



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:39 PM UTC

PDB ID : 1EOI / pdb_00001eoi
Title : CRYSTAL STRUCTURE OF ACID PHOSPHATASE FROM ES-
CHERICHIA BLATTAE COMPLEXED WITH THE TRANSITION
STATE ANALOG MOLYBDATE
Authors : Ishikawa, K.; Mihara, Y.; Gondoh, K.; Suzuki, E.; Asano, Y.
Deposited on : 2000-03-23
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

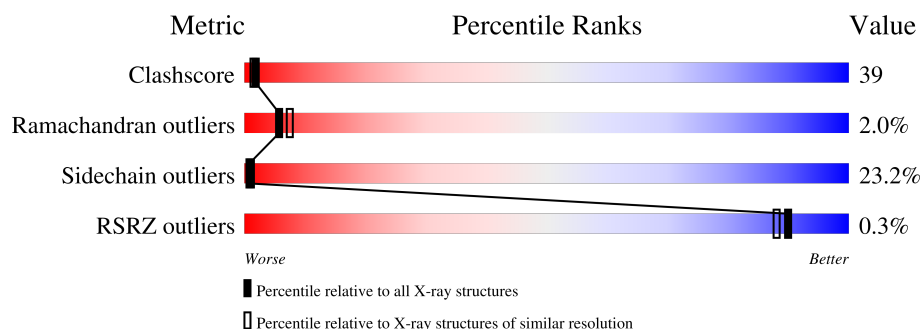
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	231	
1	B	231	
1	C	231	

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	MOO	C	1003	-	-	X	-

2 Entry composition [i](#)

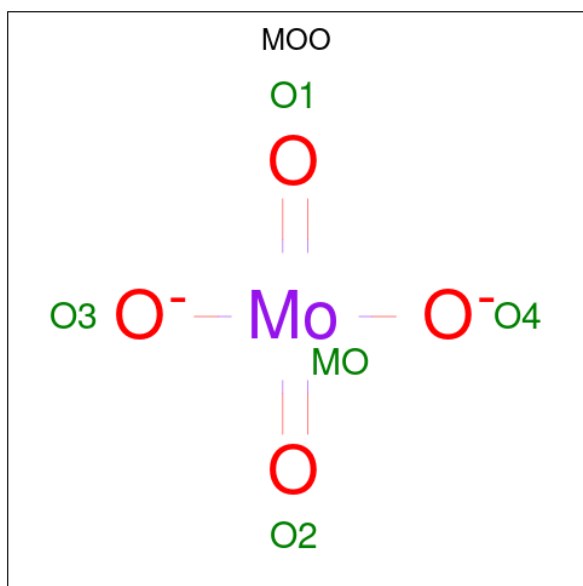
There are 3 unique types of molecules in this entry. The entry contains 5222 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ACID PHOSPHATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	0	0
			1694	1058	302	329	5			
1	B	222	Total	C	N	O	S	0	0	0
			1694	1058	302	329	5			
1	C	222	Total	C	N	O	S	0	0	0
			1694	1058	302	329	5			

- Molecule 2 is MOLYBDATE ION (CCD ID: MOO) (formula: MoO_4).



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

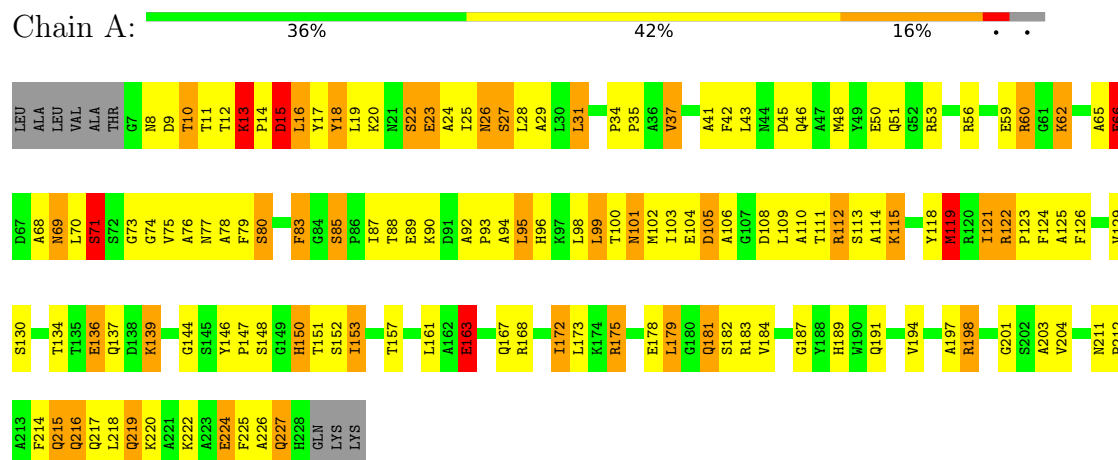
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	41	Total 41	O 41	0	0
3	B	41	Total 41	O 41	0	0
3	C	43	Total 43	O 43	0	0

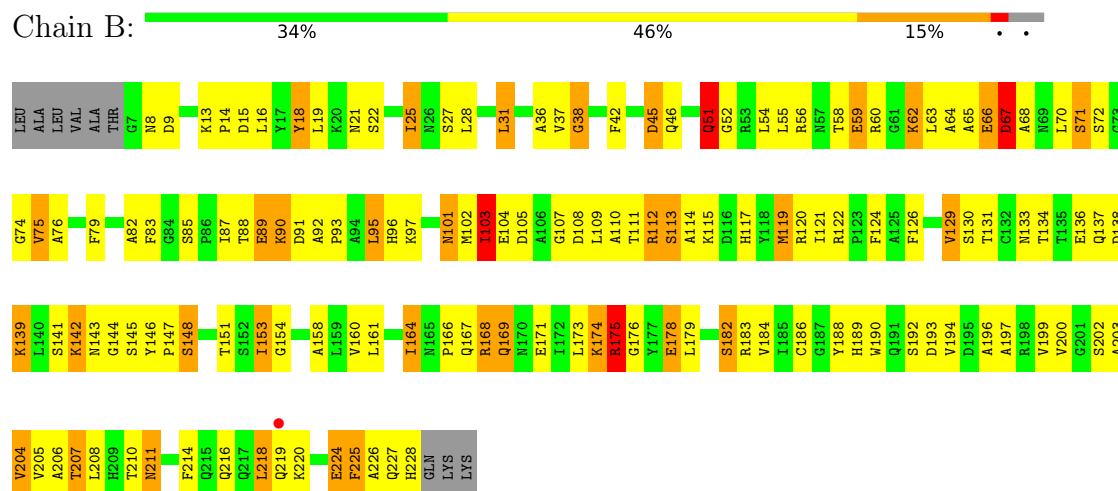
3 Residue-property plots

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.

