



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:43 PM UTC

PDB ID : 2VMK / pdb_00002vmk
Title : Crystal Structure of E. coli RNase E Apoprotein - Catalytic Domain
Authors : Koslover, D.J.; Callaghan, A.J.; Marcaida, M.J.; Martick, M.; Scott, W.G.;
Luisi, B.F.
Deposited on : 2008-01-28
Resolution : 3.30 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)
Xtrriage (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

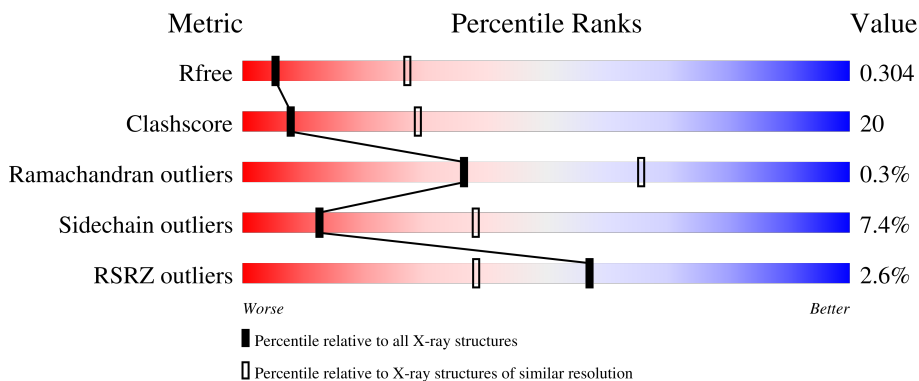
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	515	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 65%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 24%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">2% 65% 24% 5% • 5%</p>
1	B	515	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 63%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 27%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">3% 63% 27% 5% • •</p>
1	C	515	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 60%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 25%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">4% 60% 25% 7% 8%</p>
1	D	515	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 63%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 24%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">% 63% 24% • • 8%</p>

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	SO4	A	1509	-	-	X	-
2	SO4	C	1507	-	-	X	-

2 Entry composition [i](#)

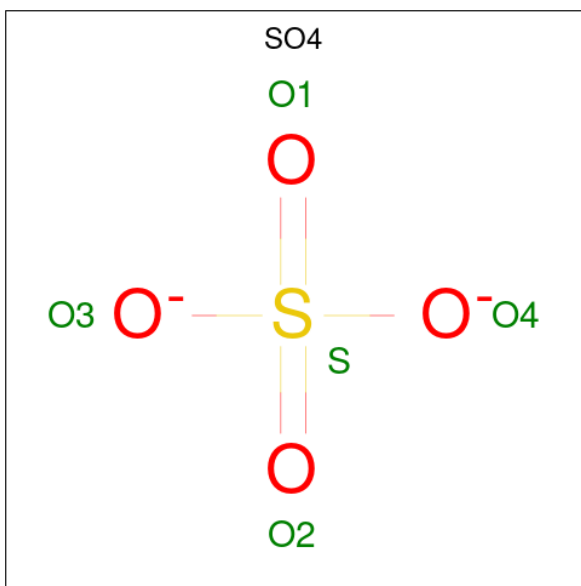
There are 3 unique types of molecules in this entry. The entry contains 14187 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RIBONUCLEASE E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	489	Total 3507	C 2207	N 621	O 669	S 10	0	0	0
1	B	495	Total 3653	C 2303	N 657	O 681	S 12	0	0	0
1	C	474	Total 3507	C 2198	N 633	O 665	S 11	0	0	0
1	D	472	Total 3503	C 2210	N 626	O 655	S 12	0	0	0

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	73.24Å 75.57Å 109.37Å 94.95° 102.03° 91.77°	Depositor
Resolution (Å)	47.84 – 3.30 47.84 – 3.30	Depositor EDS
% Data completeness (in resolution range)	96.9 (47.84-3.30) 96.9 (47.84-3.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 3.32Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.267 , 0.293 0.275 , 0.304	Depositor DCC
R_{free} test set	1664 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	96.3	Xtrriage
Anisotropy	0.100	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 75.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	14187	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ZN

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	1.40	28/3560 (0.8%)	0.84	9/4859 (0.2%)
1	B	1.35	26/3711 (0.7%)	0.80	3/5048 (0.1%)
1	C	1.58	51/3558 (1.4%)	0.84	7/4835 (0.1%)
1	D	1.20	19/3553 (0.5%)	0.76	4/4828 (0.1%)
All	All	1.39	124/14382 (0.9%)	0.81	23/19570 (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	A	0	13
1	B	1	6
1	C	0	13
1	D	0	6
All	All	1	38

All (124) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	140	SER	CA-CB	-11.22	1.34	1.53
1	B	307	ALA	C-O	-10.02	1.11	1.24
1	C	342	LEU	CG-CD1	-9.99	1.19	1.52
1	B	342	LEU	CG-CD1	-9.68	1.20	1.52
1	A	342	LEU	CG-CD1	-9.27	1.22	1.52
1	C	298	ALA	CA-CB	-9.25	1.38	1.53
1	D	342	LEU	CG-CD2	-9.07	1.22	1.52
1	B	229	ILE	CA-CB	8.75	1.63	1.53
1	A	95	ARG	CZ-NH1	8.73	1.45	1.32
1	A	140	SER	CA-CB	-8.65	1.39	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	342	LEU	CG-CD1	-8.35	1.25	1.52
1	D	38	LYS	C-O	-8.18	1.14	1.23
1	A	307	ALA	C-O	-8.17	1.14	1.24
1	C	339	LEU	C-O	8.09	1.33	1.23
1	C	95	ARG	NE-CZ	8.02	1.41	1.33
1	B	141	ARG	N-CA	-7.66	1.36	1.46
1	A	38	LYS	C-O	-7.52	1.14	1.23
1	A	321	ASN	CG-OD1	-7.29	1.09	1.23
1	D	474	VAL	CB-CG2	-7.19	1.28	1.52
1	D	77	TYR	CG-CD1	-7.12	1.24	1.39
1	A	342	LEU	CG-CD2	-7.02	1.29	1.52
1	B	342	LEU	CA-C	7.00	1.61	1.52
1	A	439	VAL	CB-CG1	-6.97	1.29	1.52
1	A	117	THR	CB-CG2	-6.96	1.29	1.52
1	C	258	LEU	CG-CD2	-6.87	1.29	1.52
1	C	363	LEU	C-O	-6.84	1.16	1.24
1	B	38	LYS	C-O	-6.83	1.15	1.23
1	C	41	ILE	CA-CB	6.83	1.62	1.54
1	C	247	LEU	CG-CD1	-6.82	1.30	1.52
1	A	439	VAL	CB-CG2	-6.82	1.30	1.52
1	A	102	VAL	CA-CB	6.77	1.64	1.54
1	B	485	HIS	CA-CB	-6.73	1.41	1.53
1	D	474	VAL	CB-CG1	-6.70	1.30	1.52
1	C	367	VAL	CA-CB	6.66	1.62	1.54
1	A	321	ASN	CG-ND2	-6.62	1.19	1.33
1	C	372	ALA	CA-CB	-6.58	1.43	1.53
1	A	280	GLN	C-O	-6.57	1.16	1.23
1	D	77	TYR	CG-CD2	-6.57	1.25	1.39
1	C	226	ILE	N-CA	-6.52	1.38	1.46
1	C	77	TYR	CG-CD2	-6.40	1.25	1.39
1	C	77	TYR	CG-CD1	-6.39	1.25	1.39
1	A	140	SER	N-CA	-6.36	1.37	1.45
1	D	367	VAL	CB-CG1	-6.34	1.31	1.52
1	C	342	LEU	CG-CD2	-6.33	1.31	1.52
1	C	274	GLN	CG-CD	-6.28	1.36	1.52
1	C	336	LEU	N-CA	6.22	1.54	1.46
1	C	301	ALA	CA-CB	-6.20	1.45	1.53
1	B	330	ILE	C-O	6.18	1.31	1.24
1	C	359	VAL	C-O	-6.18	1.16	1.24
1	A	77	TYR	CG-CD1	-6.15	1.26	1.39
1	C	19	VAL	C-O	-6.11	1.17	1.24
1	C	247	LEU	CG-CD2	-6.10	1.32	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	77	TYR	CE1-CZ	-6.01	1.23	1.38
1	C	437	GLN	CA-C	6.00	1.60	1.53
1	D	378	HIS	CA-C	-5.97	1.44	1.53
1	C	330	ILE	C-O	-5.94	1.17	1.24
1	B	136	ALA	C-O	-5.88	1.15	1.23
1	C	20	ASP	C-O	5.88	1.30	1.24
1	A	139	ILE	C-N	-5.86	1.25	1.33
1	D	485	HIS	CA-C	-5.85	1.45	1.52
1	C	368	ARG	N-CA	5.84	1.53	1.46
1	C	205	PHE	N-CA	5.84	1.53	1.45
1	B	139	ILE	C-O	-5.84	1.16	1.24
1	C	362	ARG	C-O	-5.82	1.17	1.24
1	B	27	LEU	C-O	-5.80	1.17	1.23
1	D	485	HIS	CA-CB	-5.78	1.43	1.53
1	A	464	THR	CB-CG2	-5.78	1.33	1.52
1	B	331	ALA	C-O	5.77	1.30	1.24
1	C	95	ARG	CD-NE	5.76	1.54	1.46
1	C	481	THR	CA-CB	5.72	1.62	1.53
1	A	139	ILE	C-O	-5.70	1.16	1.23
1	A	77	TYR	CG-CD2	-5.68	1.27	1.39
1	D	213	VAL	N-CA	5.68	1.53	1.46
1	D	77	TYR	CE2-CZ	-5.66	1.24	1.38
1	A	247	LEU	CG-CD2	-5.64	1.33	1.52
1	A	258	LEU	CG-CD2	-5.61	1.34	1.52
1	C	278	ALA	CA-CB	5.61	1.63	1.53
1	A	256	ILE	C-O	-5.58	1.18	1.24
1	C	3	ARG	C-O	5.58	1.31	1.23
1	A	77	TYR	CE2-CZ	-5.57	1.24	1.38
1	C	77	TYR	CE2-CZ	-5.55	1.25	1.38
1	C	24	LEU	N-CA	-5.55	1.39	1.46
1	C	77	TYR	CE1-CZ	-5.54	1.25	1.38
1	C	445	VAL	CA-C	5.53	1.57	1.52
1	B	1	MET	SD-CE	5.46	1.93	1.79
1	C	349	ASP	CG-OD1	-5.44	1.15	1.25
1	B	247	LEU	CG-CD1	-5.43	1.34	1.52
1	C	333	GLN	C-O	-5.43	1.17	1.24
1	B	298	ALA	CA-CB	5.41	1.62	1.53
1	D	100	VAL	CB-CG2	-5.39	1.34	1.52
1	A	15	ARG	C-O	-5.39	1.17	1.24
1	D	100	VAL	CB-CG1	-5.39	1.34	1.52
1	D	399	SER	N-CA	5.39	1.53	1.45
1	B	139	ILE	C-N	-5.38	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1	MET	CG-SD	-5.37	1.67	1.80
1	C	362	ARG	NE-CZ	5.37	1.39	1.33
1	A	95	ARG	CZ-NH2	5.36	1.40	1.33
1	C	23	ARG	C-O	-5.36	1.17	1.23
1	B	205	PHE	N-CA	5.34	1.52	1.45
1	C	362	ARG	CZ-NH1	5.33	1.40	1.32
1	A	247	LEU	CG-CD1	-5.33	1.34	1.52
1	C	295	SER	CA-C	-5.30	1.46	1.52
1	B	16	VAL	CA-CB	5.29	1.61	1.54
1	C	237	LEU	CG-CD2	-5.29	1.35	1.52
1	C	273	SER	C-O	-5.27	1.17	1.24
1	C	203	ALA	C-N	5.20	1.38	1.33
1	A	331	ALA	CA-CB	-5.19	1.45	1.53
1	C	368	ARG	CA-CB	5.19	1.61	1.53
1	B	333	GLN	C-O	5.15	1.30	1.24
1	C	474	VAL	CA-CB	5.15	1.60	1.54
1	B	419	LEU	C-O	-5.15	1.18	1.24
1	B	203	ALA	CA-C	5.15	1.59	1.52
1	B	342	LEU	CG-CD2	-5.12	1.35	1.52
1	C	204	PRO	N-CA	5.11	1.53	1.47
1	B	140	SER	N-CA	-5.11	1.39	1.45
1	D	213	VAL	CA-CB	5.10	1.62	1.54
1	C	379	ILE	N-CA	-5.09	1.40	1.46
1	C	337	ARG	N-CA	5.08	1.52	1.46
1	C	4	MET	C-O	-5.04	1.18	1.24
1	D	247	LEU	CG-CD2	-5.03	1.35	1.52
1	B	326	ALA	C-O	5.03	1.29	1.24
1	A	205	PHE	N-CA	5.03	1.51	1.45
1	C	225	ASP	CA-C	5.03	1.60	1.52
1	C	318	THR	C-O	-5.02	1.18	1.24

