23	1.83	0.80
1:C:298:ARG:HD2	1:C:316:ASP:OD1	1.83	0.79
1:A:251:PHE:O	1:A:255:VAL:HG22	1.82	0.79
1:C:284:ASP:O	1:C:288:VAL:HG23	1.83	0.79
1:D:165:THR:HB	1:D:193:HIS:CD2	2.18	0.79
1:D:213:ARG:HG3	1:D:213:ARG:HH11	1.46	0.79
1:C:241:ARG:HH11	1:C:241:ARG:CG	1.93	0.78
1:D:241:ARG:HH11	1:D:241:ARG:CG	1.96	0.78
1:B:241:ARG:HH11	1:B:241:ARG:CG	1.95	0.77
1:A:241:ARG:HG2	1:A:241:ARG:NH1	1.95	0.77
1:D:246:GLY:O	1:D:250:MET:HG3	1.85	0.75
1:A:298:ARG:HD2	1:A:316:ASP:OD1	1.87	0.75
1:C:58:ALA:O	1:D:59:THR:HB	1.87	0.75
1:A:165:THR:HB	1:A:193:HIS:CD2	2.22	0.74
1:B:179:ARG:HH11	1:B:179:ARG:CG	1.99	0.74
1:A:214:TYR:O	1:A:217:ILE:HG12	1.87	0.74
1:B:241:ARG:HG2	1:B:241:ARG:NH1	1.93	0.74
1:B:251:PHE:O	1:B:255:VAL:HG22	1.86	0.74
1:C:251:PHE:O	1:C:255:VAL:HG22	1.86	0.74
1:A:179:ARG:HH11	1:A:179:ARG:CG	1.99	0.74
1:C:179:ARG:HH11	1:C:179:ARG:CG	2.01	0.73
1:B:298:ARG:HD2	1:B:316:ASP:OD1	1.88	0.73
1:C:246:GLY:O	1:C:250:MET:HG3	1.88	0.73
1:C:279:SER:HB3	1:C:282:ASP:HB2	1.71	0.73
1:D:241:ARG:HG2	1:D:241:ARG:NH1	1.93	0.73
1:A:213:ARG:HG3	1:A:213:ARG:HH11	1.52	0.73
1:B:269:ILE:HG22	1:B:314:ALA:HA	1.71	0.73
1:D:269:ILE:HG22	1:D:314:ALA:HA	1.72	0.72
1:A:284:ASP:O	1:A:288:VAL:HG23	1.90	0.72
1:B:246:GLY:O	1:B:250:MET:HG3	1.91	0.70
1:A:67:PRO:HB2	1:A:73:MET:HG3	1.74	0.70
1:B:214:TYR:O	1:B:217:ILE:HG12	1.92	0.70
1:C:185:LEU:HD12	1:C:190:GLU:O	1.92	0.69
1:A:269:ILE:HG22	1:A:314:ALA:HA	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:TYR:O	1:C:217:ILE:HG12	1.93	0.69
1:D:279:SER:HB3	1:D:282:ASP:HB2	1.74	0.69
1:D:179:ARG:HH11	1:D:179:ARG:CG	2.03	0.68
1:A:185:LEU:HD12	1:A:190:GLU:O	1.93	0.68
1:A:146:GLU:HG2	1:A:161:HIS:ND1	2.08	0.68
1:D:214:TYR:O	1:D:217:ILE:HG12	1.93	0.68
1:C:175:VAL:HG11	1:C:198:ILE:HG23	1.75	0.67
1:D:298:ARG:HD2	1:D:316:ASP:OD1	1.94	0.67
1:C:269:ILE:HG22	1:C:314:ALA:HA	1.74	0.67
1:A:175:VAL:HG11	1:A:198:ILE:HG23	1.78	0.66
1:B:185:LEU:HD12	1:B:190:GLU:O	1.95	0.66
1:B:210:GLU:OE1	1:B:231:PRO:HG3	1.96	0.66
1:B:179:ARG:HG3	1:B:179:ARG:NH1	2.05	0.66
1:C:146:GLU:HG2	1:C:161:HIS:ND1	2.11	0.66
1:D:213:ARG:HG3	1:D:213:ARG:NH1	2.11	0.66
1:C:241:ARG:HG2	1:C:241:ARG:NH1	1.93	0.65
1:B:117:HIS:CE1	1:B:178:ALA:HB2	2.30	0.65
1:A:210:GLU:OE1	1:A:231:PRO:HG3	1.97	0.65
1:B:146:GLU:HG2	1:B:161:HIS:ND1	2.11	0.65
1:B:279:SER:HB3	1:B:282:ASP:HB2	1.79	0.65
1:A:279:SER:HB3	1:A:282:ASP:HB2	1.79	0.65
1:C:165:THR:CG2	1:C:193:HIS:HD2	2.09	0.65
1:D:185:LEU:HD12	1:D:190:GLU:C	2.21	0.65
1:B:213:ARG:HG3	1:B:213:ARG:NH1	2.11	0.64
1:A:293:ILE:CD1	1:A:318:ILE:HG23	2.28	0.64
1:C:293:ILE:CD1	1:C:318:ILE:HG23	2.28	0.64
1:D:293:ILE:CD1	1:D:318:ILE:HG23	2.28	0.64
1:C:279:SER:HB3	1:C:282:ASP:CB	2.28	0.64
1:D:289:THR:HG21	1:D:330:LEU:HA	1.78	0.63
1:A:185:LEU:HD12	1:A:190:GLU:C	2.23	0.63
