Full wwPDB X-ray Structure Validation Report ⓘ

Nov 11, 2024 – 05:52 AM EST

PDB ID	:	4L0C
Title	:	Crystal structure of the N-Fopmylmaleamic acid deformylase Nfo(S94A) from Pseudomonas putida S16
Authors	:	Chen, D.; Lu, Y.; Zhang, Z.; Wu, G.; Xu, P.
Deposited on	:	2013-05-31
Resolution	:	1.65 Å(reported)

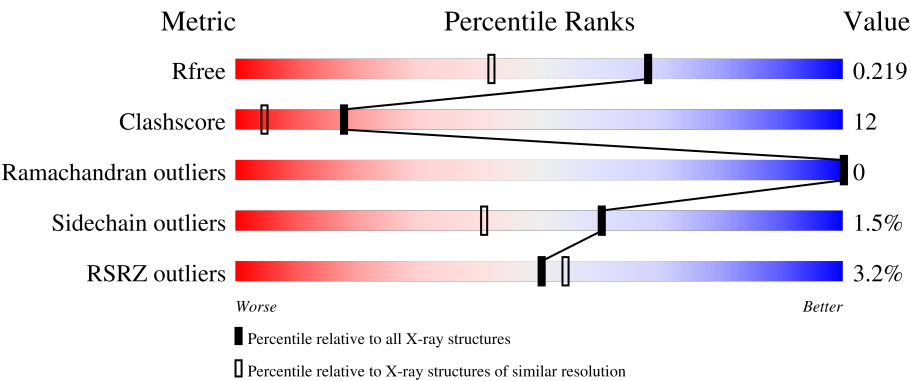The following versions of software and data (see references ⓘ) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 1.65 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.
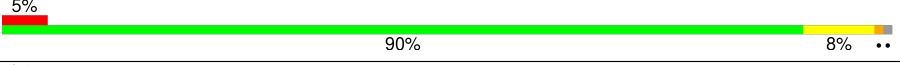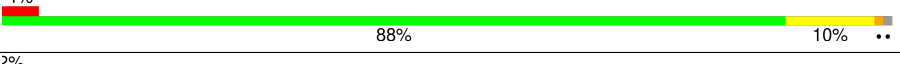
Metric	Percentile Ranks	Value
Rfree		0.219
Clashscore		12
Ramachandran outliers		0
Sidechain outliers		1.5%
RSRZ outliers		3.2%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	164625	2328 (1.66-1.66)
Clashscore	180529	2515 (1.66-1.66)
Ramachandran outliers	177936	2475 (1.66-1.66)
Sidechain outliers	177891	2475 (1.66-1.66)
RSRZ outliers	164620	2328 (1.66-1.66)

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 <=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	255	% 89% 10% •
1	B	255	3% 90% 9% •
1	C	255	3% 90% 9% •
1	D	255	5% 88% 11% •
1	E	255	2% 91% 9%

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Mol	Chain	Length	Quality of chain
1	F	255	5% ... 90% ... 8%
1	G	255	4% ... 88% ... 10%
1	H	255	2% ... 91% ... 8%

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	ACY	A	302	-	-	X	-
2	ACY	B	301	-	-	X	-

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 18024 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 Deformylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	Se	0	5	0
			1996	1272	347	368	3	6			
1	B	255	Total	C	N	O	S	Se	0	8	0
			2023	1288	351	373	3	8			
1	C	253	Total	C	N	O	S	Se	0	3	0
			1970	1258	338	363	3	8			
1	D	253	Total	C	N	O	S	Se	0	4	0
			1983	1264	340	369	3	7			
1	E	255	Total	C	N	O	S	Se	0	2	0
			1991	1270	344	367	3	7			
1	F	252	Total	C	N	O	S	Se	0	2	0
			1960	1249	341	361	3	6			
1	G	252	Total	C	N	O	S	Se	0	0	0
			1954	1245	337	363	3	6			
1	H	254	Total	C	N	O	S	Se	0	6	0
			1996	1275	343	369	3	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	ALA	SER	engineered mutation	UNP F8G0M2
B	94	ALA	SER	engineered mutation	UNP F8G0M2
C	94	ALA	SER	engineered mutation	UNP F8G0M2
D	94	ALA	SER	engineered mutation	UNP F8G0M2
E	94	ALA	SER	engineered mutation	UNP F8G0M2
F	94	ALA	SER	engineered mutation	UNP F8G0M2
G	94	ALA	SER	engineered mutation	UNP F8G0M2
H	94	ALA	SER	engineered mutation	UNP F8G0M2

- Molecule 2 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).