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	119	PHE	N-CA-C	-8.20	97.53	109.59
1	A	393	SER	CA-C-N	8.19	130.08	119.84
1	A	393	SER	C-N-CA	8.19	130.08	119.84
1	B	205	PHE	N-CA-C	6.39	118.78	110.53
1	A	24	LEU	N-CA-C	-6.21	100.98	110.30
1	C	205	PHE	N-CA-C	6.19	118.51	110.53
1	A	24	LEU	CB-CA-C	6.01	118.41	110.06
1	C	474	VAL	N-CA-C	5.96	114.53	107.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	ARG	CA-C-N	5.81	130.50	121.26
1	A	23	ARG	C-N-CA	5.81	130.50	121.26
1	C	299	LEU	N-CA-C	5.74	116.66	108.74
1	D	408	SER	N-CA-C	-5.71	106.53	112.93
1	C	119	PHE	CB-CA-C	5.62	118.69	110.26
1	A	393	SER	N-CA-C	5.44	118.13	109.64
1	D	233	ASN	CA-C-N	5.39	124.58	118.97
1	D	233	ASN	C-N-CA	5.39	124.58	118.97
1	A	233	ASN	CA-C-N	5.36	124.55	118.97
1	A	233	ASN	C-N-CA	5.36	124.55	118.97
1	B	474	VAL	N-CA-C	5.36	113.84	107.73
1	B	307	ALA	N-CA-C	5.29	122.07	110.80
1	D	205	PHE	N-CA-C	5.22	117.27	110.53
1	C	369	GLN	N-CA-C	5.10	117.57	111.71
1	C	204	PRO	N-CA-C	5.09	120.71	114.35

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	412	THR	CB

All (38) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	GLN	Mainchain
1	A	140	SER	Mainchain
1	A	202	PRO	Peptide
1	A	210	GLU	Peptide
1	A	212	ASN	Peptide
1	A	23	ARG	Peptide
1	A	243	HIS	Sidechain
1	A	29	ILE	Peptide
1	A	30	GLU	Peptide
1	A	393	SER	Mainchain
1	A	42	TYR	Peptide
1	A	480	GLU	Peptide
1	A	9	THR	Mainchain
1	B	140	SER	Mainchain
1	B	20	ASP	Peptide
1	B	202	PRO	Peptide
1	B	21	GLY	Peptide
1	B	211	SER	Peptide

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Mol	Chain	Res	Type	Group
1	B	480	GLU	Peptide
1	C	139	ILE	Peptide
1	C	202	PRO	Peptide
1	C	210	GLU	Peptide
1	C	212	ASN	Peptide
1	C	243	HIS	Sidechain
1	C	284	ARG	Sidechain
1	C	29	ILE	Mainchain
1	C	30	GLU	Mainchain
1	C	354	ARG	Mainchain
1	C	37	LYS	Peptide
1	C	378	HIS	Mainchain
1	C	405	PRO	Peptide
1	C	480	GLU	Peptide
1	D	118	THR	Peptide
1	D	136	ALA	Peptide
1	D	202	PRO	Peptide
1	D	212	ASN	Mainchain
1	D	480	GLU	Peptide
1	D	78	PHE	Sidechain

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	3507	0	3268	141	1
1	B	3653	0	3525	163	0
1	C	3507	0	3350	142	3
1	D	3503	0	3359	145	0
2	A	5	0	0	4	0
2	B	5	0	0	1	0
2	C	5	0	0	3	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
All	All	14187	0	13502	546	3

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 20.