1:A:289:THR:HG21	1:A:330:LEU:HA	1.81	0.63
1:A:332:ASN:C	1:A:334:ILE:H	2.06	0.63
1:B:216:ASN:O	1:B:220:LEU:HD13	1.98	0.63
1:D:330:LEU:O	1:D:334:ILE:HB	1.98	0.63
1:B:290:GLY:HA3	1:B:326:GLU:OE2	1.99	0.63
1:C:332:ASN:C	1:C:334:ILE:H	2.07	0.63
1:B:293:ILE:CD1	1:B:318:ILE:HG23	2.28	0.63
1:D:279:SER:HB3	1:D:282:ASP:CB	2.29	0.63
1:B:332:ASN:C	1:B:334:ILE:H	2.07	0.62
1:C:185:LEU:HD12	1:C:190:GLU:C	2.24	0.62
1:B:289:THR:O	1:B:326:GLU:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:LEU:HD12	1:D:190:GLU:O	1.99	0.62
1:A:330:LEU:O	1:A:334:ILE:HB	1.99	0.62
1:B:330:LEU:O	1:B:334:ILE:HB	2.00	0.62
1:C:179:ARG:HG3	1:C:179:ARG:NH1	2.07	0.61
1:C:210:GLU:OE1	1:C:231:PRO:HG3	2.00	0.61
1:B:175:VAL:HG11	1:B:198:ILE:HG23	1.82	0.61
1:A:289:THR:O	1:A:326:GLU:HB2	2.00	0.61
1:B:185:LEU:HD12	1:B:190:GLU:C	2.26	0.61
1:C:216:ASN:O	1:C:220:LEU:HD13	2.00	0.61
1:A:290:GLY:HA3	1:A:326:GLU:OE2	2.01	0.61
1:C:213:ARG:HG3	1:C:213:ARG:NH1	2.11	0.61
1:A:246:GLY:O	1:A:250:MET:HG3	2.01	0.60
1:C:273:SER:C	1:C:275:LEU:H	2.08	0.60
1:B:289:THR:HG21	1:B:330:LEU:HA	1.82	0.60
1:C:139:VAL:HG12	1:C:157:ALA:HB1	1.84	0.60
1:A:117:HIS:CE1	1:A:178:ALA:HB2	2.37	0.59
1:A:139:VAL:HG12	1:A:157:ALA:HB1	1.85	0.59
1:D:146:GLU:HG2	1:D:161:HIS:ND1	2.18	0.59
1:C:330:LEU:O	1:C:334:ILE:HB	2.03	0.59
1:A:213:ARG:HG3	1:A:213:ARG:NH1	2.18	0.59
1:A:34:GLY:HA2	1:A:75:PHE:HZ	1.68	0.59
1:C:289:THR:HG21	1:C:330:LEU:HA	1.84	0.59
1:D:332:ASN:C	1:D:334:ILE:H	2.11	0.58
1:A:265:VAL:HG21	1:A:327:ILE:HD12	1.85	0.58
1:B:273:SER:C	1:B:275:LEU:H	2.11	0.58
1:C:233:VAL:HG12	1:C:234:ILE:N	2.18	0.58
1:B:34:GLY:HA2	1:B:75:PHE:HZ	1.68	0.58
1:C:275:LEU:HD12	1:C:334:ILE:HG13	1.86	0.57
1:C:289:THR:O	1:C:326:GLU:HB2	2.05	0.57
1:A:222:MET:HE1	1:C:196:LEU:O	2.03	0.57
1:A:273:SER:C	1:A:275:LEU:H	2.11	0.57
1:A:279:SER:HB3	1:A:282:ASP:CB	2.35	0.57
1:C:117:HIS:CE1	1:C:178:ALA:HB2	2.39	0.57
1:C:183:VAL:HG12	1:C:191:THR:HG23	1.87	0.57
1:A:275:LEU:HA	1:A:278:VAL:HG21	1.85	0.57
1:C:279:SER:HB3	1:C:282:ASP:CG	2.30	0.57
1:D:273:SER:C	1:D:275:LEU:H	2.12	0.57
1:A:280:VAL:HG23	1:A:312:PHE:CZ	2.40	0.57
1:C:273:SER:C	1:C:275:LEU:N	2.61	0.56
1:D:34:GLY:HA2	1:D:75:PHE:HZ	1.69	0.56
1:A:192:ILE:HD12	1:C:193:HIS:ND1	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ASN:O	1:A:220:LEU:HD13	2.05	0.56
1:B:279:SER:HB3	1:B:282:ASP:CB	2.35	0.56
1:B:275:LEU:HA	1:B:278:VAL:HG21	1.87	0.56
1:D:289:THR:O	1:D:326:GLU:HB2	2.06	0.56
1:C:290:GLY:HA3	1:C:326:GLU:OE2	2.06	0.56
1:D:276:GLU:C	1:D:278:VAL:H	2.12	0.56
1:C:53:THR:O	1:C:57:ILE:HG23	2.06	0.56
1:B:166:ARG:HG2	1:B:168:SER:OG	2.06	0.56
1:A:273:SER:C	1:A:275:LEU:N	2.64	0.55
1:D:216:ASN:O	1:D:220:LEU:HD13	2.05	0.55
1:A:275:LEU:HD12	1:A:334:ILE:HG13	1.88	0.55
1:C:131:LEU:HD21	1:C:157:ALA:HB2	1.89	0.55