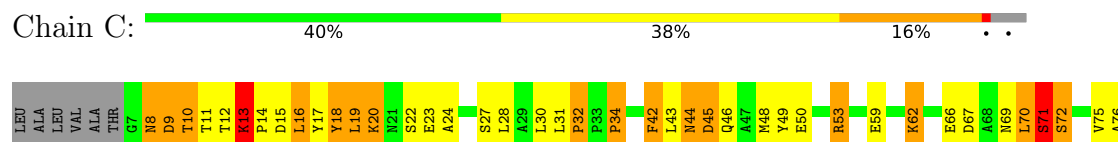
• Molecule 1: ACID PHOSPHATASE

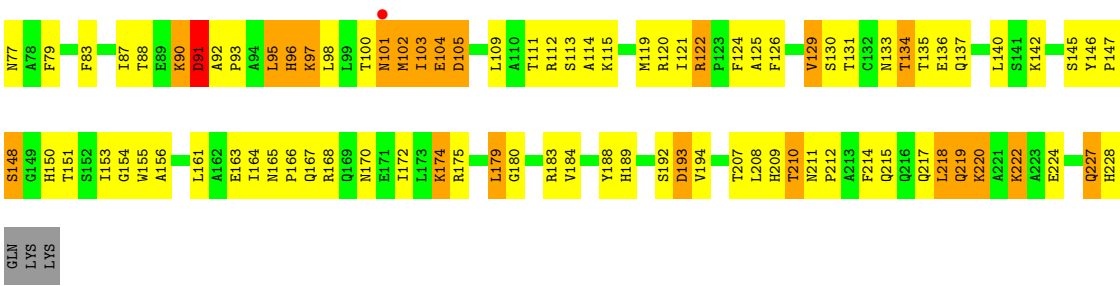


• Molecule 1: ACID PHOSPHATASE



• Molecule 1: ACID PHOSPHATASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	86.60Å 86.60Å 205.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.40 10.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	89.7 (10.00-2.40) 88.6 (10.00-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.40Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.212 , 0.280 0.201 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.591	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 75.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5222	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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: MOO

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	0.69	0/1729	1.14	11/2347 (0.5%)
1	B	0.79	0/1729	1.23	25/2347 (1.1%)
1	C	0.77	1/1729 (0.1%)	1.18	13/2347 (0.6%)
All	All	0.75	1/5187 (0.0%)	1.18	49/7041 (0.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	34	PRO	CA-C	-5.46	1.48	1.52

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112	ARG	N-CA-C	9.98	121.92	111.14
1	B	211	ASN	CA-C-N	9.27	128.88	119.24
1	B	211	ASN	C-N-CA	9.27	128.88	119.24
1	A	18	TYR	N-CA-C	-9.25	100.88	113.18
1	A	73	GLY	N-CA-C	-7.68	103.41	116.01
1	C	45	ASP	N-CA-C	-7.63	103.05	111.36
1	A	150	HIS	N-CA-C	-7.43	103.18	111.28
1	B	18	TYR	N-CA-C	-7.30	103.98	114.12
1	B	190	TRP	N-CA-C	-7.24	100.78	110.55
1	A	105	ASP	N-CA-C	-7.14	103.57	111.36
1	C	42	PHE	N-CA-C	-7.12	104.40	113.23
1	C	49	TYR	N-CA-C	-7.00	102.87	111.40
1	C	13	LYS	CA-C-N	6.92	128.49	119.84
1	C	13	LYS	C-N-CA	6.92	128.49	119.84
1	B	225	PHE	N-CA-C	-6.81	105.12	113.50
1	B	199	VAL	N-CA-C	-6.69	104.24	110.53
1	B	186	CYS	N-CA-C	6.68	118.56	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	219	GLN	N-CA-C	-6.62	103.75	110.97
1	A	163	GLU	N-CA-C	-6.53	105.32	113.28
1	C	18	TYR	N-CA-C	-6.49	104.55	113.18
1	A	15	ASP	N-CA-C	-6.46	105.43	113.38
1	B	227	GLN	N-CA-C	-5.93	104.91	113.21
1	A	13	LYS	CA-C-N	5.91	127.23	119.84
1	A	13	LYS	C-N-CA	5.91	127.23	119.84
1	B	56	ARG	N-CA-C	5.88	118.44	111.33
1	B	67	ASP	N-CA-C	-5.77	105.86	114.64
1	B	103	ILE	N-CA-C	5.77	116.23	110.23
1	B	169	GLN	N-CA-C	5.72	117.52	111.28
1	B	175	ARG	N-CA-C	-5.68	104.99	111.07
1	C	70	LEU	N-CA-C	-5.64	106.32	113.43
1	C	105	ASP	N-CA-C	-5.45	105.03	110.97
1	A	66	GLU	N-CA-C	5.44	117.96	111.71
1	B	38	GLY	N-CA-C	-5.42	107.55	115.63
1	B	45	ASP	N-CA-C	-5.38	105.31	111.07
1	B	31	LEU	CA-C-N	5.34	123.50	119.66
1	B	31	LEU	C-N-CA	5.34	123.50	119.66
1	B	70	LEU	N-CA-C	-5.26	108.12	114.75
1	A	83	PHE	N-CA-C	-5.25	106.66	113.16
1	C	44	ASN	N-CA-C	-5.20	107.11	113.50
1	B	218	LEU	N-CA-C	-5.18	105.71	111.36
1	C	43	LEU	N-CA-C	-5.14	106.27	112.54
1	B	51	GLN	N-CA-C	-5.12	105.60	111.07
1	B	130	SER	N-CA-C	5.07	117.79	110.28
1	B	204	VAL	CB-CA-C	-5.06	105.31	112.14
1	A	74	GLY	N-CA-C	-5.03	108.07	114.16
1	B	95	LEU	N-CA-C	-5.02	105.72	111.14
1	C	32	PRO	CA-C-N	-5.01	115.22	120.38
1	C	32	PRO	C-N-CA	-5.01	115.22	120.38
1	B	105	ASP	N-CA-C	-5.01	105.90	111.36

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	1694	0	1654	139	0
1	B	1694	0	1654	124	0
1	C	1694	0	1654	135	0
2	A	5	0	0	1	0
2	B	5	0	0	1	0
2	C	5	0	0	4	0
3	A	41	0	0	3	0
3	B	41	0	0	5	0
3	C	43	0	0	1	0
All	All	5222	0	4962	397	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 39.