All (546) 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:23:ARG:NH2	1:C:332:ARG:HG2	1.36	1.41
1:B:14:LEU:HD23	1:B:213:VAL:CG1	1.59	1.32
1:D:128:VAL:O	1:D:166:LEU:HD12	1.28	1.32
1:D:14:LEU:HD23	1:D:213:VAL:CG1	1.66	1.24
1:B:391:ARG:NH1	1:B:397:GLY:HA2	1.54	1.21
1:C:209:GLN:HG2	1:C:212:ASN:ND2	1.56	1.19
1:B:485:HIS:HD2	1:B:487:LEU:HD11	1.04	1.18
1:B:391:ARG:HH11	1:B:397:GLY:HA2	0.99	1.16
1:C:222:LEU:O	1:C:223:ARG:HG3	1.45	1.15
1:D:14:LEU:HD23	1:D:213:VAL:HG11	1.25	1.14
1:D:169:ARG:HG2	1:D:169:ARG:HH11	1.07	1.13
1:C:209:GLN:CG	1:C:212:ASN:HD22	1.62	1.13
1:A:231:ILE:HD12	1:A:237:LEU:HD12	1.23	1.12
1:B:391:ARG:HH11	1:B:397:GLY:CA	1.66	1.08
1:B:78:PHE:HE2	1:B:93:VAL:HG11	1.04	1.07
1:B:485:HIS:CD2	1:B:487:LEU:HD11	1.90	1.04
1:B:485:HIS:HD2	1:B:487:LEU:CD1	1.69	1.04
1:C:23:ARG:NH2	1:C:332:ARG:CG	2.21	1.04
1:B:209:GLN:HG2	1:B:212:ASN:OD1	1.59	1.03
1:B:78:PHE:CE2	1:B:93:VAL:HG11	1.95	1.01
1:D:128:VAL:C	1:D:166:LEU:CD1	2.33	1.01
1:C:25:TYR:HB2	1:C:335:ARG:HH21	1.21	1.00
1:D:231:ILE:HD12	1:D:237:LEU:HD12	1.39	0.99
1:B:14:LEU:HD23	1:B:213:VAL:HG11	1.00	0.99
1:B:166:LEU:HD21	1:B:184:LEU:HD13	1.41	0.99
1:A:5:LEU:HD22	1:A:265:LEU:HD11	1.44	0.98
1:B:78:PHE:HE2	1:B:93:VAL:CG1	1.75	0.98
1:D:128:VAL:O	1:D:166:LEU:CD1	2.11	0.97
1:B:3:ARG:NE	1:B:228:GLU:OE2	1.98	0.95
1:B:14:LEU:CD2	1:B:213:VAL:HG11	1.96	0.95
1:B:34:HIS:CE1	1:B:36:GLN:HB2	2.01	0.95
1:C:173:VAL:HG11	1:C:373:ARG:HG2	1.49	0.94
1:A:78:PHE:HE2	1:A:93:VAL:HG11	1.32	0.94
1:D:129:LEU:HA	1:D:166:LEU:HD13	1.50	0.94
1:C:272:GLU:HB3	1:D:429:GLU:CD	1.93	0.94
1:D:128:VAL:C	1:D:166:LEU:HD12	1.93	0.93
1:B:14:LEU:CD2	1:B:213:VAL:CG1	2.47	0.93
1:D:169:ARG:HH11	1:D:169:ARG:CG	1.81	0.93
1:A:78:PHE:CE2	1:A:93:VAL:HG11	2.04	0.92
1:A:99:GLU:HG2	1:A:203:ALA:HB2	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:PHE:CE2	1:B:93:VAL:CG1	2.55	0.90
1:A:273:SER:HB3	1:B:426:LEU:CD1	2.02	0.89
1:C:209:GLN:HG2	1:C:212:ASN:HD22	0.73	0.88
1:A:70:LEU:HD13	1:A:90:ILE:HG12	1.53	0.88
1:C:118:THR:O	1:C:132:ASN:ND2	2.07	0.88
1:B:406:ARG:HH21	1:B:481:THR:HG22	1.40	0.87
1:C:23:ARG:HH22	1:C:332:ARG:HG2	1.36	0.86
1:C:30:GLU:HB3	1:C:213:VAL:HG21	1.56	0.86
1:C:23:ARG:CZ	1:C:332:ARG:HG2	2.04	0.86
1:D:169:ARG:HG2	1:D:169:ARG:NH1	1.78	0.86
1:A:460:ASN:O	1:A:464:THR:HG23	1.76	0.86
1:C:382:PHE:CZ	1:D:387:MET:HA	2.10	0.85
1:C:22:GLN:O	1:C:274:GLN:NE2	2.10	0.85
1:D:363:LEU:O	1:D:367:VAL:HG23	1.76	0.85
1:D:1:MET:CE	1:D:227:GLY:HA3	2.07	0.85
1:D:237:LEU:HD11	1:D:256:ILE:HG22	1.57	0.84
1:D:1:MET:HE3	1:D:227:GLY:HA3	1.59	0.84
1:A:18:LEU:HB3	1:A:25:TYR:CZ	2.13	0.84
1:A:78:PHE:CD2	1:A:93:VAL:HG13	2.12	0.84
1:A:407:CYS:HB2	1:A:410:THR:O	1.78	0.83
1:B:3:ARG:HG2	1:B:228:GLU:HB2	1.60	0.83
1:C:30:GLU:HB3	1:C:213:VAL:CG2	2.09	0.83
1:D:118:THR:O	1:D:132:ASN:ND2	2.11	0.83
1:D:367:VAL:HG11	1:D:374:ILE:HD13	1.60	0.83
1:C:24:LEU:HD22	1:C:275:ILE:HG13	1.58	0.82
1:B:2:LYS:HD3	1:B:20:ASP:HB2	1.61	0.82
1:A:78:PHE:CE2	1:A:93:VAL:CG1	2.64	0.81
1:A:77:TYR:O	1:A:79:PRO:HD3	1.80	0.80
1:D:514:SER:O	1:D:515:GLU:HB2	1.81	0.80
1:C:382:PHE:HB3	1:D:342:LEU:HD22	1.63	0.80
1:B:460:ASN:O	1:B:464:THR:HG22	1.82	0.80
1:B:14:LEU:HD23	1:B:213:VAL:HG13	1.61	0.80
1:D:474:VAL:HG21	1:D:499:SER:O	1.83	0.79
1:A:99:GLU:HG2	1:A:203:ALA:CB	2.12	0.78
1:D:407:CYS:HB2	1:D:409:GLY:H	1.48	0.78
1:C:102:VAL:HG11	1:C:116:LEU:HD13	1.66	0.78
1:A:99:GLU:CG	1:A:203:ALA:HB2	2.13	0.78
1:A:273:SER:HB3	1:B:426:LEU:HD11	1.65	0.77
1:D:78:PHE:CD2	1:D:78:PHE:O	2.38	0.77
1:D:78:PHE:O	1:D:78:PHE:HD2	1.67	0.77
1:C:7:ASN:ND2	1:C:232:ASP:OD1	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:LEU:CA	1:D:166:LEU:HD13	2.15	0.77
1:B:24:LEU:HB2	1:B:271:ILE:CG2	2.13	0.77
1:D:367:VAL:CG1	1:D:374:ILE:HD13	2.15	0.76
1:B:22:GLN:O	1:B:22:GLN:HG2	1.85	0.76
1:C:173:VAL:HG11	1:C:373:ARG:CG	2.15	0.76
1:B:352:PRO:HG2	1:B:355:HIS:CD2	2.20	0.76
1:D:14:LEU:CD2	1:D:213:VAL:CG1	2.57	0.76
1:D:68:LEU:HD11	1:D:118:THR:CG2	2.16	0.75
1:A:77:TYR:O	1:A:79:PRO:CD	2.35	0.75
1:C:222:LEU:C	1:C:223:ARG:HG3	2.11	0.75
1:C:24:LEU:HG	1:C:336:LEU:HD21	1.68	0.75
1:B:102:VAL:HG11	1:B:116:LEU:HD13	1.68	0.75
1:A:272:GLU:HG2	1:B:425:ARG:HB2	1.69	0.75
1:D:68:LEU:HD11	1:D:118:THR:HG23	1.66	0.74
1:C:382:PHE:CD2	1:D:388:SER:HB3	2.22	0.74
1:A:99:GLU:CD	1:A:203:ALA:HB2	2.12	0.74
1:A:231:ILE:CD1	1:A:237:LEU:HD12	2.12	0.74
1:C:1:MET:HE3	1:C:227:GLY:HA3	1.70	0.74
1:D:155:LEU:HD13	1:D:168:VAL:CG2	2.18	0.73
1:D:14:LEU:HD23	1:D:213:VAL:HG13	1.65	0.73
1:C:460:ASN:O	1:C:464:THR:HG22	1.89	0.73
1:B:284:ARG:HH12	1:B:290:SER:HB3	1.53	0.73
1:B:284:ARG:NH1	1:B:290:SER:HB3	2.04	0.73
1:B:363:LEU:O	1:B:367:VAL:HG22	1.88	0.72
1:D:151:LEU:HD11	1:D:168:VAL:HG11	1.71	0.72
1:D:209:GLN:HG2	1:D:212:ASN:HD22	1.55	0.72
1:A:231:ILE:HD12	1:A:237:LEU:CD1	2.12	0.71
1:A:237:LEU:HD11	1:A:256:ILE:CG2	2.20	0.71
1:A:49:ILE:HG23	1:A:90:ILE:HG22	1.71	0.71
1:D:75:ARG:HA	1:D:78:PHE:CD1	2.25	0.71
1:C:139:ILE:O	1:C:140:SER:HB3	1.91	0.70
1:C:9:THR:HG23	1:C:232:ASP:CG	2.16	0.69
1:C:382:PHE:HB3	1:D:342:LEU:CD2	2.22	0.69
1:D:75:ARG:HA	1:D:78:PHE:CE1	2.26	0.69
1:B:5:LEU:HD23	1:B:230:LEU:HB2	1.74	0.69
1:D:438:GLU:HG2	1:D:470:ARG:HB2	1.75	0.69
1:A:460:ASN:O	1:A:464:THR:CG2	2.40	0.69
1:B:20:ASP:C	1:B:20:ASP:OD1	2.35	0.69
1:B:166:LEU:CD2	1:B:184:LEU:HD13	2.20	0.69
1:C:173:VAL:HB	1:C:373:ARG:HG3	1.74	0.69
1:D:102:VAL:HG11	1:D:116:LEU:HD13	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:TRP:CZ2	1:D:223:ARG:HA	2.28	0.68
1:D:237:LEU:HD11	1:D:256:ILE:CG2	2.22	0.68
1:A:170:THR:OG1	2:A:1509:SO4:O2	2.11	0.68
1:D:239:LEU:O	1:D:243:HIS:ND1	2.25	0.68
1:A:210:GLU:CD	1:A:219:ARG:HH12	2.02	0.68
1:A:78:PHE:CD2	1:A:93:VAL:CG1	2.76	0.68
1:C:46:ILE:HD12	1:C:98:GLN:HB3	1.75	0.68
1:A:78:PHE:HD2	1:A:93:VAL:HG13	1.55	0.67
1:D:460:ASN:O	1:D:464:THR:HG22	1.93	0.67
1:B:43:LYS:NZ	1:B:99:GLU:OE2	2.25	0.67
1:B:14:LEU:CD2	1:B:213:VAL:HG13	2.22	0.67
1:A:237:LEU:HD11	1:A:256:ILE:HG22	1.77	0.67