1:B:275:LEU:HD12	1:B:334:ILE:HG13	1.88	0.55
1:D:210:GLU:OE1	1:D:231:PRO:HG3	2.07	0.55
1:D:290:GLY:HA3	1:D:326:GLU:OE2	2.06	0.55
1:D:273:SER:C	1:D:275:LEU:N	2.65	0.54
1:D:131:LEU:HD21	1:D:157:ALA:HB2	1.90	0.54
1:D:275:LEU:HA	1:D:278:VAL:HG21	1.89	0.54
1:B:293:ILE:HD11	1:B:318:ILE:HG23	1.89	0.54
1:A:309:ASP:O	1:A:309:ASP:OD2	2.27	0.53
1:A:37:GLY:HA3	1:A:75:PHE:CE1	2.44	0.53
1:D:279:SER:HB3	1:D:282:ASP:CG	2.33	0.53
1:C:246:GLY:C	1:C:250:MET:HG3	2.33	0.53
1:A:265:VAL:CG2	1:A:327:ILE:HD12	2.39	0.53
1:B:131:LEU:HD21	1:B:157:ALA:HB2	1.89	0.53
1:B:273:SER:C	1:B:275:LEU:N	2.63	0.53
1:D:309:ASP:O	1:D:309:ASP:OD2	2.27	0.53
1:A:52:TRP:CE2	1:A:56:THR:OG1	2.60	0.53
1:A:131:LEU:HD21	1:A:157:ALA:HB2	1.91	0.53
1:D:175:VAL:HG11	1:D:198:ILE:HG23	1.91	0.52
1:A:279:SER:HB3	1:A:282:ASP:CG	2.34	0.52
1:B:139:VAL:HG12	1:B:157:ALA:HB1	1.90	0.52
1:C:280:VAL:HG23	1:C:312:PHE:CZ	2.45	0.52
1:D:179:ARG:HG3	1:D:179:ARG:NH1	2.09	0.52
1:A:276:GLU:C	1:A:278:VAL:H	2.18	0.52
1:B:37:GLY:HA3	1:B:75:PHE:CE1	2.44	0.52
1:A:166:ARG:HG2	1:A:168:SER:OG	2.10	0.52
1:B:276:GLU:C	1:B:278:VAL:H	2.17	0.52
1:A:212:GLU:HG3	1:A:232:PHE:HE2	1.75	0.52
1:C:265:VAL:HG21	1:C:327:ILE:HD12	1.92	0.52
1:C:309:ASP:O	1:C:309:ASP:OD2	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:VAL:HG21	1:B:327:ILE:HD12	1.92	0.51
1:C:131:LEU:HD11	1:C:157:ALA:HB3	1.92	0.51
1:C:293:ILE:HD11	1:C:318:ILE:HG23	1.92	0.51
1:B:246:GLY:C	1:B:250:MET:HG3	2.35	0.51
1:D:166:ARG:HG2	1:D:168:SER:OG	2.10	0.51
1:C:286:HIS:O	1:C:290:GLY:N	2.37	0.51
1:D:233:VAL:HG12	1:D:234:ILE:N	2.24	0.51
1:B:279:SER:HB3	1:B:282:ASP:CG	2.35	0.51
1:C:185:LEU:HD11	1:C:194:CYS:HB2	1.91	0.51
1:D:181:VAL:HG11	1:D:198:ILE:HD13	1.93	0.51
1:B:269:ILE:CG2	1:B:314:ALA:HA	2.40	0.50
1:D:37:GLY:HA3	1:D:75:PHE:CE1	2.46	0.50
1:D:117:HIS:CE1	1:D:178:ALA:HB2	2.46	0.50
1:C:60:VAL:O	1:D:61:GLY:HA3	2.11	0.50
1:A:167:VAL:HG13	1:A:201:ILE:HD11	1.92	0.50
1:B:265:VAL:CG2	1:B:327:ILE:HD12	2.42	0.50
1:D:246:GLY:C	1:D:250:MET:HG3	2.37	0.50
1:C:275:LEU:HD12	1:C:334:ILE:CG1	2.41	0.50
1:D:275:LEU:HD12	1:D:334:ILE:HG13	1.94	0.50
1:B:179:ARG:CG	1:B:179:ARG:NH1	2.68	0.50
1:B:309:ASP:O	1:B:309:ASP:OD2	2.30	0.49
1:B:131:LEU:HD11	1:B:157:ALA:HB3	1.94	0.49
1:B:280:VAL:HG23	1:B:312:PHE:CZ	2.47	0.49
1:B:185:LEU:HD11	1:B:194:CYS:HB2	1.93	0.49
1:C:267:VAL:O	1:C:318:ILE:HB	2.12	0.49
1:C:298:ARG:CD	1:C:316:ASP:OD1	2.58	0.49
1:D:267:VAL:O	1:D:318:ILE:HB	2.11	0.49
1:A:131:LEU:HD11	1:A:157:ALA:HB3	1.93	0.49
1:A:179:ARG:HG3	1:A:179:ARG:NH1	2.07	0.49
1:A:183:VAL:HG12	1:A:191:THR:HG23	1.93	0.49
1:A:333:TYR:CG	1:A:333:TYR:O	2.65	0.49
1:C:166:ARG:HG2	1:C:168:SER:OG	2.12	0.49
1:D:181:VAL:HG11	1:D:198:ILE:CD1	2.43	0.49
1:D:202:ASP:HB3	1:D:205:VAL:HB	1.93	0.49