ACY

OXT

OH

C

CH3

O

O

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	D	1	Total 4	C 2	O 2	0	0
2	E	1	Total 4	C 2	O 2	0	0
2	F	1	Total 4	C 2	O 2	0	0
2	G	1	Total 4	C 2	O 2	0	0
2	G	1	Total 4	C 2	O 2	0	0
2	H	1	Total 4	C 2	O 2	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	300	Total	O	0	0
			300	300		
4	B	272	Total	O	0	0
			272	272		
4	C	212	Total	O	0	0
			212	212		
4	D	237	Total	O	0	0
			237	237		
4	E	287	Total	O	0	0
			287	287		
4	F	217	Total	O	0	0
			217	217		
4	G	266	Total	O	0	0
			266	266		
4	H	313	Total	O	0	0
			313	313		

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: Deformylase

Chain A:

- Molecule 1: Deformylase

Chain B:

- Molecule 1: Deformylase

Chain C:

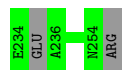- Molecule 1: Deformylase

Chain D:
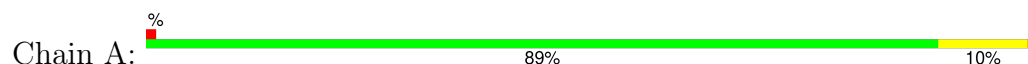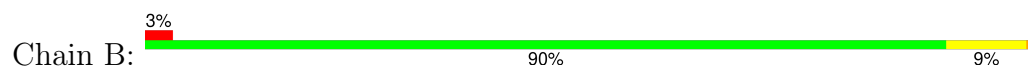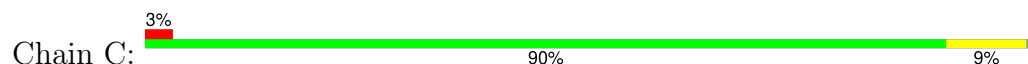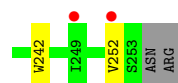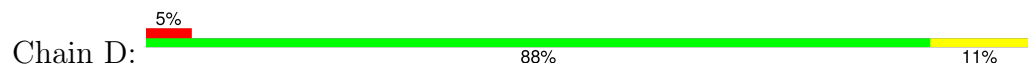
- Molecule 1: Deformylase

Chain E:

- Molecule 1: Deformylase

Chain F:

- Molecule 1: Deformylase

Chain G:

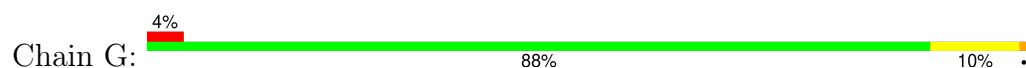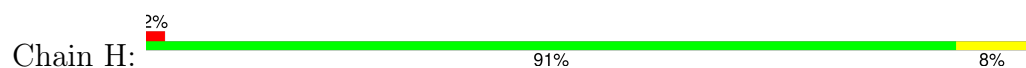- Molecule 1: Deformylase

Chain H:
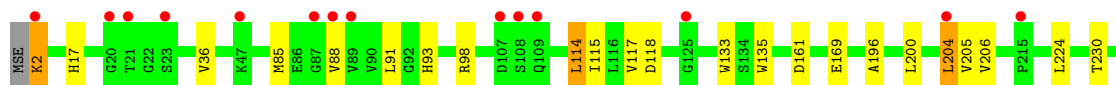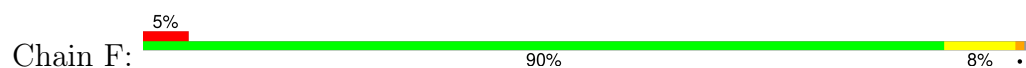
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.41Å 87.27Å 130.88Å 90.00° 94.42° 90.00°	Depositor
Resolution (Å)	44.57 – 1.65 44.57 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.2 (44.57-1.65) 99.2 (44.57-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.98 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.185 , 0.211 0.196 , 0.219	Depositor DCC
R_{free} test set	12039 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	12.5	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 36.7	EDS
L-test for twinning[2]	$< |L| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18024	wwPDB-VP
Average B, all atoms (Å^2)	15.0	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 46.38 % 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 1.1544e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: ACY, PEG

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	0.61	3/2054 (0.1%)	0.69	3/2793 (0.1%)
1	B	0.59	2/2086 (0.1%)	0.68	1/2832 (0.0%)
1	C	0.58	2/2022 (0.1%)	0.63	0/2749
1	D	0.58	1/2032 (0.0%)	0.68	0/2763
1	E	0.61	3/2040 (0.1%)	0.67	0/2773
1	F	0.60	2/2008 (0.1%)	0.63	1/2729 (0.0%)
1	G	0.60	1/1997 (0.1%)	0.67	2/2716 (0.1%)
1	H	0.60	3/2057 (0.1%)	0.69	1/2798 (0.0%)
All	All	0.59	17/16296 (0.1%)	0.67	8/22153 (0.0%)