All (397) 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:122:ARG:HG2	1:C:122:ARG:HH11	1.26	1.00
1:C:8:ASN:ND2	1:C:13:LYS:HG3	1.78	0.97
1:C:19:LEU:HD21	1:C:208:LEU:HD23	1.47	0.97
1:A:111:THR:HG22	1:A:147:PRO:HG2	1.54	0.89
1:B:166:PRO:O	1:B:169:GLN:HG2	1.72	0.88
1:C:211:ASN:O	1:C:215:GLN:HG2	1.76	0.86
1:C:91:ASP:C	1:C:93:PRO:HD3	2.02	0.85
1:C:101:ASN:HD22	1:C:101:ASN:H	1.23	0.83
1:C:8:ASN:HD21	1:C:13:LYS:HG3	1.40	0.83
1:A:184:VAL:HG23	1:A:194:VAL:HG21	1.60	0.81
1:A:80:SER:HA	1:A:87:ILE:HD12	1.64	0.80
1:B:18:TYR:CE2	1:B:101:ASN:HB3	2.16	0.80
1:B:8:ASN:HD22	1:B:13:LYS:HG3	1.45	0.79
1:A:100:THR:O	1:A:103:ILE:HG13	1.83	0.78
1:A:139:LYS:H	1:A:139:LYS:HD2	1.47	0.78
1:B:110:ALA:HB2	1:B:204:VAL:CG1	2.13	0.78
1:B:51:GLN:HG2	3:B:1031:HOH:O	1.83	0.78
1:B:62:LYS:O	1:B:66:GLU:HG3	1.85	0.76
1:A:198:ARG:HG3	1:A:198:ARG:HH11	1.48	0.76
1:B:87:ILE:HG23	1:B:95:LEU:HD23	1.67	0.76
1:C:212:PRO:O	1:C:215:GLN:HB2	1.84	0.75
1:A:181:GLN:HE22	1:A:191:GLN:HE22	1.33	0.75
1:C:168:ARG:O	1:C:172:ILE:HG13	1.86	0.75
1:A:59:GLU:O	1:A:62:LYS:HB3	1.88	0.74
1:C:215:GLN:HA	1:C:215:GLN:HE21	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:THR:HG23	1:C:180:GLY:HA3	1.67	0.74
1:C:131:THR:HG21	1:C:188:TYR:OH	1.88	0.73
1:B:110:ALA:HB2	1:B:204:VAL:HG11	1.69	0.73
1:B:75:VAL:HG11	1:B:103:ILE:HD11	1.70	0.72
1:A:211:ASN:O	1:A:215:GLN:HG2	1.89	0.72
1:C:88:THR:OG1	1:C:91:ASP:HB2	1.89	0.72
1:C:101:ASN:H	1:C:101:ASN:ND2	1.87	0.72
1:B:111:THR:O	1:B:115:LYS:HB2	1.90	0.71
1:C:150:HIS:HB2	2:C:1003:MOO:O2	1.91	0.71
1:C:184:VAL:HG23	1:C:194:VAL:HG21	1.72	0.71
1:B:19:LEU:HD21	1:B:208:LEU:HD23	1.72	0.71
1:C:122:ARG:HG2	1:C:122:ARG:NH1	2.00	0.71
1:C:12:THR:O	1:C:13:LYS:HG2	1.92	0.70
1:A:139:LYS:H	1:A:139:LYS:CD	2.02	0.70
1:C:164:ILE:O	1:C:166:PRO:HD3	1.91	0.69
1:A:34:PRO:HG3	1:A:146:TYR:CD2	2.28	0.69
1:B:136:GLU:HB3	1:B:139:LYS:HE3	1.74	0.69
1:B:183:ARG:NH1	2:B:1002:MOO:O1	2.26	0.69
1:C:44:ASN:O	1:C:48:MET:HG2	1.93	0.69
1:B:89:GLU:O	1:B:93:PRO:HB3	1.93	0.68
1:C:104:GLU:OE2	1:C:104:GLU:HA	1.93	0.68
1:B:226:ALA:HB3	3:B:1033:HOH:O	1.93	0.68
1:B:55:LEU:O	1:B:58:THR:HB	1.94	0.67
1:C:163:GLU:O	1:C:163:GLU:HG2	1.93	0.67
1:C:17:TYR:CZ	1:C:104:GLU:HB3	2.29	0.67
1:B:134:THR:HG22	1:B:137:GLN:OE1	1.94	0.67
1:A:37:VAL:HG23	3:A:1036:HOH:O	1.94	0.66
1:B:67:ASP:OD2	1:B:179:LEU:HD12	1.95	0.66
1:B:226:ALA:CB	3:B:1033:HOH:O	2.43	0.66
1:B:28:LEU:HB2	1:B:113:SER:HB2	1.78	0.66
1:C:218:LEU:HD12	1:C:218:LEU:O	1.95	0.66
1:B:184:VAL:HG23	1:B:194:VAL:HG21	1.77	0.65
1:B:122:ARG:HG2	1:B:145:SER:HB2	1.77	0.65
1:C:101:ASN:HD22	1:C:101:ASN:N	1.86	0.65
1:B:151:THR:HG21	1:B:194:VAL:O	1.97	0.65
1:A:87:ILE:CG1	1:A:95:LEU:HD13	2.27	0.65
1:B:148:SER:HB2	1:B:189:HIS:CD2	2.31	0.65
1:A:96:HIS:O	1:A:100:THR:HG23	1.97	0.64
1:C:10:THR:HG23	1:C:17:TYR:O	1.97	0.64
1:C:83:PHE:CE1	1:C:161:LEU:HD22	2.32	0.64
1:C:62:LYS:O	1:C:66:GLU:HG3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:LEU:O	1:C:101:ASN:ND2	2.30	0.64
1:C:92:ALA:N	1:C:93:PRO:HD3	2.12	0.63
1:A:178:GLU:HA	1:A:178:GLU:OE1	1.99	0.63
1:C:28:LEU:HB2	1:C:113:SER:HB2	1.80	0.63
1:A:10:THR:O	1:A:14:PRO:HB3	1.99	0.63
1:A:108:ASP:CG	1:A:112:ARG:HH21	2.07	0.63
1:A:25:ILE:HD13	1:A:203:ALA:HB3	1.80	0.63
1:C:103:ILE:HG22	1:C:104:GLU:OE2	1.99	0.63
1:C:131:THR:HG21	1:C:188:TYR:CZ	2.35	0.62
1:C:109:LEU:HD23	1:C:112:ARG:HH21	1.62	0.62
1:C:18:TYR:HB2	1:C:105:ASP:OD2	2.00	0.62
1:A:212:PRO:HA	1:A:215:GLN:HG3	1.81	0.62
1:A:118:TYR:O	1:A:119:MET:C	2.43	0.62
1:A:227:GLN:NE2	1:A:227:GLN:HA	2.15	0.62
1:C:150:HIS:CB	1:C:183:ARG:HD3	2.30	0.62
1:A:56:ARG:NH2	1:A:187:GLY:HA3	2.15	0.61
2:C:1003:MOO:O2	2:C:1003:MOO:MO	1.71	0.61
1:A:26:ASN:HB3	1:A:29:ALA:HB3	1.83	0.60
1:A:12:THR:OG1	1:A:13:LYS:HG2	2.01	0.60
1:A:37:VAL:HG13	1:A:42:PHE:CE2	2.36	0.60
1:C:122:ARG:HG2	1:C:188:TYR:O	2.02	0.60
1:B:82:ALA:O	1:B:168:ARG:NH1	2.35	0.59
1:A:17:TYR:CZ	1:A:104:GLU:HB3	2.37	0.59
1:A:27:SER:OG	1:A:113:SER:HB3	2.02	0.59
1:C:137:GLN:HA	1:C:188:TYR:HE1	1.67	0.59
1:B:63:LEU:C	1:B:63:LEU:HD23	2.27	0.59
1:B:63:LEU:HA	1:B:66:GLU:CD	2.27	0.59
1:C:164:ILE:C	1:C:166:PRO:HD3	2.27	0.59
1:A:98:LEU:HB2	1:A:217:GLN:HG3	1.85	0.59
1:B:115:LYS:NZ	1:B:144:GLY:O	2.36	0.59
1:B:216:GLN:O	1:B:220:LYS:HG3	2.03	0.59
1:C:134:THR:O	1:C:134:THR:HG22	2.03	0.59
1:A:172:ILE:HG22	1:A:173:LEU:N	2.16	0.59