1:C:179:ARG:CG	1:C:179:ARG:NH1	2.70	0.49
1:B:212:GLU:HG3	1:B:232:PHE:HE2	1.78	0.48
1:B:266:GLU:HA	1:B:318:ILE:O	2.13	0.48
1:A:175:VAL:CG1	1:A:198:ILE:HG23	2.41	0.48
1:C:175:VAL:CG1	1:C:198:ILE:HG23	2.41	0.48
1:D:212:GLU:HG3	1:D:232:PHE:HE2	1.78	0.48
1:A:246:GLY:C	1:A:250:MET:HG3	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:VAL:HG21	1:D:327:ILE:HD12	1.95	0.48
1:B:294:ILE:HD13	1:B:321:ILE:HD11	1.96	0.48
1:A:267:VAL:O	1:A:318:ILE:HB	2.13	0.48
1:A:293:ILE:HD11	1:A:318:ILE:HG23	1.95	0.48
1:D:266:GLU:HA	1:D:318:ILE:O	2.14	0.48
1:D:280:VAL:HG23	1:D:312:PHE:CZ	2.49	0.48
1:B:288:VAL:HG11	1:B:333:TYR:CE1	2.49	0.48
1:A:298:ARG:CD	1:A:316:ASP:OD1	2.61	0.48
1:B:267:VAL:O	1:B:318:ILE:HB	2.13	0.48
1:C:59:THR:OG1	1:D:59:THR:HB	2.14	0.48
1:D:265:VAL:CG2	1:D:327:ILE:HD12	2.44	0.48
1:A:222:MET:HE1	1:C:200:LYS:N	2.29	0.48
1:A:286:HIS:O	1:A:290:GLY:N	2.39	0.48
1:D:328:GLU:O	1:D:331:LYS:N	2.46	0.48
1:C:265:VAL:CG2	1:C:327:ILE:HD12	2.44	0.47
1:C:288:VAL:HG11	1:C:333:TYR:CE1	2.49	0.47
1:D:183:VAL:HG12	1:D:191:THR:HG23	1.96	0.47
1:A:269:ILE:CG2	1:A:314:ALA:HA	2.43	0.47
1:A:238:LEU:HD22	1:A:249:ALA:HA	1.94	0.47
1:C:59:THR:O	1:D:59:THR:O	2.32	0.47
1:B:175:VAL:CG1	1:B:198:ILE:HG23	2.44	0.47
1:B:183:VAL:HG12	1:B:191:THR:HG23	1.97	0.47
1:B:328:GLU:O	1:B:331:LYS:N	2.48	0.47
1:D:293:ILE:HD11	1:D:318:ILE:HG23	1.95	0.47
1:B:241:ARG:CG	1:B:241:ARG:NH1	2.63	0.47
1:A:222:MET:CE	1:C:196:LEU:O	2.63	0.46
1:B:167:VAL:HG13	1:B:201:ILE:HD11	1.95	0.46
1:A:192:ILE:CD1	1:C:193:HIS:ND1	2.79	0.46
1:C:276:GLU:C	1:C:278:VAL:H	2.24	0.46
1:C:57:ILE:HB	1:C:83:GLY:O	2.15	0.46
1:A:266:GLU:HA	1:A:318:ILE:O	2.14	0.46
1:D:131:LEU:HD11	1:D:157:ALA:HB3	1.97	0.46
1:D:298:ARG:CD	1:D:316:ASP:OD1	2.62	0.46
1:B:121:CYS:HB2	1:B:183:VAL:HG22	1.97	0.46
1:B:333:TYR:CG	1:B:333:TYR:O	2.68	0.46
1:C:212:GLU:HG3	1:C:232:PHE:HE2	1.81	0.46
1:D:280:VAL:HB	1:D:310:TYR:HB3	1.98	0.46
1:B:47:THR:O	1:B:47:THR:HG22	2.15	0.46
1:C:273:SER:O	1:C:275:LEU:N	2.49	0.46
1:D:185:LEU:HD11	1:D:194:CYS:HB2	1.96	0.46
1:D:199:ARG:HH12	1:D:205:VAL:HG12	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:LEU:HD12	1:B:334:ILE:CG1	2.46	0.46
1:D:167:VAL:HG13	1:D:201:ILE:HD11	1.98	0.46
1:A:222:MET:HE1	1:C:200:LYS:H	1.81	0.45
1:C:333:TYR:CG	1:C:333:TYR:O	2.68	0.45
1:D:134:LEU:O	1:D:135:ARG:C	2.59	0.45
1:D:278:VAL:HG12	1:D:279:SER:N	2.30	0.45
1:D:170:LEU:HD23	1:D:170:LEU:HA	1.79	0.45
1:C:275:LEU:HA	1:C:278:VAL:HG21	1.97	0.45
1:A:121:CYS:HB2	1:A:183:VAL:HG22	1.99	0.45
1:A:35:THR:HG23	1:A:49:SER:HB2	1.98	0.45
1:A:241:ARG:CG	1:A:241:ARG:NH1	2.61	0.45
1:B:134:LEU:O	1:B:135:ARG:C	2.58	0.45
1:C:266:GLU:HA	1:C:318:ILE:O	2.17	0.45
1:C:332:ASN:C	1:C:334:ILE:N	2.74	0.45
1:A:185:LEU:HD11	1:A:194:CYS:HB2	1.98	0.45
1:A:288:VAL:HG11	1:A:333:TYR:CE1	2.51	0.45