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	B	0	1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	74	MSE	C-N	-5.62	1.21	1.34
1	A	242	TRP	CD2-CE2	5.47	1.48	1.41
1	H	242	TRP	CD2-CE2	5.46	1.47	1.41
1	F	135	TRP	CD2-CE2	5.35	1.47	1.41
1	E	135	TRP	CD2-CE2	5.34	1.47	1.41
1	B	242	TRP	CD2-CE2	5.31	1.47	1.41
1	D	242	TRP	CD2-CE2	5.30	1.47	1.41
1	G	170	TRP	CD2-CE2	5.27	1.47	1.41
1	E	133	TRP	CD2-CE2	5.22	1.47	1.41
1	C	170	TRP	CD2-CE2	5.19	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	133	TRP	CD2-CE2	5.15	1.47	1.41
1	H	135	TRP	CD2-CE2	5.15	1.47	1.41
1	A	135	TRP	CD2-CE2	5.13	1.47	1.41
1	C	135	TRP	CD2-CE2	5.13	1.47	1.41
1	B	170	TRP	CD2-CE2	5.11	1.47	1.41
1	H	170	TRP	CD2-CE2	5.06	1.47	1.41
1	A	170	TRP	CD2-CE2	5.05	1.47	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	105	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	H	74	MSE	CA-CB-CG	-6.05	103.02	113.30
1	G	105	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	102[A]	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	A	102[B]	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	B	74	MSE	CA-CB-CG	-5.33	104.24	113.30
1	A	74	MSE	CA-CB-CG	-5.12	104.60	113.30
1	F	98	ARG	NE-CZ-NH2	5.02	122.81	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	85	MSE	Mainchain

5.2 Too-close contacts (i)

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	1996	0	1979	51	0
1	B	2023	0	2015	45	0
1	C	1970	0	1951	45	0
1	D	1983	0	1953	61	0
1	E	1991	0	1973	35	0
1	F	1960	0	1933	47	0
1	G	1954	0	1920	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1996	0	1985	42	0
2	A	8	0	6	3	0
2	B	4	0	3	2	0
2	C	4	0	3	1	0
2	D	4	0	3	0	0
2	E	4	0	3	0	0
2	F	4	0	3	0	0
2	G	8	0	6	0	0
2	H	4	0	3	0	0
3	H	7	0	10	2	0
4	A	300	0	0	3	0
4	B	272	0	0	3	0
4	C	212	0	0	2	0
4	D	237	0	0	2	0
4	E	287	0	0	3	0
4	F	217	0	0	1	0
4	G	266	0	0	2	0
4	H	313	0	0	3	0
All	All	18024	0	15749	384	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 12.