1:C:18:LEU:HD11	1:C:221:TYR:HD2	1.59	0.67
1:A:273:SER:HB3	1:B:426:LEU:HD13	1.74	0.67
1:D:410:THR:OG1	1:D:412:THR:HG22	1.95	0.66
1:A:377:SER:HB3	1:B:382:PHE:HE1	1.60	0.66
1:C:169:ARG:NH1	2:C:1507:SO4:O2	2.28	0.66
1:A:5:LEU:HD21	1:A:230:LEU:HD12	1.78	0.65
1:B:485:HIS:CD2	1:B:487:LEU:CD1	2.62	0.65
1:B:509:ALA:C	1:B:511:ALA:H	2.04	0.65
1:A:46:ILE:HD12	1:A:98:GLN:HB3	1.79	0.65
1:C:173:VAL:CG1	1:C:373:ARG:CG	2.75	0.65
1:B:509:ALA:O	1:B:511:ALA:N	2.30	0.64
1:C:382:PHE:CE2	1:D:388:SER:HB3	2.32	0.64
1:D:211:SER:O	1:D:211:SER:OG	2.06	0.64
1:C:179:ALA:HB2	1:C:368:ARG:HH21	1.62	0.64
1:C:237:LEU:O	1:C:241:ARG:HG3	1.97	0.64
1:A:210:GLU:CD	1:A:219:ARG:NH1	2.57	0.63
1:D:128:VAL:C	1:D:166:LEU:HD11	2.23	0.63
1:A:19:VAL:HA	1:A:23:ARG:O	1.98	0.63
1:B:20:ASP:O	1:B:23:ARG:N	2.31	0.63
1:A:169:ARG:CG	2:A:1509:SO4:O4	2.47	0.63
1:C:139:ILE:O	1:C:140:SER:CB	2.47	0.63
1:A:437:GLN:HB2	1:A:491:LYS:HA	1.81	0.63
1:A:100:VAL:HG12	1:A:102:VAL:HG23	1.80	0.62
1:A:412:THR:HG23	1:A:412:THR:O	1.98	0.62
1:B:175:LYS:HD2	1:B:175:LYS:N	2.14	0.62
1:D:419:LEU:HD21	1:D:481:THR:O	1.98	0.62
1:A:75:ARG:HA	1:A:78:PHE:HD1	1.64	0.62
1:C:351:THR:N	1:C:352:PRO:CD	2.63	0.62
1:D:137:GLY:HA2	1:D:166:LEU:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ALA:HB2	1:B:303:ASP:HB2	1.81	0.61
1:D:129:LEU:HA	1:D:166:LEU:CD1	2.28	0.61
1:A:15:ARG:NH1	1:A:272:GLU:OE2	2.24	0.61
1:D:129:LEU:N	1:D:166:LEU:CD1	2.63	0.61
1:A:421:LEU:HD13	1:B:279:PHE:CE2	2.36	0.61
1:B:166:LEU:HD21	1:B:184:LEU:CD1	2.22	0.61
1:B:244:ILE:HD13	1:B:252:PHE:HB3	1.83	0.61
1:A:5:LEU:HD23	1:A:230:LEU:HB2	1.82	0.60
1:B:46:ILE:HD12	1:B:98:GLN:HB3	1.82	0.60
1:C:4:MET:HE2	1:C:221:TYR:CB	2.31	0.60
1:C:170:THR:HG22	1:C:373:ARG:HD2	1.84	0.60
1:A:481:THR:N	1:A:482:PRO:HD2	2.15	0.60
1:C:173:VAL:CG1	1:C:373:ARG:HG3	2.31	0.60
1:A:119:PHE:HA	1:A:132:ASN:HD22	1.67	0.60
1:B:78:PHE:CE2	1:B:93:VAL:HG13	2.37	0.60
1:C:25:TYR:HB2	1:C:335:ARG:NH2	2.05	0.60
1:A:404:CYS:HB2	1:B:407:CYS:SG	2.43	0.59
1:B:146:ASP:OD1	1:B:147:ASP:N	2.35	0.59
1:A:404:CYS:CB	1:B:407:CYS:SG	2.90	0.59
1:A:428:GLU:OE1	1:A:465:ARG:NH1	2.34	0.59
1:B:24:LEU:HB2	1:B:271:ILE:HG21	1.83	0.59
1:C:8:ALA:N	1:C:232:ASP:OD2	2.28	0.59
1:C:69:PRO:HG2	1:C:72:GLU:HG2	1.85	0.59
1:B:99:GLU:O	1:B:100:VAL:HG23	2.02	0.59
1:D:222:LEU:O	1:D:223:ARG:HG2	2.02	0.59
1:B:5:LEU:HD22	1:B:265:LEU:HD11	1.85	0.59
1:C:4:MET:HE2	1:C:221:TYR:HB2	1.85	0.59
1:B:70:LEU:HA	1:B:73:ILE:HD12	1.83	0.58
1:D:190:HIS:ND1	1:D:247:LEU:HA	2.18	0.58
1:D:14:LEU:CD2	1:D:213:VAL:HG13	2.31	0.58
1:B:36:GLN:HG2	1:B:211:SER:HB3	1.84	0.58
1:C:43:LYS:HD2	1:C:203:ALA:HA	1.86	0.58
1:A:282:GLU:CD	1:B:512:LEU:HB3	2.29	0.58
1:A:49:ILE:CG2	1:A:90:ILE:HG22	2.33	0.57
1:C:23:ARG:HH21	1:C:332:ARG:HB3	1.69	0.57
1:C:23:ARG:HG2	1:C:332:ARG:NH2	2.20	0.57
1:B:75:ARG:HA	1:B:78:PHE:HB2	1.86	0.57
1:A:169:ARG:HG2	2:A:1509:SO4:O4	2.04	0.57
1:A:212:ASN:OD1	1:A:212:ASN:C	2.46	0.57
1:A:5:LEU:CD2	1:A:230:LEU:HD12	2.34	0.57
1:A:404:CYS:HB3	1:A:407:CYS:SG	2.44	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:406:ARG:HH21	1:D:481:THR:HG22	1.70	0.57
1:B:437:GLN:HB2	1:B:491:LYS:HA	1.86	0.56
1:C:243:HIS:O	1:C:247:LEU:HD12	2.05	0.56
1:A:47:THR:O	1:A:96:GLU:OE1	2.23	0.56
1:B:5:LEU:CD2	1:B:230:LEU:HB2	2.35	0.56
1:D:127:LEU:HD13	1:D:166:LEU:HD21	1.85	0.56
1:C:437:GLN:HB2	1:C:491:LYS:HA	1.88	0.56
1:C:481:THR:N	1:C:482:PRO:HD2	2.20	0.56
1:B:34:HIS:HE1	1:B:36:GLN:OE1	1.89	0.56
1:C:213:VAL:CG2	1:C:213:VAL:O	2.54	0.56
1:C:239:LEU:O	1:C:243:HIS:ND1	2.39	0.56
1:D:239:LEU:HB3	1:D:243:HIS:HE1	1.71	0.56
1:D:69:PRO:HG2	1:D:72:GLU:HG2	1.87	0.56
1:A:5:LEU:HD11	1:A:269:TYR:CG	2.40	0.56
1:B:391:ARG:NH2	1:B:395:SER:CB	2.69	0.56
1:D:119:PHE:HD1	1:D:133:ASN:HB3	1.71	0.55
1:C:95:ARG:HG2	1:C:98:GLN:HB2	1.88	0.55
1:A:18:LEU:HB3	1:A:25:TYR:OH	2.06	0.55
1:B:407:CYS:HB3	1:B:410:THR:H	1.71	0.55
1:C:173:VAL:CG1	1:C:174:GLY:N	2.69	0.55
1:D:474:VAL:HG12	1:D:474:VAL:O	2.05	0.55
1:A:69:PRO:HG2	1:A:72:GLU:HG2	1.89	0.55
1:D:474:VAL:CG2	1:D:499:SER:O	2.52	0.55
1:C:173:VAL:CB	1:C:373:ARG:HG3	2.36	0.55
1:B:391:ARG:NH2	1:B:395:SER:HB3	2.21	0.55
1:D:291:ILE:HG22	1:D:304:ILE:HG12	1.88	0.55
1:A:406:ARG:NH1	1:B:480:GLU:OE2	2.41	0.54
1:B:171:ALA:C	1:B:173:VAL:H	2.15	0.54
1:C:30:GLU:HG2	1:C:213:VAL:HB	1.88	0.54
1:D:426:LEU:HD23	1:D:486:VAL:HG21	1.90	0.54
1:B:2:LYS:HB2	1:B:226:ILE:HA	1.89	0.54
1:C:23:ARG:CG	1:C:332:ARG:NH2	2.70	0.54
1:A:66:GLY:HA3	1:A:116:LEU:HD11	1.89	0.54
1:D:334:LEU:HD23	1:D:339:LEU:HD12	1.90	0.54
1:B:141:ARG:HD2	1:B:141:ARG:N	2.22	0.54
1:A:208:HIS:CE1	1:A:215:VAL:HG11	2.44	0.54
1:D:428:GLU:OE1	1:D:465:ARG:NH1	2.39	0.54
1:B:171:ALA:HB2	1:B:371:ARG:O	2.08	0.53
1:B:127:LEU:CD1	1:B:184:LEU:HB2	2.39	0.53
1:B:170:THR:OG1	2:B:1515:SO4:O2	2.25	0.53
1:C:24:LEU:CD2	1:C:275:ILE:HA	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:LEU:CD1	1:D:256:ILE:CG2	2.86	0.53
1:D:414:ARG:HH22	1:D:422:SER:HB2	1.73	0.53
1:C:231:ILE:HD12	1:C:237:LEU:HD12	1.90	0.53
1:C:18:LEU:CD1	1:C:221:TYR:HD2	2.20	0.53
1:D:209:GLN:HG2	1:D:212:ASN:ND2	2.22	0.53
1:D:239:LEU:HB3	1:D:243:HIS:CE1	2.43	0.53
1:A:381:ARG:HH12	1:B:375:GLN:NE2	2.06	0.53
1:D:46:ILE:HD12	1:D:98:GLN:HB3	1.91	0.53
1:D:14:LEU:CD2	1:D:213:VAL:HG11	2.18	0.53
1:A:18:LEU:HB3	1:A:25:TYR:CE2	2.44	0.53
1:B:170:THR:O	1:B:173:VAL:HB	2.09	0.53
1:D:119:PHE:CD1	1:D:133:ASN:HB3	2.43	0.52
1:D:352:PRO:HG2	1:D:355:HIS:CD2	2.44	0.52
1:B:2:LYS:CD	1:B:20:ASP:HB2	2.37	0.52
1:D:367:VAL:CG1	1:D:374:ILE:CD1	2.87	0.52
1:A:102:VAL:HG11	1:A:116:LEU:HD13	1.90	0.52
1:A:407:CYS:CB	1:A:410:THR:O	2.55	0.52
1:B:24:LEU:HB2	1:B:271:ILE:HG22	1.89	0.52
1:A:49:ILE:HG23	1:A:90:ILE:CG2	2.38	0.52
1:C:304:ILE:HD12	1:C:347:PHE:HA	1.91	0.52
1:D:24:LEU:HD21	1:D:336:LEU:HD22	1.92	0.52
1:B:43:LYS:CE	1:B:99:GLU:OE2	2.58	0.52
1:A:46:ILE:HD13	1:A:94:LEU:HD13	1.90	0.52
1:C:291:ILE:HG22	1:C:304:ILE:HG12	1.90	0.52
1:A:317:GLU:O	1:A:321:ASN:HB2	2.09	0.52
1:C:270:GLN:HE22	1:D:433:LYS:HG2	1.74	0.52