1:B:332:ASN:C	1:B:334:ILE:N	2.74	0.45
1:D:123:TRP:HE1	1:D:151:LYS:NZ	2.15	0.45
1:A:275:LEU:HD12	1:A:334:ILE:CG1	2.46	0.45
1:B:153:LEU:HD13	1:B:153:LEU:HA	1.72	0.45
1:B:275:LEU:O	1:B:278:VAL:HB	2.16	0.45
1:D:276:GLU:C	1:D:278:VAL:N	2.75	0.45
1:B:123:TRP:HE1	1:B:151:LYS:NZ	2.15	0.45
1:C:167:VAL:HG13	1:C:201:ILE:HD11	1.98	0.45
1:D:286:HIS:O	1:D:290:GLY:N	2.37	0.45
1:A:328:GLU:O	1:A:329:ARG:C	2.58	0.44
1:B:35:THR:HG23	1:B:49:SER:HB2	1.99	0.44
1:C:215:GLU:H	1:C:215:GLU:HG3	1.66	0.44
1:D:215:GLU:H	1:D:215:GLU:HG3	1.65	0.44
1:B:117:HIS:CE1	1:B:178:ALA:CB	2.98	0.44
1:B:233:VAL:HG12	1:B:234:ILE:N	2.30	0.44
1:C:283:ALA:O	1:C:284:ASP:C	2.61	0.44
1:D:139:VAL:HG12	1:D:157:ALA:HB1	1.99	0.44
1:B:141:VAL:HB	1:B:152:VAL:HG11	1.98	0.44
1:C:328:GLU:O	1:C:329:ARG:C	2.60	0.44
1:B:63:GLY:C	1:B:65:TYR:H	2.25	0.44
1:C:199:ARG:HH12	1:C:205:VAL:HG12	1.82	0.44
1:C:202:ASP:HB3	1:C:205:VAL:HB	1.99	0.44
1:D:241:ARG:CG	1:D:241:ARG:NH1	2.63	0.44
1:C:35:THR:HG23	1:C:49:SER:HB2	2.00	0.44
1:D:116:ARG:O	1:D:179:ARG:NH1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:PRO:HA	1:A:73:MET:HB2	1.99	0.44
1:B:298:ARG:CD	1:B:316:ASP:OD1	2.62	0.44
1:D:269:ILE:CG2	1:D:314:ALA:HA	2.43	0.43
1:B:195:ILE:HD13	1:B:225:ALA:HB2	2.00	0.43
1:C:131:LEU:HD11	1:C:157:ALA:CB	2.48	0.43
1:C:293:ILE:HD13	1:C:293:ILE:HA	1.84	0.43
1:A:123:TRP:HE1	1:A:151:LYS:NZ	2.16	0.43
1:B:202:ASP:HB3	1:B:205:VAL:HB	2.00	0.43
1:C:170:LEU:HD23	1:C:170:LEU:HA	1.72	0.43
1:C:165:THR:CB	1:C:193:HIS:CD2	2.56	0.43
1:A:134:LEU:O	1:A:135:ARG:C	2.58	0.43
1:A:199:ARG:HH12	1:A:205:VAL:HG12	1.84	0.43
1:D:200:LYS:O	1:D:200:LYS:CG	2.66	0.43
1:D:275:LEU:HD12	1:D:334:ILE:CG1	2.49	0.43
1:B:215:GLU:H	1:B:215:GLU:HG3	1.64	0.43
1:D:281:LEU:HB3	1:D:308:ARG:O	2.19	0.43
1:A:275:LEU:O	1:A:278:VAL:HB	2.19	0.43
1:B:332:ASN:O	1:B:334:ILE:N	2.52	0.43
1:B:35:THR:HG22	1:B:35:THR:O	2.18	0.43
1:D:333:TYR:O	1:D:333:TYR:CG	2.72	0.43
1:B:328:GLU:O	1:B:329:ARG:C	2.62	0.43
1:D:176:ARG:NH2	1:D:201:ILE:HG23	2.34	0.43
1:A:195:ILE:HD13	1:A:225:ALA:HB2	2.01	0.42
1:D:276:GLU:O	1:D:278:VAL:N	2.52	0.42
1:A:153:LEU:HA	1:A:153:LEU:HD13	1.72	0.42
1:C:153:LEU:HD13	1:C:153:LEU:HA	1.73	0.42
1:C:238:LEU:HD22	1:C:249:ALA:HA	2.00	0.42
1:A:328:GLU:O	1:A:331:LYS:N	2.52	0.42
1:B:273:SER:O	1:B:275:LEU:N	2.52	0.42
1:B:283:ALA:O	1:B:284:ASP:C	2.62	0.42
1:C:269:ILE:CG2	1:C:314:ALA:HA	2.44	0.42
1:C:294:ILE:HD13	1:C:321:ILE:HD11	2.02	0.42
1:B:176:ARG:HA	1:B:202:ASP:HB2	2.02	0.42
1:D:63:GLY:C	1:D:65:TYR:H	2.27	0.42
1:A:34:GLY:HA2	1:A:75:PHE:CZ	2.53	0.42
1:A:63:GLY:C	1:A:65:TYR:H	2.27	0.42
1:B:127:THR:CG2	1:B:184:ASP:HB3	2.50	0.42
1:C:63:GLY:C	1:C:65:TYR:H	2.27	0.42
1:A:296:VAL:CG1	1:A:306:PRO:HG3	2.50	0.42
1:C:123:TRP:HE1	1:C:151:LYS:NZ	2.17	0.42