1:C:83:PHE:O	1:C:168:ARG:HD3	2.03	0.59
1:A:15:ASP:C	1:A:16:LEU:HG	2.28	0.58
1:A:25:ILE:HD13	1:A:203:ALA:CB	2.32	0.58
1:B:37:VAL:HG22	1:B:42:PHE:CE2	2.38	0.58
1:C:183:ARG:HH21	1:C:188:TYR:CB	2.16	0.58
1:B:136:GLU:HG2	1:B:139:LYS:NZ	2.17	0.58
2:C:1003:MOO:MO	2:C:1003:MOO:O4	1.73	0.58
1:C:111:THR:O	1:C:115:LYS:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:GLY:O	1:A:204:VAL:HG12	2.02	0.58
1:B:31:LEU:CD1	1:B:147:PRO:HG3	2.33	0.58
1:C:105:ASP:OD1	1:C:109:LEU:HD12	2.04	0.58
1:C:114:ALA:HB3	1:C:147:PRO:HD3	1.86	0.58
1:B:220:LYS:O	1:B:224:GLU:HB3	2.03	0.57
1:A:51:GLN:HG2	3:C:1026:HOH:O	2.04	0.57
1:A:17:TYR:HD1	1:A:109:LEU:CD1	2.17	0.57
1:A:136:GLU:HA	1:A:139:LYS:HD3	1.87	0.57
1:C:131:THR:HG22	1:C:137:GLN:OE1	2.05	0.57
1:A:163:GLU:O	1:A:163:GLU:HG3	2.04	0.56
1:C:9:ASP:OD2	1:C:9:ASP:N	2.39	0.56
1:C:218:LEU:O	1:C:222:LYS:HD3	2.04	0.56
1:A:69:ASN:N	1:A:69:ASN:ND2	2.52	0.56
1:C:27:SER:O	1:C:31:LEU:HB2	2.05	0.56
1:C:122:ARG:NH1	1:C:122:ARG:CG	2.67	0.56
1:B:224:GLU:O	1:B:224:GLU:HG3	2.03	0.56
1:C:10:THR:HG23	1:C:17:TYR:C	2.30	0.56
1:A:53:ARG:HG2	1:A:53:ARG:NH2	2.21	0.56
1:C:34:PRO:HB3	1:C:146:TYR:CG	2.41	0.56
1:C:98:LEU:HG	1:C:102:MET:HE3	1.87	0.55
1:A:18:TYR:CZ	1:A:101:ASN:HB3	2.40	0.55
1:A:94:ALA:HA	1:A:217:GLN:NE2	2.21	0.55
1:A:157:THR:HG22	1:A:157:THR:O	2.05	0.55
1:B:171:GLU:N	1:B:171:GLU:OE1	2.35	0.55
1:A:53:ARG:HG2	1:A:53:ARG:HH21	1.72	0.55
1:A:99:LEU:HG	1:A:157:THR:HG23	1.89	0.55
1:A:17:TYR:HD1	1:A:109:LEU:HD11	1.71	0.55
1:A:108:ASP:OD2	1:A:112:ARG:NH2	2.29	0.55
1:B:64:ALA:HA	1:B:182:SER:OG	2.06	0.55
1:A:114:ALA:O	1:A:118:TYR:HD2	1.90	0.54
1:B:31:LEU:HD12	1:B:147:PRO:HG3	1.90	0.54
1:A:19:LEU:HD12	1:A:105:ASP:HB3	1.89	0.54
1:A:50:GLU:OE2	1:A:50:GLU:HA	2.07	0.54
1:C:75:VAL:HG13	1:C:76:ALA:N	2.23	0.53
1:A:9:ASP:HA	1:A:17:TYR:CD1	2.44	0.53
1:A:24:ALA:HB2	1:A:109:LEU:HD22	1.90	0.53
1:B:83:PHE:CD2	1:B:161:LEU:HD22	2.43	0.53
1:C:87:ILE:HG23	1:C:95:LEU:HG	1.91	0.53
1:C:16:LEU:O	1:C:104:GLU:HB2	2.08	0.53
1:A:102:MET:HA	1:A:105:ASP:OD2	2.08	0.53
1:B:131:THR:HG21	1:B:188:TYR:CE1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:GLU:OE2	1:C:104:GLU:CA	2.55	0.53
1:A:106:ALA:O	1:A:110:ALA:HB3	2.07	0.53
1:B:63:LEU:HA	1:B:66:GLU:OE2	2.09	0.53
1:B:136:GLU:CB	1:B:139:LYS:HE3	2.39	0.53
1:A:98:LEU:HB2	1:A:217:GLN:CG	2.39	0.52
1:A:15:ASP:OD2	1:A:15:ASP:N	2.43	0.52
1:B:134:THR:HG22	1:B:137:GLN:CD	2.34	0.52
1:C:72:SER:O	1:C:72:SER:OG	2.26	0.52
1:C:148:SER:HB2	1:C:189:HIS:CD2	2.43	0.52
1:A:87:ILE:HG12	1:A:95:LEU:HD13	1.90	0.52
1:B:9:ASP:HB3	1:B:21:ASN:ND2	2.24	0.52
1:B:204:VAL:HG23	1:B:205:VAL:N	2.23	0.52
1:B:121:ILE:CG1	1:B:122:ARG:H	2.23	0.52
1:A:19:LEU:HA	1:A:23:GLU:OE2	2.09	0.52
1:B:131:THR:HG21	1:B:188:TYR:CZ	2.44	0.52
1:B:8:ASN:ND2	1:B:13:LYS:HG3	2.21	0.52
1:A:13:LYS:NZ	1:A:13:LYS:HB3	2.25	0.52
1:C:215:GLN:HA	1:C:215:GLN:NE2	2.22	0.52
1:A:9:ASP:OD1	1:A:9:ASP:C	2.53	0.52
1:B:184:VAL:CG2	1:B:194:VAL:HG21	2.40	0.52
1:B:154:GLY:HA2	1:B:179:LEU:HD23	1.91	0.51
1:C:120:ARG:NH1	1:C:193:ASP:OD1	2.42	0.51
1:B:45:ASP:OD1	1:B:120:ARG:NH2	2.41	0.51
1:A:10:THR:HA	1:A:17:TYR:HB2	1.91	0.51
1:A:214:PHE:CZ	1:A:218:LEU:HD22	2.46	0.51
1:C:120:ARG:HB3	1:C:145:SER:HB3	1.93	0.51
1:A:59:GLU:OE1	1:A:62:LYS:HD2	2.11	0.51
1:C:16:LEU:HA	1:C:101:ASN:HA	1.93	0.51
1:C:140:LEU:HD13	2:C:1003:MOO:O3	2.11	0.51
1:A:227:GLN:NE2	1:A:227:GLN:CA	2.73	0.51
1:B:88:THR:OG1	1:B:91:ASP:HB2	2.11	0.51
1:C:129:VAL:O	1:C:129:VAL:HG12	2.11	0.51
1:A:92:ALA:HB1	1:A:95:LEU:HB2	1.93	0.51
1:A:227:GLN:N	1:A:227:GLN:CD	2.68	0.51
1:B:58:THR:HG22	1:B:60:ARG:H	1.76	0.50
1:B:72:SER:C	1:B:74:GLY:H	2.19	0.50
1:B:42:PHE:O	1:B:45:ASP:HB2	2.11	0.50
1:C:183:ARG:NH2	1:C:188:TYR:CG	2.78	0.50
1:B:90:LYS:NZ	1:B:90:LYS:HB3	2.26	0.49
1:B:102:MET:HE1	1:B:160:VAL:HG21	1.94	0.49
1:C:83:PHE:O	1:C:165:ASN:ND2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ARG:HG3	1:A:198:ARG:NH1	2.23	0.49
1:C:120:ARG:HH12	1:C:192:SER:HG	1.56	0.49
1:A:87:ILE:HG13	1:A:95:LEU:HD13	1.94	0.49
1:A:28:LEU:HA	1:A:114:ALA:HB2	1.93	0.49
1:B:31:LEU:HD13	1:B:196:ALA:HB1	1.94	0.49
1:A:34:PRO:HG3	1:A:146:TYR:CG	2.47	0.49
1:A:62:LYS:O	1:A:65:ALA:HB3	2.11	0.49
1:C:150:HIS:CG	1:C:183:ARG:NH1	2.81	0.49
1:C:9:ASP:HA	1:C:17:TYR:CD1	2.48	0.49
1:A:75:VAL:HG13	1:A:76:ALA:N	2.28	0.49
