



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:19 PM UTC

PDB ID : 1PS7 / pdb_00001ps7
Title : Crystal structure of E.coli PdxA
Authors : Sivaraman, J.; Li, Y.; Banks, J.; Cane, D.E.; Matte, A.; Cygler, M.
Deposited on : 2003-06-20
Resolution : 2.47 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

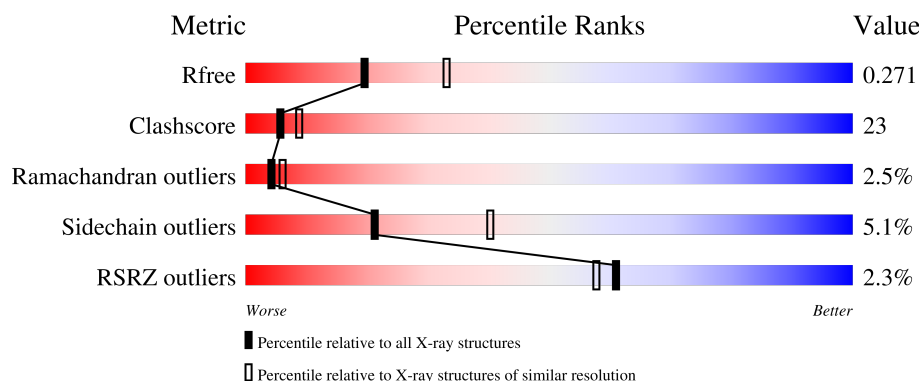
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.47 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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	329	2% 58% 37% . .
1	B	329	% 63% 31% 5%
1	C	329	5% 50% 44% 5%
1	D	329	2% 57% 38% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10026 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 4-hydroxythreonine-4-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	Se	0	0	0
			2396	1525	418	442	4	7			
1	B	328	Total	C	N	O	S	Se	0	0	0
			2388	1521	418	438	4	7			
1	C	328	Total	C	N	O	S	Se	0	0	0
			2396	1525	418	442	4	7			
1	D	328	Total	C	N	O	S	Se	0	0	0
			2388	1521	418	438	4	7			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	49	MSE	MET	modified residue	UNP P19624
A	151	MSE	MET	modified residue	UNP P19624
A	152	MSE	MET	modified residue	UNP P19624
A	218	MSE	MET	modified residue	UNP P19624
A	238	MSE	MET	modified residue	UNP P19624
A	264	MSE	MET	modified residue	UNP P19624
A	324	MSE	MET	modified residue	UNP P19624
B	49	MSE	MET	modified residue	UNP P19624
B	151	MSE	MET	modified residue	UNP P19624
B	152	MSE	MET	modified residue	UNP P19624
B	218	MSE	MET	modified residue	UNP P19624
B	238	MSE	MET	modified residue	UNP P19624
B	264	MSE	MET	modified residue	UNP P19624
B	324	MSE	MET	modified residue	UNP P19624
C	49	MSE	MET	modified residue	UNP P19624
C	151	MSE	MET	modified residue	UNP P19624
C	152	MSE	MET	modified residue	UNP P19624
C	218	MSE	MET	modified residue	UNP P19624
C	238	MSE	MET	modified residue	UNP P19624
C	264	MSE	MET	modified residue	UNP P19624
C	324	MSE	MET	modified residue	UNP P19624

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Chain	Residue	Modelled	Actual	Comment	Reference
D	49	MSE	MET	modified residue	UNP P19624
D	151	MSE	MET	modified residue	UNP P19624
D	152	MSE	MET	modified residue	UNP P19624
D	218	MSE	MET	modified residue	UNP P19624
D	238	MSE	MET	modified residue	UNP P19624
D	264	MSE	MET	modified residue	UNP P19624
D	324	MSE	MET	modified residue	UNP P19624

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

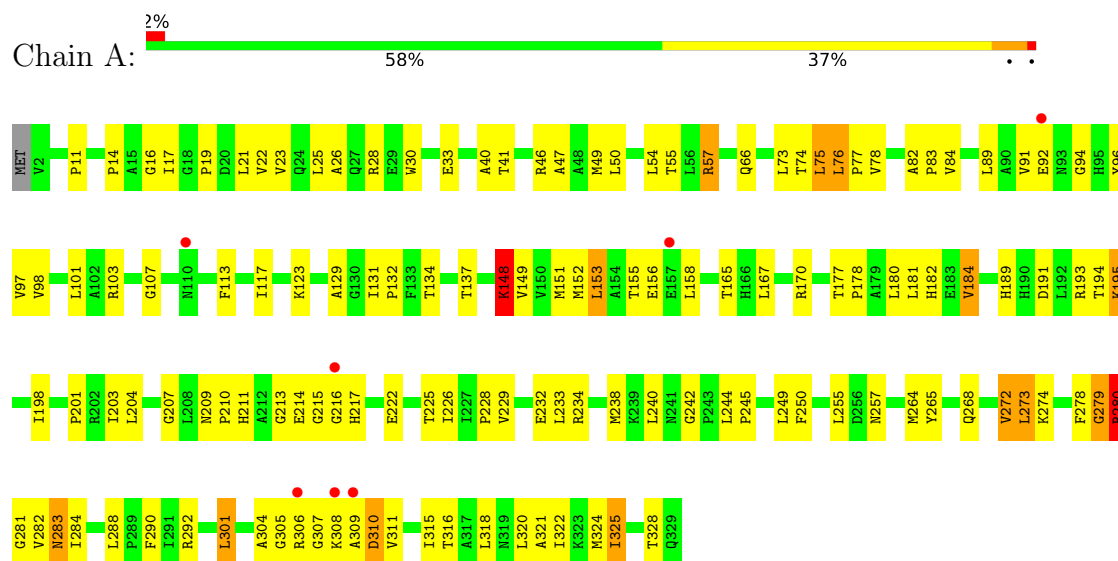
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	80	Total 80	O 80	0	0
3	B	129	Total 129	O 129	0	0
3	C	107	Total 107	O 107	0	0
3	D	138	Total 138	O 138	0	0

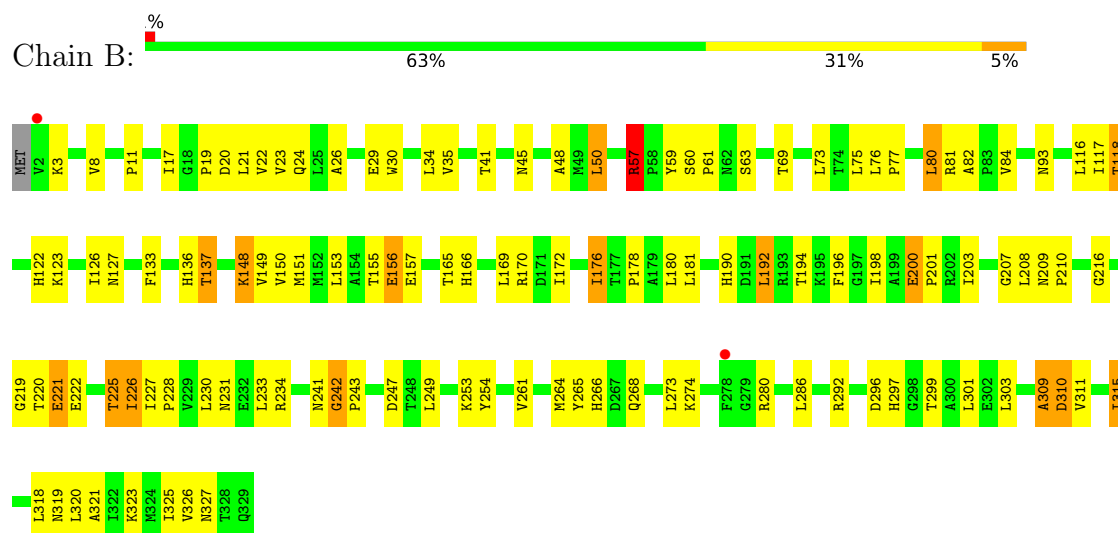
3 Residue-property plots [i](#)