1:C:328:GLU:O	1:C:331:LYS:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:GLN:HA	1:D:222:MET:HB2	2.02	0.42
1:C:280:VAL:HB	1:C:310:TYR:HB3	2.00	0.42
1:A:281:LEU:HB3	1:A:308:ARG:O	2.20	0.41
1:A:86:THR:O	1:A:90:ALA:HB3	2.21	0.41
1:A:202:ASP:HB3	1:A:205:VAL:HB	2.02	0.41
1:A:283:ALA:O	1:A:284:ASP:C	2.62	0.41
1:B:285:ILE:O	1:B:289:THR:OG1	2.35	0.41
1:C:142:LEU:HD12	1:C:160:VAL:O	2.20	0.41
1:A:35:THR:O	1:A:35:THR:HG22	2.20	0.41
1:A:53:THR:HG23	1:A:79:LEU:HD21	2.02	0.41
1:A:141:VAL:HB	1:A:152:VAL:HG11	2.01	0.41
1:A:215:GLU:H	1:A:215:GLU:HG3	1.66	0.41
1:A:275:LEU:C	1:A:278:VAL:HG23	2.45	0.41
1:D:176:ARG:HA	1:D:202:ASP:HB2	2.02	0.41
1:A:273:SER:O	1:A:275:LEU:N	2.53	0.41
1:D:293:ILE:HD13	1:D:293:ILE:HA	1.87	0.41
1:D:328:GLU:O	1:D:329:ARG:C	2.63	0.41
1:C:116:ARG:O	1:C:179:ARG:NH1	2.54	0.41
1:D:332:ASN:C	1:D:334:ILE:N	2.78	0.41
1:A:27:VAL:O	1:A:31:ILE:HG13	2.21	0.41
1:A:131:LEU:HA	1:A:131:LEU:HD23	1.84	0.41
1:A:196:LEU:O	1:C:222:MET:HE1	2.20	0.41
1:A:285:ILE:O	1:A:289:THR:OG1	2.35	0.41
1:B:116:ARG:O	1:B:179:ARG:NH1	2.54	0.41
1:B:188:ASP:OD2	1:B:216:ASN:OD1	2.38	0.41
1:B:238:LEU:HD22	1:B:249:ALA:HA	2.03	0.41
1:C:165:THR:CG2	1:C:193:HIS:CD2	2.97	0.41
1:D:131:LEU:HD11	1:D:157:ALA:CB	2.51	0.41
1:D:131:LEU:HA	1:D:131:LEU:HD23	1.80	0.41
1:D:288:VAL:HG11	1:D:333:TYR:CE1	2.55	0.41
1:B:280:VAL:HB	1:B:310:TYR:HB3	2.02	0.41
1:C:116:ARG:HD2	1:C:116:ARG:HA	1.84	0.41
1:A:34:GLY:HA3	1:A:79:LEU:HD21	2.02	0.40
1:A:131:LEU:HD11	1:A:157:ALA:CB	2.50	0.40
1:A:276:GLU:C	1:A:278:VAL:N	2.80	0.40
1:B:34:GLY:HA2	1:B:75:PHE:CZ	2.53	0.40
1:B:216:ASN:HA	1:B:219:GLN:OE1	2.21	0.40
1:C:256:LEU:HD23	1:C:256:LEU:HA	1.73	0.40
1:A:116:ARG:HD2	1:A:116:ARG:HA	1.82	0.40
1:A:296:VAL:HG12	1:A:306:PRO:HG3	2.02	0.40
1:A:264:MET:HE3	1:A:319:LEU:HD21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ASP:OD2	1:A:216:ASN:OD1	2.40	0.40
1:C:35:THR:O	1:C:35:THR:HG22	2.21	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:D:204:SER:OG	1:D:309:ASP:O[12_555]	1.95	0.25

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	285/340 (84%)	253 (89%)	26 (9%)	6 (2%)	5	24
1	B	277/340 (82%)	244 (88%)	27 (10%)	6 (2%)	5	24
1	C	282/340 (83%)	250 (89%)	26 (9%)	6 (2%)	5	24
1	D	281/340 (83%)	246 (88%)	27 (10%)	8 (3%)	4	19
All	All	1125/1360 (83%)	993 (88%)	106 (9%)	26 (2%)	5	23

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	TYR
1	A	277	GLY
1	B	65	TYR
1	B	277	GLY
1	B	333	TYR
1	B	335	SER
1	C	65	TYR
1	C	277	GLY

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Mol	Chain	Res	Type
1	C	333	TYR
1	C	335	SER
1	D	65	TYR
1	D	277	GLY
1	D	333	TYR
1	A	274	LYS
1	A	333	TYR
1	A	335	SER
1	B	274	LYS
1	C	274	LYS
1	D	274	LYS
1	D	335	SER
1	A	312	PHE
1	B	312	PHE
1	D	27	VAL
1	D	200	LYS
1	C	312	PHE
1	D	312	PHE