1:C:95:LEU:O	1:C:96:HIS:C	2.55	0.49
1:A:10:THR:HG22	1:A:20:LYS:HG2	1.95	0.48
1:A:83:PHE:CE1	1:A:95:LEU:HD11	2.48	0.48
1:A:121:ILE:HG13	1:A:122:ARG:O	2.13	0.48
1:A:25:ILE:HD11	1:A:203:ALA:C	2.39	0.48
1:A:79:PHE:O	1:A:80:SER:C	2.57	0.48
1:B:151:THR:HB	1:B:197:ALA:CB	2.44	0.48
1:B:79:PHE:CE2	1:B:158:ALA:HB2	2.48	0.48
1:C:83:PHE:HE1	1:C:161:LEU:HD22	1.76	0.48
1:A:126:PHE:HE1	1:B:54:LEU:HD11	1.77	0.48
1:C:88:THR:C	1:C:90:LYS:H	2.20	0.48
1:A:122:ARG:H	1:A:122:ARG:HG2	1.28	0.48
1:C:109:LEU:HD23	1:C:112:ARG:NH2	2.28	0.48
1:B:121:ILE:CG1	1:B:122:ARG:N	2.76	0.48
1:C:95:LEU:O	1:C:97:LYS:N	2.47	0.48
1:A:35:PRO:HB3	1:A:41:ALA:CB	2.44	0.48
1:A:62:LYS:O	1:A:66:GLU:OE2	2.31	0.48
1:B:58:THR:HG22	1:B:59:GLU:N	2.28	0.48
1:B:107:GLY:HA3	1:B:153:ILE:HD11	1.96	0.48
1:B:126:PHE:O	1:C:53:ARG:NH2	2.46	0.48
1:B:89:GLU:OE2	1:B:90:LYS:N	2.48	0.47
1:C:87:ILE:HA	1:C:92:ALA:HB3	1.95	0.47
1:C:122:ARG:NH1	1:C:188:TYR:O	2.47	0.47
1:B:207:THR:O	1:B:210:THR:OG1	2.26	0.47
1:B:208:LEU:O	1:B:214:PHE:CD1	2.68	0.47
1:B:95:LEU:CD1	1:B:164:ILE:HD13	2.44	0.47
1:B:75:VAL:CG1	1:B:76:ALA:N	2.78	0.47
1:C:227:GLN:HA	1:C:227:GLN:OE1	2.15	0.47
1:B:52:GLY:O	1:B:55:LEU:HB2	2.14	0.47
1:B:203:ALA:O	1:B:206:ALA:HB3	2.14	0.47
1:C:83:PHE:C	1:C:168:ARG:HD3	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:HIS:HB3	1:C:183:ARG:HD3	1.95	0.47
1:A:78:ALA:HB1	1:A:179:LEU:HD11	1.96	0.47
1:A:124:PHE:CD1	1:A:125:ALA:N	2.82	0.47
1:B:148:SER:HB2	1:B:189:HIS:CG	2.50	0.47
1:B:16:LEU:O	1:B:104:GLU:HB2	2.16	0.46
1:B:21:ASN:ND2	1:B:109:LEU:HD21	2.30	0.46
1:C:102:MET:O	1:C:103:ILE:C	2.57	0.46
1:C:102:MET:HE2	1:C:214:PHE:HE1	1.81	0.46
1:C:184:VAL:CG2	1:C:194:VAL:HG21	2.44	0.46
1:A:25:ILE:HD11	1:A:204:VAL:N	2.31	0.46
1:B:13:LYS:N	1:B:14:PRO:CD	2.77	0.46
1:B:119:MET:O	1:B:120:ARG:C	2.57	0.46
1:A:150:HIS:HB2	2:A:1001:MOO:O2	2.15	0.46
1:C:150:HIS:CD2	1:C:183:ARG:HH11	2.34	0.46
1:B:142:LYS:HD3	1:B:142:LYS:HA	1.73	0.46
1:C:95:LEU:O	1:C:98:LEU:N	2.49	0.46
1:C:134:THR:O	1:C:135:THR:C	2.58	0.46
1:A:92:ALA:N	1:A:93:PRO:CD	2.78	0.46
1:B:63:LEU:HD23	1:B:63:LEU:O	2.15	0.46
1:A:83:PHE:C	1:A:85:SER:H	2.23	0.46
1:C:79:PHE:CZ	1:C:179:LEU:HD23	2.50	0.46
1:A:95:LEU:HD21	1:A:161:LEU:HD21	1.98	0.46
1:C:17:TYR:HE1	1:C:109:LEU:HG	1.80	0.46
1:C:75:VAL:HG11	1:C:103:ILE:HD11	1.98	0.46
1:C:219:GLN:O	1:C:220:LYS:C	2.59	0.46
1:B:121:ILE:HG12	1:B:122:ARG:H	1.80	0.46
1:B:143:ASN:O	1:B:144:GLY:C	2.59	0.46
1:C:19:LEU:HA	1:C:20:LYS:HE3	1.98	0.46
1:C:88:THR:C	1:C:90:LYS:N	2.73	0.46
1:A:60:ARG:NH2	1:A:178:GLU:OE1	2.50	0.45
1:A:8:ASN:OD1	1:A:13:LYS:HD3	2.16	0.45
1:A:45:ASP:O	1:A:48:MET:HB2	2.16	0.45
1:C:8:ASN:HD22	1:C:13:LYS:HG3	1.75	0.45
1:C:170:ASN:O	1:C:174:LYS:HB2	2.15	0.45
1:A:95:LEU:HD21	1:A:161:LEU:CD2	2.47	0.45
1:A:148:SER:HA	1:A:189:HIS:CE1	2.52	0.45
1:B:28:LEU:HD13	1:B:117:HIS:HB3	1.98	0.45
1:B:166:PRO:O	1:B:168:ARG:N	2.49	0.45
1:A:60:ARG:NH1	1:A:182:SER:OG	2.48	0.45
1:A:151:THR:C	1:A:153:ILE:H	2.25	0.45
1:B:121:ILE:HG12	1:B:122:ARG:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:GLN:N	1:C:167:GLN:OE1	2.50	0.45
1:A:17:TYR:CD1	1:A:109:LEU:HD11	2.50	0.45
1:B:66:GLU:HG3	1:B:66:GLU:H	1.57	0.45
1:B:92:ALA:HB2	1:B:228:HIS:HE1	1.80	0.45
1:B:166:PRO:C	1:B:168:ARG:H	2.24	0.45
1:C:13:LYS:N	1:C:14:PRO:CD	2.79	0.45
1:C:92:ALA:N	1:C:93:PRO:CD	2.79	0.45
1:B:28:LEU:CB	1:B:113:SER:HB2	2.45	0.45
1:B:173:LEU:HD23	1:B:173:LEU:HA	1.82	0.45
1:C:131:THR:HG23	1:C:133:ASN:H	1.82	0.45
1:A:134:THR:O	1:A:137:GLN:HB3	2.17	0.45
1:B:28:LEU:HD13	1:B:117:HIS:CB	2.47	0.45
1:B:51:GLN:CG	3:B:1031:HOH:O	2.52	0.45
1:A:129:VAL:HG12	1:A:130:SER:N	2.32	0.45
1:B:93:PRO:HA	1:B:96:HIS:HB3	1.97	0.45
1:B:117:HIS:C	1:B:117:HIS:ND1	2.75	0.45
1:C:18:TYR:OH	1:C:98:LEU:HD12	2.17	0.45
1:C:50:GLU:OE1	1:C:50:GLU:HA	2.16	0.45
1:A:139:LYS:HD2	1:A:139:LYS:N	2.22	0.44
1:A:225:PHE:C	1:A:227:GLN:N	2.74	0.44
1:A:17:TYR:CD1	1:A:109:LEU:CD1	2.99	0.44
1:A:88:THR:O	1:A:96:HIS:HB2	2.17	0.44
1:A:227:GLN:HA	1:A:227:GLN:HE21	1.82	0.44
1:B:58:THR:CG2	1:B:59:GLU:N	2.80	0.44
1:C:42:PHE:O	1:C:46:GLN:HG3	2.18	0.44
1:C:70:LEU:O	1:C:71:SER:C	2.60	0.44
1:A:92:ALA:N	1:A:93:PRO:HD3	2.33	0.44
1:C:87:ILE:CG2	1:C:95:LEU:HG	2.47	0.44
1:C:133:ASN:OD1	1:C:133:ASN:C	2.61	0.44
1:C:207:THR:O	1:C:210:THR:HB	2.17	0.44
1:A:16:LEU:O	1:A:104:GLU:HB2	2.17	0.44