1:C:382:PHE:CE2	1:D:388:SER:CB	2.93	0.52
1:B:224:GLN:O	1:B:224:GLN:HG2	2.09	0.51
1:C:382:PHE:HD2	1:D:388:SER:HB3	1.74	0.51
1:C:406:ARG:HG2	1:C:406:ARG:O	2.10	0.51
1:D:155:LEU:HD13	1:D:168:VAL:HG23	1.92	0.51
1:D:377:SER:O	1:D:385:LEU:HD11	2.09	0.51
1:A:2:LYS:O	1:A:227:GLY:N	2.40	0.51
1:A:404:CYS:SG	1:B:406:ARG:HB3	2.49	0.51
1:C:30:GLU:HB3	1:C:213:VAL:HG23	1.89	0.51
1:C:131:PRO:HA	1:C:164:MET:HB3	1.92	0.51
1:C:382:PHE:CE2	1:D:388:SER:N	2.78	0.51
1:C:463:GLU:HG2	1:C:469:VAL:O	2.10	0.51
1:B:352:PRO:HG2	1:B:355:HIS:HD2	1.69	0.51
1:C:5:LEU:HD12	1:C:271:ILE:HD13	1.93	0.51
1:A:18:LEU:CB	1:A:25:TYR:CZ	2.89	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:LEU:O	1:A:367:VAL:HG22	2.11	0.51
1:C:25:TYR:O	1:C:335:ARG:NE	2.35	0.51
1:A:70:LEU:HD12	1:A:73:ILE:HD12	1.93	0.51
1:B:509:ALA:C	1:B:511:ALA:N	2.69	0.51
1:C:352:PRO:HG2	1:C:355:HIS:CD2	2.46	0.51
1:D:203:ALA:N	1:D:204:PRO:HD3	2.26	0.51
1:D:217:ALA:O	1:D:221:TYR:HB2	2.10	0.51
1:D:239:LEU:O	1:D:243:HIS:CE1	2.64	0.51
1:D:481:THR:N	1:D:482:PRO:HD2	2.25	0.51
1:A:75:ARG:HA	1:A:78:PHE:CD1	2.45	0.51
1:B:330:ILE:O	1:B:334:LEU:HG	2.11	0.50
1:C:43:LYS:HZ3	1:C:198:ALA:C	2.19	0.50
1:A:273:SER:CB	1:B:426:LEU:HD11	2.40	0.50
1:B:27:LEU:HD22	1:B:275:ILE:HG12	1.92	0.50
1:D:437:GLN:HB2	1:D:491:LYS:HA	1.91	0.50
1:A:427:ILE:HG23	1:A:439:VAL:HG11	1.94	0.50
1:C:412:THR:HG21	1:D:281:ARG:HE	1.76	0.50
1:B:3:ARG:HA	1:B:228:GLU:O	2.10	0.50
1:C:131:PRO:HA	1:C:164:MET:CB	2.41	0.50
1:B:231:ILE:HB	1:B:237:LEU:HD12	1.94	0.50
1:B:337:ARG:NH1	1:B:400:SER:CB	2.74	0.50
1:C:30:GLU:CB	1:C:213:VAL:CG2	2.88	0.50
1:D:407:CYS:HB2	1:D:410:THR:H	1.76	0.50
1:D:514:SER:O	1:D:515:GLU:CB	2.56	0.50
1:A:105:ASP:OD2	1:A:117:THR:HG21	2.12	0.50
1:C:23:ARG:NH2	1:C:332:ARG:CB	2.74	0.49
1:C:428:GLU:OE1	1:C:465:ARG:NH1	2.41	0.49
1:A:208:HIS:HE1	1:A:215:VAL:HG11	1.75	0.49
1:C:173:VAL:HG21	1:C:373:ARG:HE	1.77	0.49
1:A:212:ASN:OD1	1:A:215:VAL:HB	2.13	0.49
1:C:23:ARG:HH22	1:C:332:ARG:CG	2.08	0.49
1:A:15:ARG:NH2	1:A:272:GLU:OE1	2.29	0.49
1:D:304:ILE:HD12	1:D:347:PHE:HA	1.93	0.49
1:C:119:PHE:HA	1:C:132:ASN:HD22	1.76	0.49
1:C:212:ASN:OD1	1:C:212:ASN:O	2.30	0.49
1:A:105:ASP:OD2	1:A:117:THR:CG2	2.61	0.49
1:A:414:ARG:HG3	1:B:401:HIS:CE1	2.47	0.49
1:B:37:LYS:O	1:B:38:LYS:C	2.56	0.49
1:A:212:ASN:OD1	1:A:212:ASN:O	2.30	0.49
1:A:481:THR:N	1:A:482:PRO:CD	2.76	0.49
1:B:438:GLU:HG2	1:B:470:ARG:CB	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:TYR:O	1:D:79:PRO:HD3	2.13	0.49
1:D:129:LEU:CA	1:D:166:LEU:CD1	2.88	0.49
1:A:282:GLU:OE2	1:B:512:LEU:HB3	2.13	0.48
1:B:391:ARG:HH21	1:B:395:SER:HB2	1.77	0.48
1:B:393:SER:O	1:B:395:SER:O	2.31	0.48
1:C:272:GLU:HB3	1:D:429:GLU:OE2	2.11	0.48
1:C:406:ARG:HD3	1:C:413:VAL:HG21	1.95	0.48
1:D:127:LEU:HB3	1:D:166:LEU:HD21	1.95	0.48
1:A:405:PRO:HG2	1:B:406:ARG:NH1	2.28	0.48
1:C:173:VAL:HG12	1:C:174:GLY:N	2.28	0.48
1:D:5:LEU:HB3	1:D:265:LEU:HD21	1.94	0.48
1:D:146:ASP:CG	1:D:146:ASP:O	2.56	0.48
1:A:237:LEU:CD1	1:A:256:ILE:CG2	2.92	0.48
1:B:391:ARG:NH1	1:B:397:GLY:CA	2.39	0.48
1:D:512:LEU:O	1:D:515:GLU:N	2.45	0.48
1:B:8:ALA:HB2	1:B:14:LEU:CD1	2.43	0.48
1:B:137:GLY:CA	1:B:166:LEU:O	2.62	0.48
1:A:412:THR:HG21	1:B:281:ARG:HD2	1.96	0.48
1:A:502:LEU:N	1:A:503:PRO:CD	2.76	0.48
1:B:432:LEU:O	1:B:432:LEU:HG	2.13	0.48
1:A:77:TYR:O	1:A:79:PRO:HD2	2.11	0.48
1:C:272:GLU:HB3	1:D:429:GLU:OE1	2.14	0.48
1:B:69:PRO:HG2	1:B:72:GLU:HG2	1.95	0.48
1:C:95:ARG:CG	1:C:98:GLN:HB2	2.43	0.48
1:B:119:PHE:HA	1:B:132:ASN:HD22	1.79	0.47
1:D:38:LYS:HB2	1:D:107:GLU:OE1	2.14	0.47
1:B:139:ILE:HB	1:B:148:ARG:HH11	1.79	0.47
1:B:174:GLY:O	1:B:368:ARG:HD3	2.14	0.47
1:C:18:LEU:HD21	1:C:221:TYR:HB3	1.97	0.47
1:C:203:ALA:N	1:C:204:PRO:HD3	2.29	0.47
1:D:351:THR:N	1:D:352:PRO:CD	2.78	0.47
1:C:6:ILE:HG12	1:C:16:VAL:HG22	1.97	0.47
1:A:8:ALA:HB2	1:A:14:LEU:CD1	2.45	0.47
1:A:14:LEU:HB3	1:A:30:GLU:O	2.14	0.47
1:B:34:HIS:O	1:B:34:HIS:CG	2.67	0.47
1:B:391:ARG:HH12	1:B:397:GLY:HA2	1.68	0.47
1:B:406:ARG:HG3	1:B:482:PRO:HG3	1.96	0.47
1:C:8:ALA:HB2	1:C:14:LEU:CD1	2.44	0.47
1:D:42:TYR:CD2	1:D:206:LEU:HA	2.49	0.47
1:A:118:THR:O	1:A:132:ASN:ND2	2.48	0.47
1:B:391:ARG:NH2	1:B:395:SER:HB2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:LEU:HD12	1:C:161:PRO:HD2	1.97	0.47
1:B:182:TRP:NE1	1:B:186:PHE:HE2	2.13	0.47
1:B:485:HIS:HD2	1:B:487:LEU:HD12	1.72	0.47
1:C:213:VAL:O	1:C:213:VAL:HG22	2.15	0.47
1:D:407:CYS:CB	1:D:410:THR:H	2.28	0.46
1:B:100:VAL:HG12	1:B:102:VAL:HG23	1.97	0.46
1:C:369:GLN:O	1:C:369:GLN:HG3	2.15	0.46
1:B:99:GLU:C	1:B:100:VAL:HG23	2.41	0.46
1:D:8:ALA:HB2	1:D:14:LEU:CD1	2.46	0.46
1:A:27:LEU:HG	1:A:28:ASP:N	2.30	0.46
1:B:182:TRP:O	1:B:186:PHE:HD2	1.99	0.46
1:C:179:ALA:HB2	1:C:368:ARG:NH2	2.30	0.46
1:C:282:GLU:OE1	1:D:513:PRO:HD2	2.15	0.46
1:C:375:GLN:NE2	1:D:381:ARG:HH12	2.14	0.46
1:D:354:ARG:HH11	1:D:354:ARG:HG2	1.79	0.46
1:B:182:TRP:CZ2	1:B:223:ARG:HA	2.50	0.46
1:C:455:LYS:O	1:C:459:VAL:HG23	2.16	0.46
1:B:201:ARG:HG2	1:B:202:PRO:HD2	1.98	0.46
1:C:334:LEU:HD23	1:C:339:LEU:HD12	1.96	0.46
1:D:129:LEU:N	1:D:166:LEU:HD13	2.30	0.46
1:D:189:LYS:HB3	1:D:248:GLY:O	2.15	0.46
1:B:34:HIS:HE1	1:B:36:GLN:HB2	1.71	0.46
1:B:139:ILE:HB	1:B:148:ARG:NH1	2.31	0.46
1:C:382:PHE:HE2	1:D:388:SER:CB	2.28	0.46
1:C:24:LEU:HD22	1:C:275:ILE:CG1	2.39	0.46
1:C:43:LYS:NZ	1:C:198:ALA:O	2.46	0.46
1:B:118:THR:O	1:B:132:ASN:ND2	2.49	0.46
1:C:6:ILE:HD12	1:C:229:ILE:CG2	2.46	0.46
1:C:31:SER:HA	1:C:32:PRO:HD3	1.81	0.46
1:D:367:VAL:HG12	1:D:374:ILE:CD1	2.45	0.46
1:A:70:LEU:HB2	1:A:90:ILE:CG1	2.46	0.45
1:A:143:ILE:O	1:A:143:ILE:HG22	2.16	0.45
1:B:217:ALA:O	1:B:221:TYR:HB2	2.17	0.45
1:A:338:ASP:O	1:A:391:ARG:HD2	2.16	0.45
1:A:210:GLU:OE1	1:A:219:ARG:NH1	2.49	0.45
1:D:212:ASN:OD1	1:D:215:VAL:HG23	2.17	0.45
1:C:140:SER:O	1:C:140:SER:OG	2.30	0.45
1:D:127:LEU:HD22	1:D:166:LEU:HD21	1.98	0.45
1:A:203:ALA:N	1:A:204:PRO:CD	2.80	0.45
1:B:393:SER:O	1:B:394:PRO:C	2.60	0.45