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	201/291 (69%)	172 (86%)	29 (14%)	3	13
1	B	194/291 (67%)	169 (87%)	25 (13%)	4	16
1	C	191/291 (66%)	167 (87%)	24 (13%)	4	18
1	D	190/291 (65%)	165 (87%)	25 (13%)	4	16
All	All	776/1164 (67%)	673 (87%)	103 (13%)	4	15

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	MET
1	A	74	TYR
1	A	127	THR

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Mol	Chain	Res	Type
1	A	131	LEU
1	A	146	GLU
1	A	148	VAL
1	A	151	LYS
1	A	153	LEU
1	A	179	ARG
1	A	212	GLU
1	A	215	GLU
1	A	216	ASN
1	A	222	MET
1	A	230	SER
1	A	233	VAL
1	A	240	SER
1	A	241	ARG
1	A	245	ASP
1	A	253	GLN
1	A	255	VAL
1	A	274	LYS
1	A	280	VAL
1	A	281	LEU
1	A	284	ASP
1	A	292	ILE
1	A	296	VAL
1	A	302	LEU
1	A	318	ILE
1	A	334	ILE
1	B	127	THR
1	B	131	LEU
1	B	146	GLU
1	B	148	VAL
1	B	153	LEU
1	B	179	ARG
1	B	212	GLU
1	B	215	GLU
1	B	216	ASN
1	B	222	MET
1	B	230	SER
1	B	233	VAL
1	B	240	SER
1	B	241	ARG
1	B	253	GLN
1	B	255	VAL

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Mol	Chain	Res	Type
1	B	274	LYS
1	B	280	VAL
1	B	281	LEU
1	B	284	ASP
1	B	292	ILE
1	B	296	VAL
1	B	302	LEU
1	B	318	ILE
1	B	334	ILE
1	C	127	THR
1	C	131	LEU
1	C	146	GLU
1	C	148	VAL
1	C	153	LEU
1	C	179	ARG
1	C	212	GLU
1	C	215	GLU
1	C	216	ASN
1	C	222	MET
1	C	230	SER
1	C	233	VAL
1	C	240	SER
1	C	241	ARG
1	C	253	GLN
1	C	255	VAL
1	C	280	VAL
1	C	281	LEU
1	C	284	ASP
1	C	292	ILE
1	C	296	VAL
1	C	302	LEU
1	C	318	ILE
1	C	334	ILE
1	D	127	THR
1	D	131	LEU
1	D	146	GLU
1	D	148	VAL
1	D	153	LEU
1	D	179	ARG
1	D	212	GLU
1	D	215	GLU
1	D	216	ASN

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Mol	Chain	Res	Type
1	D	222	MET
1	D	230	SER
1	D	233	VAL
1	D	240	SER
1	D	241	ARG
1	D	253	GLN
1	D	255	VAL
1	D	274	LYS
1	D	280	VAL
1	D	281	LEU
1	D	284	ASP
1	D	292	ILE
1	D	296	VAL
1	D	302	LEU
1	D	318	ILE
1	D	334	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	ASN
1	A	193	HIS
1	B	117	HIS
1	B	147	ASN
1	B	193	HIS
1	C	147	ASN
1	D	147	ASN
1	D	193	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 12 ligands modelled in this entry, 12 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	289/340 (85%)	0.93	43 (14%) 5 7	47, 111, 252, 252	0
1	B	281/340 (82%)	0.78	42 (14%) 5 7	40, 107, 252, 264	0
1	C	286/340 (84%)	0.62	35 (12%) 8 9	48, 97, 252, 257	0
1	D	285/340 (83%)	0.61	26 (9%) 15 14	43, 86, 252, 252	0
All	All	1141/1360 (83%)	0.74	146 (12%) 7 9	40, 100, 252, 264	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	65	TYR	9.1
1	C	64	ASP	7.5
1	C	333	TYR	6.9
1	D	259	GLU	6.7
1	B	27	VAL	5.6
1	B	43	GLY	5.2
1	D	51	TYR	4.9
1	A	66	SER	4.9
1	B	62	TYR	4.7
1	A	263	ARG	4.7
1	D	54	PHE	4.5
1	C	336	ALA	4.5
1	B	82	LEU	4.4
1	A	89	VAL	4.4
1	B	247	TYR	4.3
1	B	64	ASP	4.3
1	A	322	GLY	4.3
1	C	26	LEU	4.2
1	B	138	GLU	4.2