1:B:114:ALA:HB3	1:B:147:PRO:HD3	2.00	0.44
1:C:148:SER:HB2	1:C:189:HIS:CG	2.53	0.44
1:C:164:ILE:HG12	1:C:222:LYS:HG3	1.99	0.44
1:A:37:VAL:HG13	1:A:42:PHE:CD2	2.52	0.44
1:C:98:LEU:HA	1:C:101:ASN:HD21	1.82	0.44
1:A:115:LYS:NZ	1:A:144:GLY:O	2.51	0.44
1:C:17:TYR:CE1	1:C:104:GLU:HB3	2.53	0.44
1:A:20:LYS:C	1:A:22:SER:N	2.73	0.44
1:A:198:ARG:HG3	3:A:1012:HOH:O	2.17	0.44
1:B:25:ILE:HD13	1:B:203:ALA:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:ALA:O	1:B:115:LYS:C	2.60	0.44
1:C:121:ILE:HG21	1:C:126:PHE:HD1	1.83	0.44
1:B:36:ALA:O	1:B:42:PHE:HB2	2.16	0.43
1:A:198:ARG:NH1	1:A:198:ARG:CG	2.81	0.43
1:B:108:ASP:O	1:B:112:ARG:HB2	2.18	0.43
1:B:131:THR:HG23	1:B:137:GLN:OE1	2.18	0.43
1:A:70:LEU:O	1:A:71:SER:C	2.59	0.43
1:A:121:ILE:HG22	3:A:1019:HOH:O	2.18	0.43
1:A:151:THR:CG2	1:A:197:ALA:HB3	2.48	0.43
1:B:137:GLN:HA	1:B:188:TYR:HE1	1.84	0.43
1:C:31:LEU:HA	1:C:32:PRO:HD3	1.81	0.43
1:C:124:PHE:CD1	1:C:125:ALA:N	2.86	0.43
1:C:131:THR:OG1	1:C:188:TYR:CE2	2.67	0.43
1:C:208:LEU:HD13	1:C:214:PHE:CE1	2.53	0.43
1:A:126:PHE:CE1	1:B:54:LEU:HD11	2.53	0.43
1:A:224:GLU:O	1:A:224:GLU:HG2	2.18	0.43
1:A:123:PRO:HG2	1:A:187:GLY:O	2.19	0.43
1:A:151:THR:HG21	1:A:197:ALA:HB3	2.01	0.43
1:B:8:ASN:HD22	1:B:13:LYS:HE3	1.83	0.43
1:B:67:ASP:CG	1:B:175:ARG:HH22	2.27	0.43
1:B:154:GLY:CA	1:B:179:LEU:HD23	2.49	0.43
1:C:136:GLU:O	1:C:137:GLN:C	2.61	0.43
1:A:105:ASP:HA	1:A:109:LEU:HD12	2.00	0.43
1:A:108:ASP:OD1	1:A:108:ASP:C	2.61	0.43
1:B:18:TYR:O	1:B:211:ASN:ND2	2.52	0.43
1:C:83:PHE:HD1	1:C:161:LEU:HD13	1.84	0.43
1:A:111:THR:O	1:A:112:ARG:C	2.62	0.43
1:C:98:LEU:HD13	1:C:217:GLN:HB3	2.01	0.43
1:A:98:LEU:HD11	1:A:214:PHE:CE1	2.54	0.42
1:C:75:VAL:CG1	1:C:103:ILE:HD11	2.48	0.42
1:C:92:ALA:HB2	1:C:228:HIS:CE1	2.53	0.42
1:B:146:TYR:HB2	1:B:193:ASP:OD1	2.19	0.42
1:B:166:PRO:C	1:B:168:ARG:N	2.78	0.42
1:C:8:ASN:ND2	1:C:12:THR:OG1	2.52	0.42
1:B:115:LYS:HE2	1:B:147:PRO:O	2.19	0.42
1:B:124:PHE:CD2	1:B:131:THR:HG22	2.55	0.42
1:C:70:LEU:HD21	1:C:179:LEU:HD11	2.01	0.42
1:A:216:GLN:O	1:A:219:GLN:HB3	2.19	0.42
1:A:66:GLU:C	1:A:68:ALA:H	2.27	0.42
1:B:124:PHE:HB2	1:B:129:VAL:O	2.19	0.42
1:C:42:PHE:HA	1:C:45:ASP:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:GLU:OE1	1:C:209:HIS:HE1	2.02	0.42
1:B:87:ILE:CG2	1:B:95:LEU:HD23	2.44	0.42
1:C:153:ILE:O	1:C:154:GLY:C	2.63	0.42
1:C:155:TRP:O	1:C:156:ALA:C	2.62	0.42
1:C:165:ASN:OD1	1:C:165:ASN:C	2.62	0.42
1:A:25:ILE:HD11	1:A:204:VAL:HA	2.01	0.41
1:A:219:GLN:HG2	1:A:220:LYS:N	2.34	0.41
1:A:224:GLU:O	1:A:227:GLN:HB2	2.20	0.41
1:A:183:ARG:HA	1:A:183:ARG:HD2	1.77	0.41
1:B:38:GLY:N	3:B:1009:HOH:O	2.33	0.41
1:C:70:LEU:O	1:C:72:SER:N	2.52	0.41
1:A:168:ARG:O	1:A:172:ILE:HD12	2.20	0.41
1:A:25:ILE:HD11	1:A:204:VAL:CA	2.51	0.41
1:C:9:ASP:O	1:C:13:LYS:N	2.53	0.41
1:A:31:LEU:HA	1:A:31:LEU:HD12	1.87	0.41
1:B:95:LEU:HD11	1:B:164:ILE:HD13	2.01	0.41
1:B:115:LYS:HA	1:B:146:TYR:O	2.20	0.41
1:A:136:GLU:O	1:A:139:LYS:HG2	2.20	0.41
1:A:79:PHE:CD2	1:A:175:ARG:HG2	2.55	0.41
1:A:121:ILE:HG12	1:A:126:PHE:HB2	2.02	0.41
1:B:65:ALA:C	1:B:67:ASP:H	2.29	0.41
1:B:27:SER:O	1:B:28:LEU:C	2.64	0.41
1:C:67:ASP:C	1:C:69:ASN:H	2.28	0.41
1:A:17:TYR:CZ	1:A:104:GLU:CB	3.03	0.41
1:A:35:PRO:HB3	1:A:41:ALA:HB3	2.02	0.41
1:A:146:TYR:HA	1:A:147:PRO:HA	1.81	0.41
1:B:174:LYS:O	1:B:178:GLU:HB2	2.20	0.41
1:C:24:ALA:HB2	1:C:109:LEU:HD22	2.02	0.41
1:A:75:VAL:CG1	1:A:76:ALA:N	2.83	0.41
1:B:18:TYR:CZ	1:B:101:ASN:HB3	2.54	0.41
1:B:68:ALA:HB3	1:B:133:ASN:OD1	2.21	0.41
1:B:110:ALA:HB2	1:B:204:VAL:HG13	2.01	0.41
1:B:197:ALA:O	1:B:200:VAL:HG23	2.21	0.41
1:A:225:PHE:O	1:A:226:ALA:C	2.63	0.40
1:B:204:VAL:CG2	1:B:205:VAL:N	2.83	0.40
1:C:102:MET:HE2	1:C:214:PHE:CE1	2.56	0.40
1:C:150:HIS:CD2	1:C:183:ARG:NH1	2.89	0.40
1:C:17:TYR:CE1	1:C:109:LEU:HG	2.56	0.40
1:A:42:PHE:CE2	1:A:46:GLN:NE2	2.89	0.40
1:A:108:ASP:OD1	1:A:112:ARG:HB2	2.21	0.40
1:B:15:ASP:C	1:B:101:ASN:ND2	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:ARG:O	1:B:176:GLY:C	2.65	0.40
1:C:113:SER:O	1:C:114:ALA:C	2.63	0.40
1:A:66:GLU:H	1:A:66:GLU:HG2	1.43	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	220/231 (95%)	193 (88%)	24 (11%)	3 (1%)	9	13
1	B	220/231 (95%)	192 (87%)	26 (12%)	2 (1%)	14	22
1	C	220/231 (95%)	180 (82%)	32 (14%)	8 (4%)	2	2
All	All	660/693 (95%)	565 (86%)	82 (12%)	13 (2%)	6	7