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: 4-hydroxythreonine-4-phosphate dehydrogenase

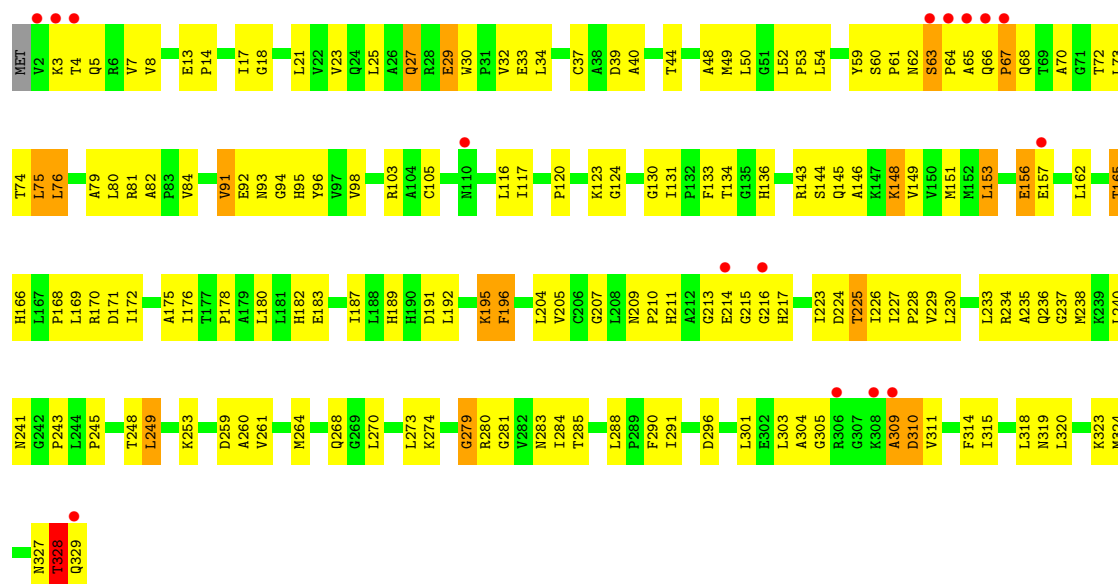


- Molecule 1: 4-hydroxythreonine-4-phosphate dehydrogenase

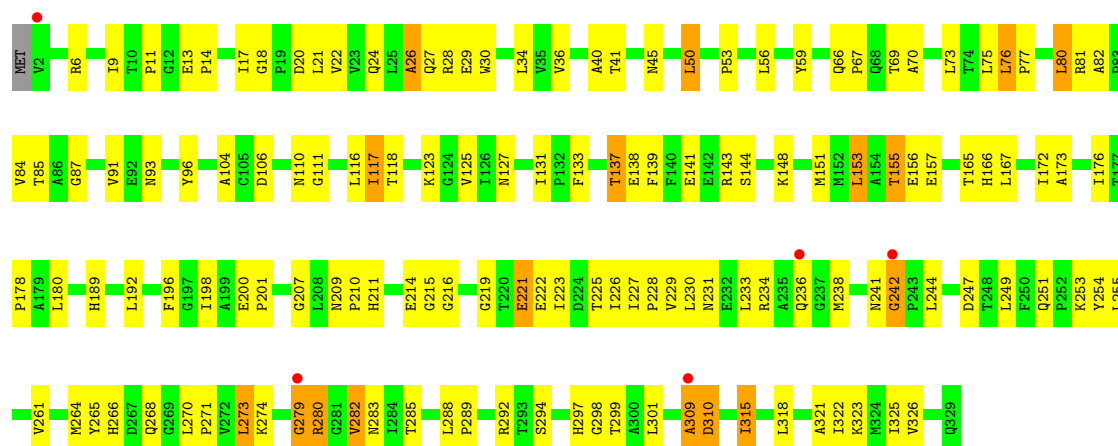


- Molecule 1: 4-hydroxythreonine-4-phosphate dehydrogenase





• Molecule 1: 4-hydroxythreonine-4-phosphate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.05Å 76.69Å 95.42Å 90.00° 109.73° 90.00°	Depositor
Resolution (Å)	45.00 – 2.47 45.00 – 2.47	Depositor EDS
% Data completeness (in resolution range)	95.5 (45.00-2.47) 97.7 (45.00-2.47)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.91 (at 2.48Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.213 , 0.272 0.213 , 0.271	Depositor DCC
R_{free} test set	2204 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	18.8	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10026	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.26 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8109e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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:
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	0.50	0/2436	1.06	12/3318 (0.4%)
1	B	0.53	0/2428	1.05	13/3307 (0.4%)
1	C	0.52	0/2436	1.05	15/3318 (0.5%)
1	D	0.51	0/2428	1.07	15/3307 (0.5%)
All	All	0.51	0/9728	1.06	55/13250 (0.4%)

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	309	ALA	N-CA-C	8.45	120.27	111.14
1	A	78	VAL	N-CA-C	-7.76	97.63	108.27
1	A	280	ARG	N-CA-C	7.54	126.85	110.80
1	B	207	GLY	N-CA-C	-7.40	101.20	112.89
1	A	84	VAL	N-CA-C	7.34	118.38	108.11
1	D	280	ARG	N-CA-C	7.29	126.32	110.80
1	A	77	PRO	N-CA-C	7.12	122.41	111.15
1	C	165	THR	N-CA-C	6.97	114.50	108.78
1	B	75	LEU	N-CA-C	6.82	120.02	108.90
1	B	200	GLU	CA-C-N	6.75	126.67	119.85
1	B	200	GLU	C-N-CA	6.75	126.67	119.85
1	A	76	LEU	CA-C-N	6.72	126.76	119.90
1	A	76	LEU	C-N-CA	6.72	126.76	119.90
1	C	207	GLY	N-CA-C	-6.71	102.36	113.02
1	D	207	GLY	N-CA-C	-6.70	102.06	112.85
1	D	221	GLU	N-CA-C	6.69	118.58	111.28
1	B	118	THR	N-CA-C	6.38	119.64	109.24
1	C	79	ALA	N-CA-C	6.29	119.76	109.76
1	C	75	LEU	N-CA-C	5.98	118.48	108.73
1	B	203	ILE	N-CA-C	5.92	116.40	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	303	LEU	N-CA-C	-5.86	105.98	114.12
1	C	196	PHE	N-CA-C	-5.84	106.20	113.38
1	D	118	THR	N-CA-C	5.82	119.31	109.76
1	A	75	LEU	N-CA-C	5.62	118.12	109.07
1	D	111	GLY	N-CA-C	-5.59	107.04	115.32
1	B	226	ILE	N-CA-C	5.53	115.67	110.30
1	A	57	ARG	N-CA-C	-5.52	101.81	110.14
1	D	84	VAL	N-CA-C	5.51	115.88	108.17
1	C	18	GLY	CA-C-N	5.49	125.58	119.32
1	C	18	GLY	C-N-CA	5.49	125.58	119.32
1	D	77	PRO	N-CA-C	5.49	120.21	111.26
1	C	226	ILE	N-CA-C	5.46	115.55	110.42
1	A	184	VAL	N-CA-C	5.44	115.58	110.30
1	C	205	VAL	N-CA-C	5.42	115.65	107.80
1	B	192	LEU	N-CA-C	-5.40	105.50	111.71
1	B	221	GLU	N-CA-C	5.39	117.16	111.28
1	C	224	ASP	N-CA-C	5.38	118.30	111.69
1	A	325	ILE	N-CA-C	-5.36	105.27	110.42
1	D	76	LEU	CA-C-N	5.34	125.65	119.93
1	D	76	LEU	C-N-CA	5.34	125.65	119.93
1	C	25	LEU	N-CA-C	-5.33	105.55	111.36
1	D	251	GLN	N-CA-C	-5.33	102.41	110.50
1	A	207	GLY	N-CA-C	-5.30	104.59	113.02
1	C	165	THR	CB-CA-C	-5.30	109.44	117.07
1	D	255	LEU	N-CA-C	5.23	117.66	111.33
1	C	145	GLN	N-CA-C	-5.22	107.28	113.38
1	A	181	LEU	N-CA-C	5.21	116.95	111.28
1	D	155	THR	N-CA-C	5.19	116.54	110.41
1	B	80	LEU	N-CA-C	-5.17	103.71	110.53
1	C	168	PRO	N-CA-C	-5.09	103.28	111.38
1	B	77	PRO	N-CA-C	5.08	119.07	111.14
1	D	282	VAL	N-CA-C	5.04	116.62	108.85
1	D	26	ALA	N-CA-C	5.02	119.12	113.15
1	B	176	ILE	N-CA-C	5.01	113.81	106.55
1	B	57	ARG	N-CA-C	-5.00	100.72	109.48