1	B	54	PHE	4.1
1	A	62	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	215	GLU	4.0
1	D	57	ILE	3.9
1	C	90	ALA	3.9
1	A	88	ALA	3.9
1	B	52	TRP	3.9
1	D	68	SER	3.8
1	C	259	GLU	3.8
1	C	77	VAL	3.7
1	A	336	ALA	3.7
1	D	58	ALA	3.7
1	C	230	SER	3.7
1	A	319	LEU	3.7
1	B	116	ARG	3.6
1	B	67	PRO	3.6
1	B	140	PHE	3.6
1	B	147	ASN	3.6
1	A	259	GLU	3.6
1	B	51	TYR	3.6
1	C	275	LEU	3.6
1	C	76	THR	3.5
1	A	261	THR	3.5
1	A	223	ALA	3.3
1	C	260	SER	3.3
1	C	288	VAL	3.3
1	A	228	VAL	3.3
1	A	64	ASP	3.2
1	D	31	ILE	3.2
1	A	42	GLU	3.2
1	B	131	LEU	3.2
1	B	151	LYS	3.2
1	B	139	VAL	3.2
1	B	69	THR	3.2
1	C	258	GLU	3.2
1	B	152	VAL	3.2
1	C	66	SER	3.2
1	A	218	GLU	3.1
1	D	30	VAL	3.1
1	A	227	GLN	3.1
1	B	66	SER	3.1
1	A	255	VAL	3.1
1	B	81	VAL	3.1
1	B	310	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	300	ASP	3.1
1	B	325	GLU	3.0
1	B	73	MET	3.0
1	A	51	TYR	3.0
1	A	41	ILE	3.0
1	A	47	THR	3.0
1	A	317	ILE	3.0
1	C	80	ILE	3.0
1	A	302	LEU	2.9
1	A	46	TRP	2.9
1	C	81	VAL	2.9
1	C	269	ILE	2.9
1	A	85	ALA	2.9
1	A	225	ALA	2.9
1	B	186	GLU	2.9
1	A	221	ARG	2.9
1	B	127	THR	2.9
1	D	67	PRO	2.8
1	B	258	GLU	2.8
1	C	272	GLY	2.8
1	A	68	SER	2.8
1	D	335	SER	2.8
1	A	252	VAL	2.8
1	C	36	ALA	2.8
1	B	74	TYR	2.8
1	C	56	THR	2.7
1	A	82	LEU	2.7
1	D	64	ASP	2.7
1	B	118	VAL	2.7
1	C	47	THR	2.7
1	D	261	THR	2.7
1	A	324	PRO	2.6
1	C	278	VAL	2.6
1	C	79	LEU	2.6
1	B	148	VAL	2.6
1	D	56	THR	2.6
1	A	272	GLY	2.5
1	B	68	SER	2.5
1	B	242	SER	2.5
1	B	84	ILE	2.5
1	B	29	ALA	2.5
1	B	46	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	52	TRP	2.5
1	C	40	PHE	2.4
1	B	70	PRO	2.4
1	D	37	GLY	2.4
1	B	218	GLU	2.4
1	B	85	ALA	2.4
1	A	67	PRO	2.4
1	A	116	ARG	2.3
1	C	75	PHE	2.3
1	D	298	ARG	2.3
1	C	204	SER	2.3
1	A	318	ILE	2.3
1	B	56	THR	2.3
1	A	249	ALA	2.3
1	C	271	GLU	2.2
1	C	68	SER	2.2
1	D	66	SER	2.2
1	D	323	LYS	2.2
1	B	58	ALA	2.2
1	B	123	TRP	2.2
1	D	47	THR	2.2
1	D	280	VAL	2.2
1	A	325	GLU	2.2
1	D	271	GLU	2.2
1	C	62	TYR	2.2
1	B	134	LEU	2.2
1	D	50	LEU	2.2
1	A	271	GLU	2.2
1	C	223	ALA	2.2
1	D	325	GLU	2.2
1	C	46	TRP	2.2
1	A	260	SER	2.1
1	A	264	MET	2.1
1	A	70	PRO	2.1
1	A	321	ILE	2.1
1	A	214	TYR	2.1
1	D	213	ARG	2.1
1	C	48	VAL	2.0
1	D	87	PHE	2.0
1	D	135	ARG	2.0
1	D	317	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($\text{\AA}^2$)	Q<0.9
2	CA	D	342	1/1	0.69	0.14	60,60,60,60	0
2	CA	D	341	1/1	0.82	0.08	60,60,60,60	0
2	CA	A	342	1/1	0.85	0.11	60,60,60,60	0
2	CA	B	341	1/1	0.86	0.09	60,60,60,60	0
2	CA	B	342	1/1	0.86	0.09	60,60,60,60	0
2	CA	C	342	1/1	0.87	0.10	60,60,60,60	0
2	CA	A	341	1/1	0.90	0.07	60,60,60,60	0
2	CA	B	343	1/1	0.91	0.09	60,60,60,60	0
2	CA	C	341	1/1	0.93	0.06	60,60,60,60	0
2	CA	D	343	1/1	0.95	0.05	60,60,60,60	0
2	CA	C	343	1/1	0.97	0.03	60,60,60,60	0
2	CA	A	343	1/1	0.98	0.04	60,60,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.