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	71	SER
1	A	112	ARG
1	C	95	LEU
1	C	96	HIS
1	C	134	THR
1	B	71	SER
1	B	167	GLN
1	C	91	ASP
1	A	71	SER
1	C	130	SER
1	A	119	MET
1	C	9	ASP
1	C	103	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	177/184 (96%)	131 (74%)	46 (26%)	0	0
1	B	177/184 (96%)	139 (78%)	38 (22%)	1	1
1	C	177/184 (96%)	138 (78%)	39 (22%)	1	1
All	All	531/552 (96%)	408 (77%)	123 (23%)	1	1

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	THR
1	A	11	THR
1	A	13	LYS
1	A	15	ASP
1	A	16	LEU
1	A	22	SER
1	A	23	GLU
1	A	26	ASN
1	A	27	SER
1	A	31	LEU
1	A	37	VAL
1	A	43	LEU
1	A	60	ARG
1	A	62	LYS
1	A	66	GLU
1	A	69	ASN
1	A	71	SER
1	A	77	ASN
1	A	80	SER
1	A	85	SER
1	A	89	GLU
1	A	90	LYS
1	A	95	LEU
1	A	99	LEU
1	A	101	ASN
1	A	115	LYS

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Mol	Chain	Res	Type
1	A	119	MET
1	A	121	ILE
1	A	122	ARG
1	A	136	GLU
1	A	139	LYS
1	A	152	SER
1	A	153	ILE
1	A	163	GLU
1	A	167	GLN
1	A	172	ILE
1	A	175	ARG
1	A	179	LEU
1	A	181	GLN
1	A	198	ARG
1	A	215	GLN
1	A	216	GLN
1	A	219	GLN
1	A	222	LYS
1	A	224	GLU
1	A	227	GLN
1	B	22	SER
1	B	25	ILE
1	B	46	GLN
1	B	51	GLN
1	B	59	GLU
1	B	62	LYS
1	B	66	GLU
1	B	67	ASP
1	B	71	SER
1	B	75	VAL
1	B	85	SER
1	B	89	GLU
1	B	90	LYS
1	B	97	LYS
1	B	101	ASN
1	B	103	ILE
1	B	113	SER
1	B	119	MET
1	B	129	VAL
1	B	138	ASP
1	B	139	LYS
1	B	141	SER