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	2396	0	2417	115	0
1	B	2388	0	2411	87	0
1	C	2396	0	2417	140	0
1	D	2388	0	2411	112	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	80	0	0	9	0
3	B	129	0	0	12	0
3	C	107	0	0	13	0
3	D	138	0	0	14	0
All	All	10026	0	9656	448	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 23.

All (448) 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:156:GLU:CD	1:C:157:GLU:H	1.69	1.01
1:C:3:LYS:HE2	1:C:65:ALA:H	1.33	0.94
1:D:82:ALA:H	1:D:93:ASN:HD21	1.16	0.93
1:C:233:LEU:HD13	1:C:236:GLN:NE2	1.83	0.91
1:C:229:VAL:O	1:C:233:LEU:HD23	1.73	0.87
1:D:236:GLN:HG3	3:D:633:HOH:O	1.76	0.86
1:A:17:ILE:HD12	1:A:304:ALA:HA	1.58	0.84
1:B:319:ASN:O	1:B:323:LYS:HG3	1.79	0.83
1:D:9:ILE:HD11	1:D:34:LEU:HD22	1.62	0.82
1:C:3:LYS:CE	1:C:65:ALA:H	1.92	0.81
1:C:4:THR:HG23	1:C:32:VAL:HA	1.61	0.81
1:D:279:GLY:HA3	3:D:335:HOH:O	1.81	0.79
1:A:229:VAL:O	1:A:233:LEU:HD23	1.84	0.78
1:A:211:HIS:HA	1:A:245:PRO:HB3	1.64	0.78
1:C:95:HIS:CE1	1:C:131:ILE:HD11	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:SER:HB3	1:C:64:PRO:HD2	1.66	0.75
1:A:54:LEU:HD12	1:A:55:THR:H	1.51	0.74
1:C:151:MSE:HB3	3:C:470:HOH:O	1.87	0.74
1:D:36:VAL:HG21	1:D:73:LEU:HD13	1.69	0.74
1:D:82:ALA:H	1:D:93:ASN:ND2	1.83	0.74
1:C:17:ILE:HD12	1:C:304:ALA:HA	1.68	0.74
1:A:194:THR:O	1:A:195:LYS:HG3	1.87	0.74
1:B:264:MSE:H	1:B:268:GLN:NE2	1.86	0.73
1:C:27:GLN:HE21	1:C:52:LEU:HD22	1.53	0.73
1:A:155:THR:HG23	1:A:273:LEU:HD11	1.71	0.73
1:B:176:ILE:HD12	1:B:208:LEU:HD13	1.72	0.72
1:C:189:HIS:CD2	1:C:238:MSE:HG3	2.24	0.71
1:C:233:LEU:HA	1:C:236:GLN:HE21	1.55	0.71
1:A:14:PRO:HG3	1:A:96:TYR:CE2	2.26	0.71
1:D:59:TYR:HD2	1:D:76:LEU:HD13	1.54	0.70
1:C:153:LEU:HD12	1:C:273:LEU:CD1	2.20	0.70
1:C:169:LEU:HD12	1:C:172:ILE:HD12	1.71	0.70
1:C:233:LEU:HD13	1:C:236:GLN:HE22	1.56	0.70
1:A:278:PHE:O	1:A:279:GLY:O	2.10	0.70
1:D:41:THR:HG22	1:D:45:ASN:HD21	1.54	0.69
1:C:225:THR:O	1:C:229:VAL:HG23	1.90	0.69
1:A:11:PRO:HG3	1:A:22:VAL:HG21	1.74	0.69
1:D:29:GLU:OE1	1:D:69:THR:HA	1.93	0.69
1:D:41:THR:HG22	1:D:45:ASN:ND2	2.07	0.69
1:B:82:ALA:H	1:B:93:ASN:HD21	1.41	0.68
1:B:29:GLU:OE2	1:B:69:THR:HA	1.93	0.68
1:A:195:LYS:HB3	1:A:324:MSE:HE3	1.75	0.68
1:C:44:THR:HG23	3:C:712:HOH:O	1.93	0.68
1:C:176:ILE:O	1:C:176:ILE:HG22	1.94	0.68
1:D:40:ALA:HB2	1:D:75:LEU:HD21	1.76	0.68
1:C:279:GLY:O	1:C:281:GLY:N	2.26	0.68
1:C:153:LEU:HD12	1:C:273:LEU:HD11	1.74	0.67
1:C:130:GLY:C	1:C:131:ILE:HD12	2.19	0.67
1:C:40:ALA:HB2	1:C:75:LEU:HD21	1.77	0.67
1:A:189:HIS:CD2	1:A:201:PRO:HG2	2.30	0.67
1:B:220:THR:HG22	3:B:580:HOH:O	1.95	0.67
1:A:54:LEU:HD12	1:A:55:THR:N	2.09	0.66
1:A:40:ALA:HB2	1:A:75:LEU:HD21	1.77	0.66
1:C:33:GLU:OE1	1:C:65:ALA:HA	1.95	0.66
1:C:40:ALA:HB2	1:C:75:LEU:CD2	2.26	0.66
1:C:327:ASN:O	1:C:328:THR:HG23	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ARG:HD2	3:B:369:HOH:O	1.96	0.66
1:A:264:MSE:H	1:A:268:GLN:NE2	1.94	0.66
1:A:308:LYS:HA	3:A:366:HOH:O	1.96	0.65
1:D:11:PRO:HG3	1:D:22:VAL:HG21	1.79	0.65
1:B:81:ARG:H	1:B:93:ASN:ND2	1.94	0.64
1:C:21:LEU:HD22	1:C:311:VAL:HA	1.77	0.64
1:D:59:TYR:CD2	1:D:76:LEU:HD13	2.32	0.64
1:C:284:ILE:HD11	1:C:320:LEU:HD21	1.80	0.64
1:C:296:ASP:CB	3:C:356:HOH:O	2.45	0.64
1:B:321:ALA:O	1:B:325:ILE:HG13	1.98	0.63
1:A:283:ASN:HD22	1:A:284:ILE:N	1.96	0.63
1:D:301:LEU:H	1:D:301:LEU:HD22	1.64	0.63
1:D:297:HIS:HD2	1:D:298:GLY:O	1.81	0.63
1:B:41:THR:HG22	1:B:45:ASN:ND2	2.13	0.63
1:C:27:GLN:NE2	1:C:52:LEU:HD22	2.14	0.63
1:A:14:PRO:HG3	1:A:96:TYR:HE2	1.62	0.62
1:D:230:LEU:O	1:D:234:ARG:HG3	1.99	0.62
1:C:8:VAL:HG13	1:C:116:LEU:HD13	1.82	0.62
1:D:91:VAL:HA	1:D:125:VAL:HG23	1.81	0.61
1:C:151:MSE:HE3	1:C:165:THR:CG2	2.30	0.61
1:C:151:MSE:HE3	1:C:165:THR:HG21	1.82	0.61
1:C:319:ASN:O	1:C:323:LYS:HG3	1.99	0.61
1:D:117:ILE:N	1:D:117:ILE:HD12	2.16	0.61
1:A:123:LYS:HG3	3:A:694:HOH:O	2.01	0.60
1:D:155:THR:C	1:D:157:GLU:H	2.08	0.60
1:A:264:MSE:H	1:A:268:GLN:HE21	1.47	0.60
1:A:311:VAL:HG13	1:A:315:ILE:HD12	1.83	0.60
1:D:56:LEU:HD13	1:D:75:LEU:HD22	1.83	0.60
1:A:16:GLY:HA2	1:A:301:LEU:HD12	1.83	0.60
1:A:26:ALA:HB2	1:A:73:LEU:HG	1.84	0.60
1:A:117:ILE:HD12	1:A:117:ILE:N	2.16	0.60
1:C:211:HIS:NE2	1:D:166:HIS:NE2	2.50	0.60
1:D:30:TRP:CH2	1:D:318:LEU:HD23	2.36	0.60
1:D:82:ALA:N	1:D:93:ASN:HD21	1.96	0.59
1:C:320:LEU:O	1:C:324:MSE:HG3	2.02	0.59
1:B:230:LEU:O	1:B:234:ARG:HG3	2.02	0.59
1:C:59:TYR:HB2	1:C:74:THR:HG22	1.85	0.59
1:D:80:LEU:HD22	1:D:82:ALA:O	2.03	0.59
1:A:46:ARG:O	1:A:50:LEU:HG	2.03	0.59
1:A:107:GLY:HA3	1:A:113:PHE:CE2	2.37	0.59
1:D:123:LYS:HE3	1:D:133:PHE:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:CYS:SG	1:C:143:ARG:HG2	2.42	0.58
1:C:148:LYS:HG2	1:C:187:ILE:CD1	2.33	0.58
1:A:92:GLU:OE2	1:A:92:GLU:HA	2.01	0.58
1:C:27:GLN:NE2	1:C:53:PRO:HD2	2.17	0.58
1:A:151:MSE:SE	1:A:165:THR:HG21	2.52	0.58
1:B:20:ASP:O	1:B:24:GLN:HG3	2.02	0.58
1:C:98:VAL:HG21	1:C:131:ILE:HG21	1.86	0.58
1:A:195:LYS:HD3	1:A:324:MSE:CE	2.33	0.58
1:C:274:LYS:HG3	1:D:247:ASP:O	2.03	0.58