1:D:393:SER:C	1:D:396:LEU:N	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ARG:C	1:A:171:ALA:N	2.74	0.45
1:C:160:LEU:HD11	1:C:164:MET:HG3	1.99	0.45
1:D:397:GLY:C	1:D:398:GLU:HG3	2.41	0.45
1:A:24:LEU:HD23	1:A:274:GLN:HB3	1.98	0.45
1:A:223:ARG:H	1:A:226:ILE:HD12	1.82	0.45
1:A:393:SER:HA	1:A:394:PRO:HD2	1.51	0.45
1:C:351:THR:N	1:C:352:PRO:HD3	2.30	0.45
1:A:269:TYR:C	1:A:270:GLN:HG2	2.42	0.45
1:A:478:GLN:NE2	1:C:478:GLN:OE1	2.50	0.45
1:D:237:LEU:O	1:D:241:ARG:HG3	2.17	0.45
1:A:276:GLU:OE1	1:B:422:SER:OG	2.35	0.45
1:B:404:CYS:HA	1:B:405:PRO:HD3	1.77	0.45
1:C:404:CYS:SG	1:D:406:ARG:HB3	2.57	0.45
1:B:203:ALA:N	1:B:204:PRO:HD3	2.32	0.44
1:B:222:LEU:HA	1:B:226:ILE:HD12	1.99	0.44
1:C:290:SER:HB3	1:D:513:PRO:HG2	1.99	0.44
1:D:18:LEU:HB3	1:D:25:TYR:CZ	2.53	0.44
1:A:78:PHE:HA	1:A:79:PRO:HD2	1.80	0.44
1:C:209:GLN:CG	1:C:212:ASN:ND2	2.43	0.44
1:C:222:LEU:C	1:C:223:ARG:CG	2.87	0.44
1:C:222:LEU:HA	1:C:226:ILE:HD12	1.99	0.44
1:D:182:TRP:CH2	1:D:222:LEU:O	2.70	0.44
1:A:99:GLU:O	1:A:100:VAL:HG23	2.18	0.44
1:A:208:HIS:HE1	1:A:215:VAL:CG1	2.31	0.44
1:B:8:ALA:HB2	1:B:14:LEU:HD13	2.00	0.44
1:B:428:GLU:OE1	1:B:465:ARG:NH1	2.50	0.44
1:D:37:LYS:H	1:D:107:GLU:CD	2.26	0.44
1:D:87:ARG:HA	1:D:88:PRO:HD3	1.85	0.44
1:A:273:SER:CB	1:B:426:LEU:CD1	2.87	0.44
1:A:406:ARG:HD3	1:A:413:VAL:HG21	1.98	0.44
1:A:407:CYS:HB3	1:B:404:CYS:SG	2.57	0.44
1:B:126:TYR:CE1	1:B:175:LYS:HE2	2.52	0.44
1:C:38:LYS:O	1:C:104:ILE:O	2.35	0.44
1:C:272:GLU:CB	1:D:429:GLU:OE1	2.64	0.44
1:A:345:ILE:HD12	1:A:385:LEU:HD23	2.00	0.44
1:A:506:HIS:C	1:A:508:GLU:N	2.76	0.44
1:C:223:ARG:NH1	1:C:369:GLN:HE21	2.16	0.44
1:A:218:PHE:O	1:A:222:LEU:HB2	2.17	0.44
1:C:342:LEU:HA	1:C:342:LEU:HD12	1.73	0.44
1:A:99:GLU:OE2	1:A:203:ALA:HB2	2.18	0.44
1:C:30:GLU:HG2	1:C:213:VAL:CG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:ARG:HG2	2:C:1507:SO4:O4	2.18	0.44
1:C:23:ARG:HG2	1:C:332:ARG:HH21	1.82	0.43
1:C:382:PHE:CZ	1:D:387:MET:CA	2.92	0.43
1:D:330:ILE:O	1:D:334:LEU:HG	2.18	0.43
1:B:37:LYS:HA	1:B:40:ASN:ND2	2.33	0.43
1:A:304:ILE:HD12	1:A:347:PHE:HA	2.01	0.43
1:C:402:HIS:O	1:C:403:VAL:C	2.62	0.43
1:C:481:THR:N	1:C:482:PRO:CD	2.82	0.43
1:A:363:LEU:HD22	1:A:385:LEU:CD2	2.49	0.43
1:B:304:ILE:HD12	1:B:326:ALA:HB1	1.99	0.43
1:B:342:LEU:C	1:B:343:ILE:HG13	2.42	0.43
1:B:352:PRO:CG	1:B:355:HIS:CD2	2.98	0.43
1:B:444:PRO:HG2	1:B:481:THR:HA	2.01	0.43
1:B:393:SER:OG	1:B:395:SER:HB2	2.19	0.43
1:B:434:GLU:O	1:B:435:ASN:HB3	2.19	0.43
1:B:445:VAL:N	1:B:446:PRO:HD2	2.33	0.43
1:C:23:ARG:HG3	1:C:332:ARG:NH2	2.34	0.42
1:A:250:PRO:C	1:A:252:PHE:N	2.77	0.42
1:A:363:LEU:CD2	1:A:385:LEU:HD21	2.49	0.42
1:C:502:LEU:N	1:C:503:PRO:CD	2.82	0.42
1:A:12:GLU:CD	1:A:12:GLU:H	2.28	0.42
1:A:250:PRO:C	1:A:252:PHE:H	2.27	0.42
1:A:343:ILE:HB	1:A:387:MET:HG3	2.00	0.42
1:B:351:THR:N	1:B:352:PRO:CD	2.82	0.42
1:D:120:ILE:O	1:D:131:PRO:HD2	2.19	0.42
1:D:203:ALA:N	1:D:204:PRO:CD	2.83	0.42
1:C:39:ALA:O	1:C:210:GLU:HB2	2.20	0.42
1:D:244:ILE:HD12	1:D:256:ILE:HD11	2.02	0.42
1:A:201:ARG:CG	1:A:202:PRO:HD2	2.50	0.42
1:D:127:LEU:HD22	1:D:166:LEU:CD2	2.49	0.42
1:A:46:ILE:CD1	1:A:94:LEU:HD13	2.50	0.42
1:B:20:ASP:OD1	1:B:21:GLY:N	2.52	0.42
1:D:377:SER:O	1:D:385:LEU:CD1	2.68	0.42
1:A:404:CYS:HA	1:A:405:PRO:HD2	1.94	0.42
1:A:412:THR:O	1:A:412:THR:CG2	2.67	0.42
1:C:8:ALA:H	1:C:232:ASP:CG	2.22	0.42
1:C:169:ARG:HG3	2:C:1507:SO4:O3	2.19	0.42
1:B:24:LEU:HD22	1:B:271:ILE:HB	2.01	0.42
1:B:227:GLY:O	1:B:255:LYS:HG2	2.19	0.42
1:A:169:ARG:O	1:A:170:THR:C	2.62	0.41
1:A:407:CYS:SG	1:A:410:THR:O	2.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:PHE:CD1	1:A:133:ASN:HB3	2.55	0.41
1:A:169:ARG:HA	2:A:1509:SO4:O4	2.20	0.41
1:B:414:ARG:HD3	1:B:419:LEU:HD13	2.02	0.41
1:B:481:THR:N	1:B:482:PRO:HD2	2.35	0.41
1:B:506:HIS:O	1:B:510:MET:HG2	2.20	0.41
1:D:28:ASP:OD2	1:D:221:TYR:HE1	2.02	0.41
1:D:407:CYS:HB2	1:D:409:GLY:N	2.26	0.41
1:A:362:ARG:NH1	1:A:362:ARG:HG2	2.34	0.41
1:B:214:ILE:HD11	1:B:236:VAL:HG13	2.02	0.41
1:B:448:ALA:HB3	1:B:475:PRO:HB3	2.02	0.41
1:B:506:HIS:O	1:B:507:GLU:C	2.63	0.41
1:C:30:GLU:CB	1:C:213:VAL:HG23	2.50	0.41
1:C:105:ASP:HB3	1:C:106:LYS:HG3	2.01	0.41
1:D:434:GLU:O	1:D:435:ASN:HB3	2.20	0.41
1:A:455:LYS:O	1:A:459:VAL:HG23	2.21	0.41
1:C:354:ARG:O	1:C:354:ARG:CG	2.69	0.41
1:C:412:THR:HG21	1:D:281:ARG:NE	2.35	0.41
1:B:43:LYS:O	1:B:203:ALA:O	2.37	0.41
1:C:183:ASP:OD1	1:C:187:ARG:NH1	2.53	0.41
1:D:74:ALA:HB2	1:D:132:ASN:ND2	2.36	0.41
1:B:78:PHE:CD2	1:B:93:VAL:HG13	2.54	0.41
1:C:23:ARG:HH22	1:C:329:GLU:HA	1.86	0.41
1:A:201:ARG:HG2	1:A:202:PRO:HD2	2.03	0.41
1:B:419:LEU:HD21	1:B:481:THR:O	2.20	0.41
1:C:237:LEU:HD11	1:C:256:ILE:HG22	2.03	0.41
1:A:330:ILE:O	1:A:334:LEU:HG	2.20	0.41
1:A:504:LYS:O	1:A:507:GLU:CB	2.68	0.41
1:B:224:GLN:O	1:B:224:GLN:CG	2.68	0.41
1:B:406:ARG:HH21	1:B:481:THR:CG2	2.21	0.41
1:C:495:THR:HB	1:C:496:PRO:HD2	2.01	0.41
1:D:146:ASP:O	1:D:146:ASP:OD1	2.39	0.41
1:D:414:ARG:NH2	1:D:422:SER:HB2	2.35	0.41
1:D:445:VAL:N	1:D:446:PRO:HD2	2.36	0.41
1:B:137:GLY:HA2	1:B:166:LEU:O	2.21	0.41
1:B:396:LEU:HD13	1:B:396:LEU:HA	1.78	0.41
1:C:276:GLU:CD	1:D:422:SER:HG	2.28	0.41
1:D:231:ILE:HG22	1:D:233:ASN:H	1.86	0.41
1:D:438:GLU:HB2	1:D:489:VAL:HB	2.02	0.41
1:B:438:GLU:OE2	1:B:494:GLU:HB2	2.21	0.41
1:D:327:ALA:HB3	1:D:362:ARG:HG3	2.02	0.41
1:A:30:GLU:O	1:A:31:SER:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:CYS:O	1:B:408:SER:CB	2.69	0.40
1:C:203:ALA:N	1:C:204:PRO:CD	2.84	0.40
1:A:15:ARG:HG2	1:A:29:ILE:HG12	2.03	0.40
1:B:130:MET:C	1:B:132:ASN:H	2.29	0.40
1:B:182:TRP:CH2	1:B:223:ARG:HA	2.56	0.40
1:B:337:ARG:HH11	1:B:400:SER:CB	2.34	0.40
1:A:14:LEU:O	1:A:29:ILE:HA	2.21	0.40
1:A:434:GLU:O	1:A:435:ASN:HB3	2.21	0.40
1:B:24:LEU:CB	1:B:271:ILE:HG22	2.51	0.40
1:B:342:LEU:HD12	1:B:342:LEU:HA	1.64	0.40
1:B:378:HIS:C	1:B:385:LEU:HD12	2.46	0.40
1:C:401:HIS:ND1	1:D:412:THR:OG1	2.49	0.40
1:D:19:VAL:HG21	1:D:271:ILE:HD13	2.03	0.40
1:D:444:PRO:HG2	1:D:481:THR:HA	2.04	0.40