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Mol	Chain	Res	Type
1	B	142	LYS
1	B	148	SER
1	B	153	ILE
1	B	164	ILE
1	B	168	ARG
1	B	174	LYS
1	B	175	ARG
1	B	178	GLU
1	B	182	SER
1	B	192	SER
1	B	202	SER
1	B	207	THR
1	B	218	LEU
1	B	219	GLN
1	B	224	GLU
1	B	225	PHE
1	C	8	ASN
1	C	10	THR
1	C	11	THR
1	C	13	LYS
1	C	15	ASP
1	C	16	LEU
1	C	19	LEU
1	C	20	LYS
1	C	22	SER
1	C	23	GLU
1	C	30	LEU
1	C	53	ARG
1	C	59	GLU
1	C	62	LYS
1	C	71	SER
1	C	72	SER
1	C	77	ASN
1	C	90	LYS
1	C	91	ASP
1	C	97	LYS
1	C	100	THR
1	C	101	ASN
1	C	102	MET
1	C	104	GLU
1	C	119	MET
1	C	122	ARG

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Mol	Chain	Res	Type
1	C	129	VAL
1	C	142	LYS
1	C	148	SER
1	C	174	LYS
1	C	175	ARG
1	C	179	LEU
1	C	193	ASP
1	C	210	THR
1	C	218	LEU
1	C	220	LYS
1	C	222	LYS
1	C	224	GLU
1	C	227	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	51	GLN
1	A	57	ASN
1	A	77	ASN
1	A	133	ASN
1	A	165	ASN
1	A	167	GLN
1	A	181	GLN
1	A	216	GLN
1	A	227	GLN
1	B	8	ASN
1	B	21	ASN
1	B	44	ASN
1	B	46	GLN
1	B	57	ASN
1	B	101	ASN
1	B	219	GLN
1	B	228	HIS
1	C	8	ASN
1	C	101	ASN
1	C	215	GLN

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 ⓘ

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	MOO	C	1003	1	2,4,4	1.10	0	-		
2	MOO	A	1001	1	2,4,4	0.22	0	-		
2	MOO	B	1002	1	2,4,4	0.46	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 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1003	MOO	4	0
2	A	1001	MOO	1	0
2	B	1002	MOO	1	0

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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	222/231 (96%)	-0.42	0 100 100	13, 38, 70, 96	0
1	B	222/231 (96%)	-0.54	1 (0%) 87 85	12, 31, 65, 98	0
1	C	222/231 (96%)	-0.37	1 (0%) 87 85	9, 34, 69, 96	0
All	All	666/693 (96%)	-0.45	2 (0%) 90 88	9, 35, 69, 98	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	101	ASN	2.3
1	B	219	GLN	2.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MOO	A	1001	5/5	0.99	0.05	11,28,41,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MOO	B	1002	5/5	1.00	0.04	14,16,30,45	0
2	MOO	C	1003	5/5	1.00	0.05	2,10,35,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.