1:B:57:ARG:HD3	3:B:767:HOH:O	2.02	0.58
1:B:178:PRO:HG3	1:B:225:THR:HB	1.86	0.58
1:D:13:GLU:OE2	1:D:14:PRO:HD2	2.04	0.58
1:A:151:MSE:HE3	1:A:165:THR:HG21	1.86	0.57
1:A:153:LEU:HD12	1:A:273:LEU:HG	1.86	0.57
1:C:39:ASP:CG	1:C:80:LEU:HG	2.28	0.57
1:C:162:LEU:HD11	1:C:270:LEU:HD11	1.86	0.57
1:C:3:LYS:HE2	1:C:65:ALA:N	2.13	0.57
1:B:11:PRO:HG3	1:B:22:VAL:HG21	1.86	0.57
1:B:231:ASN:HD22	1:B:234:ARG:NH1	2.03	0.57
1:A:249:LEU:C	1:A:249:LEU:HD23	2.30	0.57
1:C:156:GLU:CD	1:C:157:GLU:N	2.53	0.57
1:D:18:GLY:O	1:D:22:VAL:HG23	2.04	0.57
1:A:148:LYS:HE2	1:A:149:VAL:O	2.05	0.57
1:A:320:LEU:O	1:A:324:MSE:HG3	2.04	0.56
1:B:155:THR:O	1:B:157:GLU:N	2.38	0.56
1:C:148:LYS:HD2	1:C:183:GLU:OE1	2.06	0.56
1:C:204:LEU:HD23	1:C:241:ASN:HB3	1.87	0.56
1:D:279:GLY:HA3	3:D:619:HOH:O	2.04	0.56
1:C:49:MSE:HE2	1:C:305:GLY:O	2.04	0.56
1:D:20:ASP:O	1:D:24:GLN:HG3	2.05	0.56
1:A:322:ILE:HA	1:A:325:ILE:HD12	1.88	0.56
1:B:148:LYS:HG3	1:B:149:VAL:N	2.20	0.56
1:D:155:THR:O	1:D:157:GLU:N	2.38	0.56
1:C:3:LYS:O	1:C:4:THR:C	2.48	0.56
1:A:195:LYS:HD3	1:A:324:MSE:HE1	1.88	0.56
1:A:76:LEU:HD21	1:A:103:ARG:NH1	2.20	0.56
1:A:211:HIS:CA	1:A:245:PRO:HB3	2.36	0.55
1:B:48:ALA:HA	3:B:555:HOH:O	2.07	0.55
1:C:4:THR:HB	1:C:65:ALA:CB	2.36	0.55
1:D:151:MSE:SE	3:D:334:HOH:O	2.75	0.55
1:B:80:LEU:HD13	1:B:84:VAL:HG23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:ILE:HD12	1:C:117:ILE:N	2.21	0.55
1:C:189:HIS:CG	1:C:238:MSE:HE2	2.41	0.55
1:A:92:GLU:C	1:A:94:GLY:H	2.15	0.55
1:C:27:GLN:HE22	1:C:53:PRO:HD2	1.72	0.55
1:D:9:ILE:CD1	1:D:34:LEU:HD22	2.34	0.55
1:A:191:ASP:O	1:A:195:LYS:HB2	2.06	0.55
1:A:91:VAL:HG23	1:A:92:GLU:N	2.21	0.55
1:A:283:ASN:HD22	1:A:283:ASN:C	2.13	0.55
1:D:26:ALA:HB2	1:D:73:LEU:HD21	1.88	0.55
1:C:4:THR:HB	1:C:65:ALA:HB3	1.89	0.55
1:B:209:ASN:ND2	1:B:219:GLY:HA3	2.22	0.54
1:C:178:PRO:HD3	1:C:225:THR:HB	1.90	0.54
1:C:233:LEU:HD12	1:C:238:MSE:SE	2.58	0.54
1:B:117:ILE:N	1:B:117:ILE:HD12	2.22	0.54
1:C:195:LYS:HD3	1:C:324:MSE:HE2	1.90	0.54
1:D:209:ASN:ND2	1:D:219:GLY:HA3	2.23	0.54
1:D:216:GLY:HA3	3:D:507:HOH:O	2.08	0.54
1:A:177:THR:HB	1:A:178:PRO:HD2	1.89	0.54
1:A:292:ARG:HD3	1:A:292:ARG:C	2.33	0.54
1:B:241:ASN:O	1:B:242:GLY:O	2.25	0.53
1:D:87:GLY:HA2	1:D:301:LEU:HB3	1.90	0.53
1:A:155:THR:HG23	1:A:273:LEU:CD1	2.38	0.53
1:A:309:ALA:O	1:A:310:ASP:CB	2.56	0.53
1:D:165:THR:OG1	1:D:166:HIS:N	2.37	0.53
1:D:91:VAL:HA	1:D:125:VAL:CG2	2.39	0.53
1:A:151:MSE:CE	1:A:165:THR:HG21	2.39	0.53
1:A:50:LEU:HD22	1:A:307:GLY:HA2	1.90	0.53
1:A:225:THR:O	1:A:229:VAL:HG23	2.08	0.53
1:A:283:ASN:C	1:A:283:ASN:ND2	2.64	0.53
1:C:171:ASP:HB3	3:C:520:HOH:O	2.09	0.53
1:A:309:ALA:HB2	3:A:441:HOH:O	2.08	0.52
1:C:273:LEU:HD13	1:C:273:LEU:C	2.33	0.52
1:A:21:LEU:CD2	1:A:309:ALA:HB1	2.38	0.52
1:C:82:ALA:H	1:C:93:ASN:HD21	1.56	0.52
1:C:37:CYS:HA	1:C:76:LEU:HB3	1.90	0.52
1:D:17:ILE:HG12	1:D:299:THR:O	2.10	0.52
1:B:265:TYR:CZ	1:B:268:GLN:HB2	2.45	0.52
1:C:195:LYS:HE2	1:C:291:ILE:HG12	1.91	0.52
1:B:30:TRP:CD1	1:B:34:LEU:HD11	2.44	0.52
1:B:137:THR:HG22	3:B:427:HOH:O	2.09	0.52
1:B:297:HIS:HE1	3:B:367:HOH:O	1.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:LEU:HD21	1:B:261:VAL:HG22	1.92	0.52
1:C:211:HIS:HA	1:C:245:PRO:HB3	1.92	0.51
1:C:264:MSE:H	1:C:268:GLN:NE2	2.08	0.51
1:B:151:MSE:SE	1:B:165:THR:HG21	2.60	0.51
1:A:40:ALA:HB2	1:A:75:LEU:CD2	2.41	0.51
1:B:123:LYS:HE2	1:B:127:ASN:OD1	2.09	0.51
1:C:180:LEU:HD23	1:C:180:LEU:C	2.36	0.51
1:A:92:GLU:C	1:A:94:GLY:N	2.66	0.51
1:A:255:LEU:C	1:A:257:ASN:H	2.19	0.51
1:D:180:LEU:C	1:D:180:LEU:HD23	2.36	0.51
1:A:57:ARG:O	1:A:74:THR:HA	2.11	0.51
1:A:151:MSE:HG2	3:A:425:HOH:O	2.10	0.51
1:C:70:ALA:O	1:C:72:THR:HG23	2.11	0.51
1:D:81:ARG:HB2	1:D:93:ASN:HD22	1.76	0.51
1:C:227:ILE:HB	1:C:228:PRO:HD3	1.93	0.51
1:A:94:GLY:O	1:A:98:VAL:HG23	2.11	0.51
1:B:230:LEU:HD12	1:B:243:PRO:HD3	1.93	0.51
1:B:264:MSE:H	1:B:268:GLN:HE22	1.57	0.51
1:D:6:ARG:HD2	3:D:419:HOH:O	2.10	0.50
1:A:170:ARG:HD3	3:A:577:HOH:O	2.11	0.50
1:A:233:LEU:HD22	1:A:233:LEU:N	2.26	0.50
1:A:250:PHE:CD1	1:A:272:VAL:HG11	2.47	0.50
1:C:230:LEU:HD12	1:C:243:PRO:HD3	1.93	0.50
1:D:123:LYS:HE2	1:D:127:ASN:OD1	2.12	0.50
1:D:137:THR:HG22	3:D:432:HOH:O	2.11	0.50
1:C:13:GLU:CD	1:C:14:PRO:HD2	2.36	0.50
1:C:14:PRO:HG3	1:C:96:TYR:CE2	2.46	0.50
1:D:241:ASN:O	1:D:242:GLY:O	2.30	0.50
1:A:91:VAL:O	1:A:129:ALA:HB2	2.12	0.50
1:D:200:GLU:N	1:D:201:PRO:HD3	2.27	0.50
1:B:41:THR:HG22	1:B:45:ASN:HD21	1.75	0.50
1:B:192:LEU:HA	1:B:196:PHE:CD1	2.47	0.50
1:C:131:ILE:HD12	1:C:131:ILE:N	2.26	0.50
1:B:59:TYR:HD2	1:B:76:LEU:HD13	1.77	0.50
1:D:242:GLY:N	3:D:395:HOH:O	2.36	0.50
1:A:26:ALA:CB	1:A:73:LEU:HG	2.41	0.49
1:C:7:VAL:HG22	1:C:33:GLU:O	2.12	0.49
1:A:19:PRO:O	1:A:23:VAL:HG23	2.13	0.49
1:C:144:SER:C	1:C:146:ALA:N	2.71	0.49
1:C:215:GLY:O	1:C:223:ILE:HD11	2.13	0.49
1:D:131:ILE:HD11	3:D:511:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:LEU:HD12	1:D:273:LEU:CD1	2.42	0.49
1:C:66:GLN:O	1:C:67:PRO:C	2.55	0.49
1:A:204:LEU:HD13	1:A:249:LEU:HG	1.93	0.49