All (3) 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:A:260:THR:CG2	1:C:241:ARG:NH1[1_665]	1.81	0.39
1:C:65:HIS:ND1	1:C:351:THR:OG1[1_545]	1.95	0.25
1:C:362:ARG:NH2	1:C:435:ASN:OD1[1_455]	2.18	0.02

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	479/515 (93%)	452 (94%)	24 (5%)	3 (1%)	21	52
1	B	485/515 (94%)	454 (94%)	28 (6%)	3 (1%)	21	52
1	C	460/515 (89%)	428 (93%)	32 (7%)	0	100	100
1	D	452/515 (88%)	431 (95%)	21 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1876/2060 (91%)	1765 (94%)	105 (6%)	6 (0%)	36 65

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	79	PRO
1	A	170	THR
1	B	510	MET
1	A	119	PHE
1	A	78	PHE
1	B	394	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	333/438 (76%)	307 (92%)	26 (8%)	11 36
1	B	361/438 (82%)	337 (93%)	24 (7%)	15 43
1	C	347/438 (79%)	322 (93%)	25 (7%)	13 40
1	D	346/438 (79%)	319 (92%)	27 (8%)	11 36
All	All	1387/1752 (79%)	1285 (93%)	102 (7%)	13 38

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	76	GLU
1	A	90	ILE
1	A	107	GLU
1	A	117	THR
1	A	140	SER
1	A	169	ARG
1	A	175	LYS
1	A	211	SER