All (384) 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:F:204:LEU:HD21	1:F:206:VAL:CG2	1.76	1.16
1:F:204:LEU:HD21	1:F:206:VAL:HG23	1.27	1.14
1:D:84:ARG:NH2	1:E:21:THR:HG23	1.63	1.10
1:B:114:LEU:HD11	1:B:200:LEU:HD11	1.30	1.08
1:F:93:HIS:HA	1:F:117:VAL:HG22	1.33	1.05
1:F:114:LEU:HD11	1:F:200:LEU:HD11	1.34	1.03
1:G:121:VAL:HG23	1:G:192:HIS:CE1	1.94	1.03
1:F:204:LEU:CD2	1:F:206:VAL:HG23	1.88	1.02
1:F:204:LEU:C	1:F:204:LEU:HD23	1.78	1.02
1:C:85[B]:MSE:HB3	1:C:88[B]:VAL:CG1	1.90	1.01
1:B:93:HIS:HA	1:B:117:VAL:HG22	1.42	1.01
1:A:91:LEU:HD13	1:A:115:ILE:HB	1.44	0.99
1:D:93:HIS:HA	1:D:117:VAL:HG22	1.44	0.98
1:G:93:HIS:HA	1:G:117:VAL:HG22	1.42	0.98
1:F:91:LEU:HD23	1:F:115:ILE:CG2	1.91	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:114:LEU:CD1	1:F:200:LEU:HD11	1.94	0.98
1:A:12:ARG:HH12	2:A:302:ACY:H1	1.26	0.97
1:G:114:LEU:HD11	1:G:200:LEU:HD11	1.47	0.96
1:F:93:HIS:HD2	1:F:117:VAL:HG23	1.27	0.96
1:C:121:VAL:HG23	1:C:192:HIS:CE1	2.01	0.96
1:H:121:VAL:HG23	1:H:192:HIS:CE1	2.00	0.96
1:C:93:HIS:HA	1:C:117:VAL:HG13	1.46	0.95
1:A:114:LEU:HD11	1:A:200:LEU:HD11	1.48	0.94
1:F:91:LEU:HD23	1:F:115:ILE:HB	1.48	0.93
1:C:91:LEU:HD13	1:C:115:ILE:HB	1.47	0.93
1:E:93:HIS:HA	1:E:117:VAL:HG22	1.48	0.92
1:F:91:LEU:HD23	1:F:115:ILE:CB	1.99	0.91
1:B:121:VAL:HG23	1:B:192:HIS:CE1	2.05	0.90
1:D:93:HIS:HD2	1:D:117:VAL:HG23	1.34	0.90
1:B:93:HIS:HD2	1:B:117:VAL:HG23	1.34	0.90
1:F:91:LEU:CD2	1:F:115:ILE:CG2	2.50	0.90
1:B:114:LEU:CD1	1:B:200:LEU:HD11	2.01	0.90
1:G:93:HIS:HD2	1:G:117:VAL:HG23	1.36	0.90
1:E:93:HIS:HD2	1:E:117:VAL:HG23	1.38	0.89
1:A:91:LEU:CD1	1:A:115:ILE:CG2	2.52	0.88
1:H:114:LEU:N	1:H:114:LEU:HD12	1.88	0.88
1:D:84:ARG:CZ	1:E:21:THR:HG23	2.03	0.87
1:H:93:HIS:HA	1:H:117:VAL:CG1	2.04	0.87
2:C:301:ACY:H2	4:C:409:HOH:O	1.74	0.86
1:B:25:LEU:HD12	1:B:26:LEU:N	1.90	0.85
1:A:91:LEU:HD13	1:A:115:ILE:CB	2.05	0.85
1:D:114:LEU:HD21	1:D:200:LEU:HD11	1.57	0.84
1:B:91:LEU:HD13	1:B:115:ILE:CG2	2.08	0.84
1:E:6:VAL:HG21	1:E:84:ARG:CZ	2.09	0.83
1:D:91:LEU:CD2	1:D:115:ILE:CG2	2.56	0.83
1:F:93:HIS:CD2	1:F:117:VAL:HG23	2.13	0.82
1:F:85:MSE:HB2	1:F:88:VAL:HG11	1.61	0.82
1:D:84:ARG:NH2	1:E:21:THR:CG2	2.40	0.82
1:A:114:LEU:N	1:A:114:LEU:HD12	1.95	0.82
1:A:91:LEU:HD13	1:A:115:ILE:CG2	2.10	0.82
1:G:28:ILE:CD1	1:G:54:VAL:HG11	2.10	0.81
1:D:41:VAL:O	1:D:45:LEU:HD23	1.82	0.80
1:G:28:ILE:HD12	1:G:54:VAL:HG11	1.62	0.80
1:A:91:LEU:CD1	1:A:115:ILE:HB	2.09	0.80
1:G:25:LEU:HD12	1:G:26:LEU:N	1.94	0.80
1:G:114:LEU:HD12	1:G:114:LEU:N	1.96	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:93:HIS:HA	1:F:117:VAL:CG2	2.12	0.80
1:F:204:LEU:CD2	1:F:204:LEU:C	2.50	0.80