1:C:245:PRO:HG2	1:C:248:THR:HB	1.95	0.49
1:A:274:LYS:HG3	1:B:247:ASP:O	2.13	0.49
1:D:104:ALA:HB1	1:D:116:LEU:HD13	1.94	0.49
1:D:123:LYS:HG3	1:D:133:PHE:HD2	1.77	0.49
1:A:304:ALA:C	1:A:306:ARG:H	2.21	0.49
1:A:321:ALA:O	1:A:325:ILE:HG13	2.13	0.49
1:B:226:ILE:O	1:B:230:LEU:HG	2.12	0.49
1:A:21:LEU:HD21	1:A:309:ALA:HB1	1.95	0.49
1:D:28:ARG:CZ	1:D:315:ILE:HD13	2.43	0.49
1:B:118:THR:HB	1:B:136:HIS:CE1	2.48	0.48
1:A:137:THR:HG21	1:A:151:MSE:HE2	1.95	0.48
1:A:189:HIS:ND1	1:A:238:MSE:HE2	2.27	0.48
1:A:209:ASN:HB3	1:A:210:PRO:HD2	1.95	0.48
1:C:192:LEU:O	1:C:196:PHE:HB2	2.14	0.48
1:D:273:LEU:HD13	1:D:273:LEU:C	2.38	0.48
1:A:182:HIS:CE1	1:A:233:LEU:HD21	2.48	0.48
1:B:118:THR:OG1	1:B:292:ARG:NH2	2.39	0.48
1:D:148:LYS:HE2	3:D:783:HOH:O	2.12	0.48
1:B:180:LEU:C	1:B:180:LEU:HD23	2.39	0.48
1:C:284:ILE:CD1	1:C:320:LEU:HD21	2.43	0.48
1:A:26:ALA:HB2	1:A:73:LEU:CG	2.44	0.48
1:D:13:GLU:CD	1:D:14:PRO:HD2	2.39	0.48
1:C:50:LEU:O	1:C:52:LEU:HG	2.13	0.48
1:C:170:ARG:NH1	1:D:221:GLU:OE2	2.46	0.48
1:C:204:LEU:HB3	1:C:249:LEU:HD11	1.96	0.48
1:C:249:LEU:HD21	1:C:261:VAL:CG1	2.44	0.48
1:B:253:LYS:HG3	1:B:254:TYR:N	2.28	0.48
1:C:80:LEU:HD13	1:C:84:VAL:HG23	1.95	0.48
1:D:29:GLU:CD	1:D:70:ALA:H	2.21	0.48
1:A:97:VAL:O	1:A:101:LEU:HG	2.13	0.48
1:B:122:HIS:O	1:B:126:ILE:HG13	2.13	0.48
1:C:29:GLU:OE2	1:C:70:ALA:HB2	2.14	0.48
1:A:152:MSE:O	1:A:283:ASN:HA	2.12	0.48
1:A:153:LEU:HA	1:A:282:VAL:O	2.14	0.48
1:C:253:LYS:HD2	3:C:512:HOH:O	2.13	0.48
1:A:167:LEU:HD23	3:A:535:HOH:O	2.14	0.47
1:A:242:GLY:HA2	1:A:244:LEU:HG	1.96	0.47
1:C:54:LEU:HD11	1:C:73:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:ALA:O	1:C:180:LEU:HD13	2.14	0.47
1:C:309:ALA:O	1:C:310:ASP:CB	2.62	0.47
1:D:172:ILE:O	1:D:176:ILE:HD12	2.14	0.47
1:D:231:ASN:HD22	1:D:234:ARG:HH11	1.62	0.47
1:A:279:GLY:O	1:A:281:GLY:N	2.44	0.47
1:B:225:THR:HG23	3:B:499:HOH:O	2.13	0.47
1:C:123:LYS:O	1:C:124:GLY:C	2.58	0.47
1:C:166:HIS:NE2	1:D:211:HIS:CE1	2.83	0.47
1:D:265:TYR:CZ	1:D:268:GLN:HB2	2.50	0.47
1:C:60:SER:C	1:C:62:ASN:H	2.23	0.47
1:D:309:ALA:O	1:D:310:ASP:HB3	2.13	0.47
1:C:17:ILE:CD1	1:C:304:ALA:HA	2.40	0.47
1:A:25:LEU:CD2	1:A:315:ILE:HG13	2.44	0.47
1:C:249:LEU:C	1:C:249:LEU:HD23	2.40	0.47
1:D:27:GLN:HE22	1:D:53:PRO:HG2	1.80	0.47
1:D:151:MSE:HB2	3:D:334:HOH:O	2.14	0.47
1:B:190:HIS:O	1:B:194:THR:HG23	2.15	0.47
1:D:20:ASP:HB3	1:D:50:LEU:HD21	1.96	0.47
1:C:204:LEU:HB3	1:C:249:LEU:CD1	2.45	0.47
1:D:116:LEU:HD23	1:D:292:ARG:HG3	1.97	0.47
1:D:234:ARG:HD2	3:D:551:HOH:O	2.16	0.46
1:A:322:ILE:O	1:A:325:ILE:HB	2.14	0.46
1:B:200:GLU:N	1:B:201:PRO:HD3	2.30	0.46
1:D:322:ILE:O	1:D:326:VAL:HG13	2.15	0.46
1:B:148:LYS:NZ	3:B:417:HOH:O	2.47	0.46
1:C:225:THR:C	1:C:228:PRO:HD2	2.40	0.46
1:D:93:ASN:O	1:D:96:TYR:HB3	2.15	0.46
1:B:222:GLU:HA	1:B:226:ILE:HB	1.98	0.46
1:D:214:GLU:C	1:D:216:GLY:H	2.23	0.46
1:D:242:GLY:O	1:D:244:LEU:HG	2.15	0.46
1:B:133:PHE:CZ	1:B:136:HIS:HA	2.51	0.46
1:C:103:ARG:HD3	3:C:599:HOH:O	2.15	0.46
1:C:283:ASN:HD22	1:C:284:ILE:N	2.13	0.46
1:A:33:GLU:HB2	1:A:66:GLN:O	2.16	0.46
1:A:89:LEU:HD21	1:A:301:LEU:HD21	1.98	0.46
1:A:213:GLY:O	1:A:214:GLU:C	2.58	0.46
1:C:169:LEU:HD12	1:C:172:ILE:CD1	2.43	0.46
1:C:214:GLU:O	1:C:216:GLY:N	2.48	0.46
1:D:215:GLY:O	1:D:223:ILE:HD11	2.15	0.46
1:B:311:VAL:HG13	1:B:315:ILE:HG13	1.98	0.46
1:C:63:SER:HB3	1:C:64:PRO:CD	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:SER:C	1:C:146:ALA:H	2.23	0.46
1:C:249:LEU:HD21	1:C:261:VAL:HG13	1.98	0.46
1:D:144:SER:HB2	1:D:289:PRO:HG2	1.98	0.46
1:A:309:ALA:O	1:A:310:ASP:HB3	2.14	0.46
1:D:253:LYS:HG3	1:D:254:TYR:N	2.30	0.46
1:B:26:ALA:HB2	1:B:73:LEU:HD21	1.97	0.45
1:C:5:GLN:HE21	1:C:329:GLN:CB	2.30	0.45
1:D:198:ILE:O	1:D:201:PRO:HG3	2.16	0.45
1:A:228:PRO:O	1:A:232:GLU:HG3	2.16	0.45
1:A:233:LEU:N	1:A:233:LEU:CD2	2.80	0.45
1:B:59:TYR:CD2	1:B:76:LEU:HD13	2.51	0.45
1:C:234:ARG:O	1:C:237:GLY:N	2.46	0.45
1:A:234:ARG:HA	1:A:238:MSE:O	2.16	0.45
1:D:321:ALA:O	1:D:325:ILE:HG13	2.17	0.45
1:B:116:LEU:C	1:B:117:ILE:HD12	2.42	0.45
1:C:3:LYS:HE3	1:C:64:PRO:HA	1.98	0.45
1:D:189:HIS:CD2	1:D:238:MSE:HG2	2.51	0.45
1:D:253:LYS:HD2	1:D:254:TYR:CE2	2.52	0.45
1:C:290:PHE:HD1	1:C:291:ILE:O	2.00	0.45
1:D:192:LEU:HA	1:D:196:PHE:CD1	2.52	0.45
1:A:82:ALA:HB1	1:A:83:PRO:HD2	1.99	0.45
1:D:210:PRO:O	1:D:211:HIS:HB2	2.16	0.45
1:A:103:ARG:HG3	1:A:103:ARG:HH11	1.81	0.45
1:B:8:VAL:HA	1:B:35:VAL:O	2.17	0.45
1:B:155:THR:C	1:B:157:GLU:H	2.25	0.45
1:C:148:LYS:HG3	1:C:149:VAL:N	2.31	0.45
1:C:195:LYS:HE3	3:C:410:HOH:O	2.16	0.45
1:D:30:TRP:CZ2	1:D:318:LEU:HD23	2.51	0.45
1:A:180:LEU:O	1:A:184:VAL:HG23	2.16	0.45
1:B:30:TRP:CH2	1:B:318:LEU:HD23	2.52	0.45
1:A:214:GLU:O	1:A:216:GLY:N	2.49	0.44
1:C:30:TRP:CD1	1:C:34:LEU:HD11	2.52	0.44
1:C:323:LYS:NZ	3:C:751:HOH:O	2.43	0.44
1:C:48:ALA:C	1:C:50:LEU:H	2.24	0.44
1:D:200:GLU:HA	3:D:402:HOH:O	2.17	0.44
1:D:264:MSE:H	1:D:268:GLN:NE2	2.15	0.44
1:C:191:ASP:O	1:C:195:LYS:HB2	2.16	0.44
1:A:210:PRO:O	1:A:211:HIS:HB2	2.18	0.44