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Mol	Chain	Res	Type
1	A	244	ILE
1	A	247	LEU
1	A	262	GLU
1	A	270	GLN
1	A	295	SER
1	A	332	ARG
1	A	362	ARG
1	A	381	ARG
1	A	403	VAL
1	A	406	ARG
1	A	413	VAL
1	A	415	ASP
1	A	439	VAL
1	A	457	SER
1	A	464	THR
1	A	481	THR
1	A	485	HIS
1	B	1	MET
1	B	20	ASP
1	B	24	LEU
1	B	38	LYS
1	B	90	ILE
1	B	117	THR
1	B	148	ARG
1	B	173	VAL
1	B	192	GLU
1	B	212	ASN
1	B	241	ARG
1	B	244	ILE
1	B	284	ARG
1	B	304	ILE
1	B	332	ARG
1	B	342	LEU
1	B	368	ARG
1	B	369	GLN
1	B	396	LEU
1	B	425	ARG
1	B	457	SER
1	B	464	THR
1	B	485	HIS
1	B	505	LEU
1	C	43	LYS

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Mol	Chain	Res	Type
1	C	48	ARG
1	C	117	THR
1	C	135	ARG
1	C	150	GLU
1	C	169	ARG
1	C	173	VAL
1	C	176	SER
1	C	209	GLN
1	C	211	SER
1	C	213	VAL
1	C	223	ARG
1	C	241	ARG
1	C	244	ILE
1	C	297	GLU
1	C	332	ARG
1	C	342	LEU
1	C	349	ASP
1	C	357	ARG
1	C	365	GLU
1	C	378	HIS
1	C	403	VAL
1	C	457	SER
1	C	480	GLU
1	C	481	THR
1	D	1	MET
1	D	23	ARG
1	D	38	LYS
1	D	68	LEU
1	D	78	PHE
1	D	100	VAL
1	D	107	GLU
1	D	117	THR
1	D	133	ASN
1	D	169	ARG
1	D	210	GLU
1	D	211	SER
1	D	241	ARG
1	D	244	ILE
1	D	253	SER
1	D	332	ARG
1	D	349	ASP
1	D	362	ARG

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Mol	Chain	Res	Type
1	D	367	VAL
1	D	369	GLN
1	D	398	GLU
1	D	407	CYS
1	D	429	GLU
1	D	457	SER
1	D	470	ARG
1	D	474	VAL
1	D	485	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	ASN
1	A	208	HIS
1	A	243	HIS
1	A	280	GLN
1	A	355	HIS
1	A	483	HIS
1	B	34	HIS
1	B	132	ASN
1	B	133	ASN
1	B	181	GLN
1	B	208	HIS
1	B	280	GLN
1	B	355	HIS
1	B	375	GLN
1	B	401	HIS
1	B	402	HIS
1	B	416	ASN
1	B	453	ASN
1	B	483	HIS
1	B	485	HIS
1	C	132	ASN
1	C	208	HIS
1	C	212	ASN
1	C	280	GLN
1	C	355	HIS
1	C	369	GLN
1	C	375	GLN
1	C	416	ASN
1	C	466	GLN

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Mol	Chain	Res	Type
1	C	483	HIS
1	D	65	HIS
1	D	208	HIS
1	D	280	GLN
1	D	355	HIS
1	D	483	HIS

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](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

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	SO4	C	1507	-	4,4,4	0.58	0	6,6,6	0.19	0
2	SO4	B	1515	-	4,4,4	0.42	0	6,6,6	0.15	0
2	SO4	A	1509	-	4,4,4	0.70	0	6,6,6	0.14	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.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1507	SO4	3	0
2	B	1515	SO4	1	0
2	A	1509	SO4	4	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	489/515 (94%)	0.26	10 (2%) 65 46	44, 99, 133, 176	0
1	B	495/515 (96%)	0.30	13 (2%) 57 38	56, 98, 129, 171	0
1	C	474/515 (92%)	0.44	23 (4%) 35 23	59, 99, 130, 172	0
1	D	472/515 (91%)	0.26	5 (1%) 78 60	54, 101, 130, 172	0
All	All	1930/2060 (93%)	0.31	51 (2%) 57 38	44, 99, 130, 176	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	174	GLY	4.4
1	B	93	VAL	4.2
1	C	319	ALA	3.9
1	B	49	ILE	3.7
1	C	339	LEU	3.6
1	B	89	ASN	3.5
1	B	80	ALA	3.5
1	C	39	ALA	3.4
1	C	166	LEU	3.1
1	A	416	ASN	3.0
1	C	11	GLN	2.9
1	A	259	TYR	2.9
1	A	420	SER	2.9
1	C	124	GLY	2.9
1	C	393	SER	2.8
1	B	154	ALA	2.8
1	B	252	PHE	2.8
1	C	353	VAL	2.7
1	B	177	ALA	2.7
1	A	226	ILE	2.7
1	A	228	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	26	ASP	2.7
1	C	382	PHE	2.6
1	C	55	ALA	2.5
1	D	49	ILE	2.5
1	C	24	LEU	2.5
1	B	279	PHE	2.5
1	C	203	ALA	2.4
1	D	171	ALA	2.4
1	A	225	ASP	2.4
1	C	327	ALA	2.3
1	A	24	LEU	2.3
1	C	37	LYS	2.2
1	C	125	SER	2.2
1	C	214	ILE	2.2
1	C	224	GLN	2.2
1	B	6	ILE	2.2
1	A	125	SER	2.1
1	A	252	PHE	2.1
1	C	413	VAL	2.1
1	D	90	ILE	2.1
1	A	398	GLU	2.1
1	B	88	PRO	2.1
1	C	127	LEU	2.1
1	C	90	ILE	2.1
1	C	77	TYR	2.1
1	D	100	VAL	2.0
1	B	432	LEU	2.0
1	B	150	GLU	2.0
1	B	315	ILE	2.0
1	D	52	SER	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(\AA^2)	Q<0.9
2	SO4	A	1509	5/5	0.72	0.09	148,150,154,159	0
2	SO4	C	1507	5/5	0.75	0.10	108,116,118,124	0
2	SO4	B	1515	5/5	0.80	0.10	134,136,140,145	0
3	ZN	B	1514	1/1	0.99	0.07	58,58,58,58	1
3	ZN	D	1516	1/1	1.00	0.08	64,64,64,64	1

6.5 Other polymers [i](#)

There are no such residues in this entry.