1:G:121:VAL:HG22	1:G:121:VAL:O	1.79	0.80
1:D:83:GLN:HE22	1:D:110:VAL:HG11	1.46	0.80
1:E:114:LEU:HD21	1:E:200:LEU:HD21	1.62	0.79
1:F:91:LEU:CD2	1:F:115:ILE:HG22	2.11	0.79
1:D:83:GLN:NE2	1:D:110:VAL:HG11	1.97	0.79
1:G:204:LEU:HD11	1:G:206:VAL:HG22	1.64	0.79
1:D:121:VAL:HG23	1:D:192:HIS:CE1	2.18	0.78
1:F:204:LEU:HD21	1:F:206:VAL:HG22	1.65	0.78
1:E:121:VAL:HG13	1:E:192:HIS:CE1	2.18	0.78
1:G:204:LEU:HD12	1:G:206:VAL:HG23	1.65	0.78
1:C:91:LEU:HD13	1:C:115:ILE:CB	2.13	0.78
1:E:6:VAL:HG23	4:E:600:HOH:O	1.84	0.77
1:E:114:LEU:CD2	1:E:200:LEU:HD21	2.14	0.77
1:H:92:GLY:O	1:H:117:VAL:HG12	1.84	0.77
1:D:114:LEU:HD21	1:D:200:LEU:HD21	1.67	0.77
1:F:204:LEU:HD23	1:F:205:VAL:N	2.00	0.77
1:H:121:VAL:HG21	4:H:517:HOH:O	1.84	0.77
1:D:114:LEU:CD2	1:D:200:LEU:HD11	2.15	0.76
1:H:114:LEU:HD11	1:H:200:LEU:HD11	1.65	0.76
1:G:115:ILE:HD13	1:G:252:VAL:CG2	2.15	0.76
1:H:93:HIS:HA	1:H:117:VAL:HG13	1.67	0.75
1:B:121:VAL:HG22	1:B:121:VAL:O	1.86	0.75
1:A:14:HIS:HD2	1:A:55:ASP:OD1	1.69	0.75
1:A:121:VAL:HG13	1:A:192:HIS:CE1	2.21	0.75
1:B:25:LEU:HD13	1:B:89:VAL:O	1.86	0.75
1:G:93:HIS:CD2	1:G:117:VAL:HG23	2.22	0.74
1:A:114:LEU:HD11	1:A:200:LEU:CD1	2.17	0.74
1:D:115:ILE:HD13	1:D:252:VAL:HG23	1.69	0.74
1:C:14:HIS:HD2	1:C:55:ASP:OD2	1.71	0.74
1:B:93:HIS:CD2	1:B:117:VAL:HG23	2.21	0.74
1:D:105:ARG:HD3	1:F:161:ASP:OD1	1.87	0.74
1:D:121:VAL:HG21	4:D:582:HOH:O	1.88	0.74
1:B:25:LEU:CD1	1:B:89:VAL:O	2.36	0.74
1:B:252:VAL:HG12	1:B:252:VAL:O	1.85	0.73
1:E:14:HIS:HD2	1:E:55:ASP:OD2	1.71	0.73
1:C:91:LEU:HD13	1:C:115:ILE:CG2	2.18	0.72
1:G:121:VAL:CG2	1:G:192:HIS:CE1	2.72	0.72
1:H:131:ALA:HA	3:H:302:PEG:H32	1.72	0.72
1:D:115:ILE:HG21	1:D:252:VAL:HG23	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:91:LEU:HD13	1:G:115:ILE:CG2	2.19	0.72
1:C:121:VAL:HG23	1:C:192:HIS:NE2	2.05	0.71
1:F:91:LEU:CD2	1:F:115:ILE:HB	2.20	0.71
1:C:121:VAL:CG2	1:C:192:HIS:CE1	2.72	0.71
1:D:93:HIS:CD2	1:D:117:VAL:HG23	2.22	0.71
1:E:121:VAL:HG12	1:E:121:VAL:O	1.91	0.71
1:G:114:LEU:CD1	1:G:200:LEU:HD11	2.19	0.71
1:G:121:VAL:HG23	1:G:192:HIS:NE2	2.06	0.71
1:A:121:VAL:HG12	1:A:121:VAL:O	1.91	0.70
1:A:91:LEU:CD1	1:A:115:ILE:HG22	2.20	0.70
1:G:204:LEU:CD1	1:G:206:VAL:CG2	2.69	0.70
1:C:85[B]:MSE:CB	1:C:88[B]:VAL:CG1	2.69	0.70
1:G:204:LEU:CD1	1:G:206:VAL:HG23	2.21	0.70
1:A:252:VAL:O	1:A:252:VAL:HG22	1.90	0.70
1:H:121:VAL:O	1:H:121:VAL:HG22	1.92	0.70
1:D:114:LEU:CD2	1:D:200:LEU:HD21	2.22	0.69
1:D:115:ILE:HD13	1:D:252:VAL:CG2	2.22	0.69
1:G:204:LEU:C	1:G:204:LEU:HD13	2.13	0.69
1:G:91:LEU:HD13	1:G:115:ILE:HB	1.75	0.69
1:A:162:GLU:HA	1:A:165:GLU:OE2	1.92	0.69
1:B:14:HIS:HD2	1:B:55:ASP:OD2	1.76	0.69
1:H:114:LEU:HD11	1:H:200:LEU:HD21	1.75	0.68