1:B:155:THR:C	1:B:157:GLU:N	2.72	0.44
1:B:169:LEU:HD22	1:B:172:ILE:HD12	1.99	0.44
1:C:91:VAL:HG23	1:C:92:GLU:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:PRO:C	1:B:63:SER:H	2.26	0.44
1:A:189:HIS:CG	1:A:238:MSE:HE2	2.52	0.44
1:A:21:LEU:HD22	1:A:311:VAL:HA	2.00	0.44
1:C:148:LYS:HG2	1:C:187:ILE:HD11	1.99	0.43
1:C:259:ASP:O	1:C:260:ALA:HB2	2.18	0.43
1:D:153:LEU:HG	1:D:270:LEU:HD22	1.99	0.43
1:A:153:LEU:HD12	1:A:273:LEU:CG	2.48	0.43
1:B:296:ASP:CB	3:B:687:HOH:O	2.65	0.43
1:C:5:GLN:NE2	1:C:329:GLN:CB	2.81	0.43
1:D:178:PRO:HA	1:D:229:VAL:HG21	2.00	0.43
1:C:182:HIS:CD2	1:C:233:LEU:HD21	2.54	0.43
1:D:172:ILE:HG23	1:D:176:ILE:HD11	1.99	0.43
1:B:198:ILE:O	1:B:201:PRO:HG3	2.18	0.43
1:C:49:MSE:O	1:C:49:MSE:HG2	2.19	0.43
1:C:284:ILE:HD11	1:C:320:LEU:CD2	2.47	0.43
1:D:271:PRO:HD2	3:D:439:HOH:O	2.18	0.43
1:A:280:ARG:O	1:A:316:THR:HG21	2.18	0.43
1:C:123:LYS:HG2	1:C:133:PHE:HD2	1.84	0.43
1:C:211:HIS:CA	1:C:245:PRO:HB3	2.47	0.43
1:D:266:HIS:CE1	1:D:270:LEU:HD12	2.54	0.43
1:C:3:LYS:CE	1:C:64:PRO:HA	2.49	0.43
1:D:282:VAL:CG1	1:D:283:ASN:N	2.81	0.43
1:A:193:ARG:HA	1:A:198:ILE:O	2.18	0.43
1:D:292:ARG:NH2	1:D:294:SER:HB2	2.34	0.43
1:B:118:THR:HB	1:B:136:HIS:HE1	1.84	0.43
1:C:285:THR:HG22	1:C:288:LEU:HG	2.00	0.43
1:A:255:LEU:C	1:A:257:ASN:N	2.76	0.43
1:D:249:LEU:HD23	1:D:249:LEU:C	2.43	0.43
1:D:283:ASN:HB3	1:D:294:SER:HB3	2.01	0.43
1:B:60:SER:HA	1:B:61:PRO:HD2	1.85	0.42
1:B:242:GLY:N	3:B:361:HOH:O	2.52	0.42
1:B:19:PRO:O	1:B:23:VAL:HG23	2.18	0.42
1:B:209:ASN:HB3	1:B:210:PRO:HD2	2.02	0.42
1:D:227:ILE:HB	1:D:228:PRO:HD3	2.02	0.42
1:A:23:VAL:HG11	1:A:47:ALA:HA	2.02	0.42
1:B:249:LEU:C	1:B:249:LEU:HD23	2.43	0.42
1:B:3:LYS:HE3	1:B:3:LYS:HB2	1.88	0.42
1:B:231:ASN:ND2	1:B:234:ARG:NH1	2.68	0.42
1:C:165:THR:HB	3:C:409:HOH:O	2.20	0.42
1:D:285:THR:CG2	1:D:288:LEU:HG	2.49	0.42
1:D:323:LYS:O	1:D:326:VAL:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:GLN:HA	1:D:27:GLN:NE2	2.34	0.42
1:A:265:TYR:HB2	3:A:371:HOH:O	2.20	0.42
1:D:172:ILE:O	1:D:173:ALA:C	2.63	0.42
1:A:30:TRP:CH2	1:A:318:LEU:HD23	2.55	0.42
1:B:225:THR:CG2	3:B:499:HOH:O	2.67	0.42
1:B:234:ARG:HH21	1:B:242:GLY:H	1.68	0.42
1:D:309:ALA:O	1:D:310:ASP:CB	2.67	0.42
1:B:20:ASP:HB3	1:B:50:LEU:HD21	2.02	0.41
1:B:155:THR:O	1:B:156:GLU:C	2.63	0.41
1:B:323:LYS:O	1:B:326:VAL:HG22	2.20	0.41
1:D:222:GLU:HA	1:D:226:ILE:HB	2.01	0.41
1:A:222:GLU:HA	1:A:226:ILE:HB	2.02	0.41
1:C:120:PRO:HG2	3:C:601:HOH:O	2.19	0.41
1:C:235:ALA:C	1:C:237:GLY:H	2.28	0.41
1:A:203:ILE:HB	1:A:240:LEU:HD23	2.02	0.41
1:B:81:ARG:H	1:B:93:ASN:HD21	1.66	0.41
1:D:249:LEU:HD21	1:D:261:VAL:HG22	2.02	0.41
1:A:211:HIS:CD2	1:B:166:HIS:HD2	2.39	0.41
1:A:324:MSE:O	1:A:328:THR:HG23	2.21	0.41
1:C:39:ASP:CB	1:C:80:LEU:HG	2.50	0.41
1:C:40:ALA:HB2	1:C:75:LEU:HD22	1.99	0.41
1:C:227:ILE:N	1:C:228:PRO:CD	2.84	0.41
1:A:21:LEU:HD23	1:A:309:ALA:HB1	2.03	0.41
1:B:216:GLY:N	3:B:572:HOH:O	2.53	0.41
1:C:153:LEU:HD12	1:C:273:LEU:HD12	1.97	0.41
1:A:288:LEU:C	1:A:290:PHE:H	2.28	0.41
1:B:59:TYR:OH	1:B:61:PRO:HB3	2.20	0.41
1:B:242:GLY:O	1:B:243:PRO:C	2.62	0.41
1:A:28:ARG:HD3	3:A:378:HOH:O	2.21	0.41
1:A:131:ILE:HA	1:A:132:PRO:HD3	1.84	0.41
1:A:158:LEU:HD23	1:A:273:LEU:HD22	2.02	0.41
1:A:216:GLY:HA3	3:A:389:HOH:O	2.20	0.41
1:B:221:GLU:OE1	1:B:221:GLU:N	2.48	0.41
1:B:323:LYS:O	1:B:327:ASN:HB2	2.20	0.41
1:C:209:ASN:HB3	1:C:210:PRO:HD2	2.03	0.41
1:C:213:GLY:O	1:C:214:GLU:C	2.64	0.41
1:C:223:ILE:HG13	3:C:538:HOH:O	2.20	0.41
1:D:66:GLN:O	1:D:67:PRO:C	2.64	0.41
1:D:155:THR:HG23	1:D:273:LEU:HD21	2.03	0.41
1:C:92:GLU:C	1:C:94:GLY:H	2.27	0.41
1:D:116:LEU:C	1:D:117:ILE:HD12	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:ILE:HB	1:B:228:PRO:HD3	2.03	0.40
1:B:301:LEU:HD22	1:B:301:LEU:H	1.85	0.40
1:C:81:ARG:NH1	3:C:595:HOH:O	2.53	0.40
1:C:253:LYS:NZ	3:C:685:HOH:O	2.27	0.40
1:D:155:THR:C	1:D:157:GLU:N	2.73	0.40
1:D:264:MSE:H	1:D:268:GLN:HE22	1.68	0.40
1:D:301:LEU:HD22	1:D:301:LEU:N	2.35	0.40
1:A:194:THR:O	1:A:195:LYS:CG	2.66	0.40
1:B:17:ILE:HG12	1:B:299:THR:O	2.22	0.40
1:B:133:PHE:HZ	1:B:136:HIS:HA	1.86	0.40
1:B:309:ALA:O	1:B:310:ASP:CB	2.69	0.40
1:C:273:LEU:HD13	1:C:273:LEU:O	2.21	0.40
1:D:106:ASP:O	1:D:110:ASN:ND2	2.55	0.40
1:D:138:GLU:O	1:D:141:GLU:HB3	2.21	0.40
1:D:270:LEU:N	1:D:271:PRO:CD	2.83	0.40
1:C:230:LEU:HD22	1:C:240:LEU:HD13	2.03	0.40
1:D:139:PHE:CZ	1:D:143:ARG:HD2	2.56	0.40
1:D:153:LEU:HD22	1:D:153:LEU:HA	1.95	0.40
1:A:14:PRO:HD3	1:A:97:VAL:CG2	2.52	0.40
1:A:91:VAL:CG2	1:A:92:GLU:N	2.85	0.40
1:B:192:LEU:O	1:B:196:PHE:HB2	2.22	0.40
1:B:150:VAL:HB	1:B:286:LEU:HB2	2.03	0.40
1:C:30:TRP:CH2	1:C:318:LEU:HD23	2.57	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	326/329 (99%)	284 (87%)	34 (10%)	8 (2%)	4 6
1	B	326/329 (99%)	300 (92%)	20 (6%)	6 (2%)	6 11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	326/329 (99%)	272 (83%)	40 (12%)	14 (4%)	2	2
1	D	326/329 (99%)	288 (88%)	33 (10%)	5 (2%)	8	14
All	All	1304/1316 (99%)	1144 (88%)	127 (10%)	33 (2%)	4	6

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	217	HIS
1	A	279	GLY
1	A	280	ARG
1	A	310	ASP
1	B	242	GLY
1	B	309	ALA
1	B	310	ASP
1	C	195	LYS
1	C	309	ALA
1	C	310	ASP
1	D	242	GLY
1	D	280	ARG
1	A	195	LYS
1	A	215	GLY
1	B	156	GLU
1	B	280	ARG
1	C	27	GLN
1	C	156	GLU
1	C	217	HIS
1	C	280	ARG
1	C	328	THR
1	A	305	GLY
1	D	310	ASP
1	A	148	LYS
1	C	61	PRO
1	C	63	SER
1	C	68	GLN
1	B	266	HIS
1	C	67	PRO
1	D	156	GLU
1	C	91	VAL
1	C	279	GLY
1	D	279	GLY

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	246/255 (96%)	236 (96%)	10 (4%)	27	50
1	B	245/255 (96%)	231 (94%)	14 (6%)	18	36
1	C	246/255 (96%)	233 (95%)	13 (5%)	20	39
1	D	245/255 (96%)	232 (95%)	13 (5%)	20	39
All	All	982/1020 (96%)	932 (95%)	50 (5%)	21	40

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	49	MSE
1	A	134	THR
1	A	148	LYS
1	A	153	LEU
1	A	156	GLU
1	A	272	VAL
1	A	273	LEU
1	A	283	ASN
1	A	301	LEU
1	B	21	LEU
1	B	50	LEU
1	B	57	ARG
1	B	137	THR
1	B	148	LYS
1	B	153	LEU
1	B	181	LEU
1	B	225	THR
1	B	233	LEU
1	B	273	LEU
1	B	274	LYS
1	B	303	LEU
1	B	315	ILE
1	B	320	LEU