1:D:14:HIS:HD2	1:D:55:ASP:OD2	1.75	0.68
1:G:14:HIS:HD2	1:G:55:ASP:OD2	1.75	0.68
1:G:27:LEU:O	1:G:54:VAL:HG12	1.93	0.68
1:E:93:HIS:HD2	1:E:117:VAL:CG2	2.06	0.68
1:H:121:VAL:HG23	1:H:192:HIS:NE2	2.08	0.68
1:C:85[B]:MSE:CB	1:C:88[B]:VAL:HG11	2.24	0.67
1:B:115:ILE:HD13	1:B:252:VAL:HG13	1.75	0.67
1:D:91:LEU:HD23	1:D:115:ILE:CG2	2.24	0.67
1:A:12:ARG:HH12	2:A:302:ACY:CH3	2.06	0.67
1:D:93:HIS:HD2	1:D:117:VAL:CG2	2.08	0.67
1:G:121:VAL:HG23	1:G:192:HIS:HE1	1.55	0.67
1:F:93:HIS:CD2	1:F:117:VAL:CG2	2.78	0.67
1:G:114:LEU:HD11	1:G:200:LEU:CD1	2.22	0.66
1:B:93:HIS:HA	1:B:117:VAL:CG2	2.22	0.66
1:F:85:MSE:HB2	1:F:88:VAL:CG1	2.26	0.65
1:F:114:LEU:CD1	1:F:200:LEU:CD1	2.74	0.65
1:B:91:LEU:HD13	1:B:115:ILE:HB	1.77	0.65
1:G:204:LEU:HD11	1:G:206:VAL:CG2	2.27	0.65
1:G:115:ILE:HD13	1:G:252:VAL:HG23	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:LEU:HD11	1:A:200:LEU:HD21	1.79	0.65
1:D:93:HIS:HA	1:D:117:VAL:CG2	2.24	0.65
1:E:117:VAL:HG23	1:E:117:VAL:O	1.95	0.65
1:F:91:LEU:HD23	1:F:115:ILE:HG21	1.76	0.64
1:E:114:LEU:HD21	1:E:200:LEU:HD11	1.78	0.64
1:F:93:HIS:CA	1:F:117:VAL:HG22	2.21	0.64
1:D:252:VAL:O	1:D:252:VAL:HG22	1.96	0.64
1:H:117:VAL:HG13	1:H:117:VAL:O	1.98	0.64
1:A:115:ILE:HD13	1:A:252:VAL:HG23	1.80	0.64
1:D:91:LEU:HD23	1:D:115:ILE:HG21	1.79	0.64
1:C:92:GLY:O	1:C:117:VAL:HG12	1.97	0.64
1:C:85[B]:MSE:HB3	1:C:88[B]:VAL:HG11	1.76	0.63
1:E:117:VAL:CG2	1:E:117:VAL:O	2.46	0.63
1:A:12:ARG:NH1	2:A:302:ACY:H1	2.06	0.63
1:D:121:VAL:HG22	1:D:121:VAL:O	1.97	0.63
1:B:93:HIS:CD2	1:B:117:VAL:CG2	2.82	0.63
1:G:121:VAL:HG21	4:G:587:HOH:O	1.98	0.63
1:B:93:HIS:HD2	1:B:117:VAL:CG2	2.10	0.63
1:H:85:MSE:HB3	1:H:88:VAL:CG1	2.28	0.62
1:H:121:VAL:HG23	1:H:192:HIS:HE1	1.63	0.62
1:A:169:GLU:OE1	1:G:14:HIS:HE1	1.81	0.62
1:C:121:VAL:O	1:C:121:VAL:HG22	1.99	0.62
1:A:91:LEU:HD11	1:A:115:ILE:HG22	1.81	0.62
1:B:91:LEU:HD13	1:B:115:ILE:CB	2.29	0.62
1:E:93:HIS:CD2	1:E:117:VAL:CG2	2.83	0.62
1:G:114:LEU:HD11	1:G:200:LEU:HD21	1.80	0.61
1:A:91:LEU:CD1	1:A:115:ILE:CB	2.71	0.61
1:D:91:LEU:CD2	1:D:115:ILE:HB	2.29	0.61
1:D:93:HIS:CD2	1:D:117:VAL:CG2	2.83	0.61
1:D:121:VAL:HG23	1:D:192:HIS:NE2	2.16	0.61
1:C:91:LEU:CD1	1:C:115:ILE:CG2	2.78	0.61
1:D:91:LEU:CD2	1:D:115:ILE:HG22	2.31	0.61
1:B:121:VAL:HG23	1:B:192:HIS:HE1	1.62	0.60
1:H:91:LEU:CD2	1:H:115:ILE:CG2	2.79	0.60
1:G:93:HIS:CA	1:G:117:VAL:HG22	2.27	0.60
1:E:14:HIS:HE1	1:F:169:GLU:OE1	1.83	0.60
1:A:91:LEU:HD11	1:A:115:ILE:CG2	2.31	0.60
1:A:114:LEU:HD11	1:A:200:LEU:CG	2.32	0.60
1:H:91:LEU:HD23	1:H:115:ILE:CG2	2.31	0.60
1:E:6:VAL:CG2	1:E:84:ARG:CZ	2.80	0.60