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Mol	Chain	Res	Type
1	C	23	VAL
1	C	29	GLU
1	C	76	LEU
1	C	134	THR
1	C	136	HIS
1	C	148	LYS
1	C	153	LEU
1	C	225	THR
1	C	249	LEU
1	C	301	LEU
1	C	314	PHE
1	C	315	ILE
1	C	328	THR
1	D	21	LEU
1	D	50	LEU
1	D	80	LEU
1	D	85	THR
1	D	117	ILE
1	D	137	THR
1	D	153	LEU
1	D	167	LEU
1	D	225	THR
1	D	233	LEU
1	D	273	LEU
1	D	274	LYS
1	D	315	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	93	ASN
1	A	190	HIS
1	A	231	ASN
1	A	268	GLN
1	A	283	ASN
1	B	5	GLN
1	B	27	GLN
1	B	45	ASN
1	B	66	GLN
1	B	93	ASN
1	B	166	HIS

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Mol	Chain	Res	Type
1	B	190	HIS
1	B	231	ASN
1	B	268	GLN
1	B	297	HIS
1	C	5	GLN
1	C	68	GLN
1	C	93	ASN
1	C	95	HIS
1	C	127	ASN
1	C	182	HIS
1	C	231	ASN
1	C	236	GLN
1	C	251	GLN
1	C	268	GLN
1	C	283	ASN
1	C	297	HIS
1	D	24	GLN
1	D	27	GLN
1	D	45	ASN
1	D	93	ASN
1	D	145	GLN
1	D	211	HIS
1	D	231	ASN
1	D	268	GLN
1	D	297	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	321/329 (97%)	0.22	7 (2%) 62 59	9, 22, 36, 42	0
1	B	321/329 (97%)	-0.20	2 (0%) 85 83	3, 14, 24, 36	0
1	C	321/329 (97%)	0.34	16 (4%) 34 30	5, 22, 42, 49	0
1	D	321/329 (97%)	-0.13	5 (1%) 70 68	4, 15, 28, 37	0
All	All	1284/1316 (97%)	0.06	30 (2%) 61 58	3, 18, 36, 49	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	308	LYS	3.8
1	D	242	GLY	3.6
1	C	4	THR	3.5
1	D	279	GLY	3.5
1	C	64	PRO	3.3
1	A	110	ASN	3.1
1	A	309	ALA	3.0
1	C	309	ALA	3.0
1	C	308	LYS	3.0
1	A	92	GLU	2.9
1	B	278	PHE	2.9
1	A	216	GLY	2.9
1	C	214	GLU	2.8
1	C	329	GLN	2.7
1	C	66	GLN	2.6
1	C	65	ALA	2.5
1	D	2	VAL	2.5
1	A	306	ARG	2.5
1	C	67	PRO	2.4
1	C	216	GLY	2.4
1	B	2	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	236	GLN	2.3
1	C	110	ASN	2.3
1	C	157	GLU	2.2
1	C	2	VAL	2.2
1	C	3	LYS	2.1
1	D	309	ALA	2.1
1	C	306	ARG	2.1
1	A	157	GLU	2.1
1	C	63	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($\text{\AA}^2$)	Q<0.9
2	ZN	D	332	1/1	0.97	0.03	43,43,43,43	0
2	ZN	A	331	1/1	0.98	0.03	29,29,29,29	0
2	ZN	C	333	1/1	0.99	0.04	26,26,26,26	0
2	ZN	B	330	1/1	0.99	0.02	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.