1:G:93:HIS:HA	1:G:117:VAL:CG2	2.27	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:LEU:CD2	1:D:115:ILE:HG21	2.30	0.60
1:G:204:LEU:HD13	1:G:205:VAL:N	2.15	0.60
1:A:14:HIS:HE1	1:G:169:GLU:OE1	1.85	0.59
1:C:85[A]:MSE:HB2	1:C:88[A]:VAL:HG21	1.84	0.59
1:A:121:VAL:O	1:A:121:VAL:CG1	2.50	0.59
1:G:28:ILE:HD13	1:G:54:VAL:CG1	2.31	0.59
1:B:113:ARG:C	1:B:114:LEU:HD12	2.23	0.59
1:A:25:LEU:HD23	1:A:89:VAL:HB	1.83	0.59
1:C:121:VAL:HG22	4:C:462:HOH:O	2.03	0.59
1:B:121:VAL:HG21	4:B:504:HOH:O	2.03	0.59
1:E:121:VAL:O	1:E:121:VAL:CG1	2.51	0.59
1:H:93:HIS:HA	1:H:117:VAL:HG12	1.85	0.59
1:G:204:LEU:CD1	1:G:204:LEU:C	2.71	0.59
1:F:91:LEU:CD2	1:F:115:ILE:CB	2.76	0.58
1:F:114:LEU:HD12	1:F:114:LEU:N	2.17	0.58
1:C:6:VAL:HG21	1:C:84:ARG:CZ	2.32	0.58
1:G:91:LEU:HD13	1:G:115:ILE:CB	2.33	0.58
1:G:204:LEU:HD12	1:G:206:VAL:CG2	2.33	0.58
1:B:114:LEU:CD1	1:B:200:LEU:CD1	2.79	0.58
1:E:114:LEU:CD2	1:E:200:LEU:HD11	2.34	0.58
1:C:85[B]:MSE:HB3	1:C:88[B]:VAL:HG13	1.80	0.58
1:B:114:LEU:HD12	1:B:114:LEU:N	2.19	0.58
1:B:121:VAL:HG23	1:B:192:HIS:NE2	2.17	0.58
1:C:91:LEU:CD1	1:C:115:ILE:HB	2.28	0.58
1:G:121:VAL:O	1:G:121:VAL:CG2	2.50	0.58
1:G:28:ILE:HD13	1:G:54:VAL:HG11	1.86	0.58
1:G:115:ILE:HG21	1:G:252:VAL:HG23	1.84	0.58
1:G:93:HIS:CD2	1:G:117:VAL:CG2	2.86	0.58
1:B:114:LEU:HD11	1:B:200:LEU:CD1	2.21	0.57
1:H:114:LEU:N	1:H:114:LEU:CD1	2.64	0.57
1:E:93:HIS:CD2	1:E:117:VAL:HG23	2.28	0.57
1:F:2:LYS:HG3	1:F:17:HIS:HB3	1.87	0.57
1:A:25:LEU:HD22	1:A:89:VAL:O	2.04	0.57
1:H:121:VAL:CG2	1:H:192:HIS:CE1	2.84	0.56
1:G:121:VAL:HG22	4:G:440:HOH:O	2.04	0.56
1:B:117:VAL:HG23	1:B:117:VAL:O	2.04	0.56
1:D:117:VAL:HG23	1:D:117:VAL:O	2.04	0.56
1:B:121:VAL:CG2	1:B:192:HIS:CE1	2.84	0.56
1:D:114:LEU:HD21	1:D:200:LEU:CD1	2.33	0.56
1:C:93:HIS:HA	1:C:117:VAL:CG1	2.28	0.56
1:E:93:HIS:HA	1:E:117:VAL:CG2	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:LEU:CD1	1:A:200:LEU:HD11	2.28	0.56
1:C:93:HIS:CA	1:C:117:VAL:HG13	2.30	0.56
1:G:114:LEU:N	1:G:114:LEU:CD1	2.68	0.56
1:H:114:LEU:HD11	1:H:200:LEU:CD1	2.35	0.56
1:F:85:MSE:CB	1:F:88:VAL:HG11	2.35	0.56
1:B:91:LEU:CD1	1:B:115:ILE:CG2	2.83	0.55
1:B:25:LEU:HD12	1:B:25:LEU:C	2.26	0.55
1:F:85:MSE:CB	1:F:88:VAL:CG1	2.84	0.55
1:D:91:LEU:HD23	1:D:115:ILE:HB	1.88	0.55
1:A:121:VAL:HG12	4:A:425:HOH:O	2.06	0.54
1:B:252:VAL:O	1:B:252:VAL:CG1	2.55	0.54
1:C:85[A]:MSE:HB2	1:C:88[A]:VAL:CG2	2.37	0.54
1:A:14:HIS:CD2	1:A:55:ASP:OD1	2.57	0.54
1:F:91:LEU:HD21	1:F:115:ILE:HG22	1.89	0.54
1:E:222:ILE:HD11	1:E:230:THR:HG21	1.90	0.54
1:B:91:LEU:CD1	1:B:115:ILE:HG22	2.37	0.54
1:C:121:VAL:CG2	1:C:192:HIS:NE2	2.71	0.53
1:A:91:LEU:HD13	1:A:115:ILE:HG21	1.89	0.53
1:B:117:VAL:CG2	1:B:117:VAL:O	2.57	0.53
1:C:14:HIS:CD2	1:C:55:ASP:OD2	2.58	0.53
1:G:25:LEU:HD12	1:G:25:LEU:C	2.25	0.53
1:D:114:LEU:N	1:D:114:LEU:HD22	2.24	0.52
1:B:121:VAL:O	1:B:121:VAL:CG2	2.56	0.52
1:C:121:VAL:HG23	1:C:192:HIS:HE1	1.67	0.52
1:C:28:ILE:HD12	1:C:54:VAL:HG21	1.91	0.52
1:A:114:LEU:HD11	1:A:200:LEU:CD2	2.40	0.52
1:D:117:VAL:CG2	1:D:117:VAL:O	2.57	0.52
2:B:301:ACY:H1	4:B:651:HOH:O	2.09	0.52
1:D:91:LEU:HD23	1:D:115:ILE:CB	2.39	0.52
1:A:114:LEU:N	1:A:114:LEU:CD1	2.69	0.51
1:A:121:VAL:HG11	4:A:462:HOH:O	2.10	0.51
1:H:121:VAL:O	1:H:121:VAL:CG2	2.57	0.51
1:G:14:HIS:CD2	1:G:55:ASP:OD2	2.61	0.51
1:A:114:LEU:CD1	1:A:200:LEU:CG	2.89	0.51
1:C:91:LEU:CD1	1:C:115:ILE:HG22	2.40	0.51
1:D:91:LEU:CD2	1:D:115:ILE:CB	2.87	0.51
1:A:102[B]:ARG:NH2	4:A:481:HOH:O	2.38	0.51
1:D:63:GLU:HG2	1:D:67[B]:LEU:HD11	1.91	0.51
1:F:117:VAL:HG23	1:F:117:VAL:O	2.09	0.51
1:D:1:MSE:HG3	1:D:18:PHE:CE2	2.46	0.51
1:D:114:LEU:HD21	1:D:200:LEU:CD2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:25:LEU:CD1	1:G:89:VAL:O	2.59	0.51
1:A:114:LEU:CD1	1:A:200:LEU:HD21	2.41	0.51
1:E:121:VAL:HG12	4:E:493:HOH:O	2.10	0.51
1:D:84:ARG:NH2	4:D:591:HOH:O	2.44	0.51
1:D:14:HIS:CD2	1:D:55:ASP:OD2	2.61	0.51
1:A:102[B]:ARG:HD3	1:A:194:ASP:OD2	2.11	0.50
1:A:252:VAL:O	1:A:252:VAL:CG2	2.59	0.50
1:G:113:ARG:C	1:G:114:LEU:HD12	2.31	0.50
1:F:114:LEU:HD11	1:F:200:LEU:CD1	2.23	0.50
1:F:114:LEU:CD1	1:F:114:LEU:N	2.75	0.50
1:H:114:LEU:HD11	1:H:200:LEU:CG	2.42	0.50
1:C:26:LEU:HD21	1:C:85[B]:MSE:HE1	1.93	0.50
1:C:85[A]:MSE:HB3	1:C:88[A]:VAL:HG22	1.92	0.50
1:H:91:LEU:HD23	1:H:115:ILE:HG21	1.94	0.49
1:E:6:VAL:HG22	1:E:7:TYR:N	2.27	0.49
1:H:114:LEU:HD11	1:H:200:LEU:CD2	2.42	0.49
1:B:93:HIS:CA	1:B:117:VAL:HG22	2.29	0.49
1:C:121:VAL:CG2	1:C:192:HIS:HE2	2.26	0.49
1:E:121:VAL:HG13	1:E:192:HIS:NE2	2.28	0.49
1:A:91:LEU:CD1	1:A:115:ILE:HG21	2.40	0.49
1:H:84:ARG:HD2	4:H:541:HOH:O	2.11	0.49
1:A:1:MSE:HG2	1:A:16:ILE:CG2	2.43	0.49
1:C:6:VAL:CG2	1:C:84:ARG:NH1	2.76	0.49
1:D:142:LEU:HD21	1:D:151:GLU:HB3	1.95	0.48
1:B:114:LEU:CD1	1:B:114:LEU:N	2.76	0.48
1:D:114:LEU:CD2	1:D:200:LEU:CD1	2.89	0.48
1:H:91:LEU:HD23	1:H:115:ILE:HB	1.94	0.48
1:B:30:GLY:HA3	2:B:301:ACY:H3	1.95	0.48
1:B:121:VAL:HG22	4:B:441:HOH:O	2.14	0.48
1:H:91:LEU:CD2	1:H:115:ILE:HB	2.44	0.48
1:D:91:LEU:HD22	1:D:115:ILE:HB	1.93	0.48
1:E:14:HIS:CD2	1:E:55:ASP:OD2	2.60	0.48
1:A:114:LEU:CD1	1:A:200:LEU:HG	2.44	0.47
1:E:6:VAL:CG2	1:E:84:ARG:NH2	2.78	0.47
1:F:117:VAL:CG2	1:F:117:VAL:O	2.62	0.47
1:A:6[B]:VAL:HG13	1:A:84:ARG:CZ	2.44	0.47
1:B:14:HIS:CD2	1:B:55:ASP:OD2	2.63	0.47
1:G:114:LEU:CD1	1:G:200:LEU:HD21	2.44	0.47
1:G:117:VAL:CG2	1:G:117:VAL:O	2.62	0.47
1:G:25:LEU:HD12	1:G:26:LEU:H	1.79	0.47
1:G:121:VAL:CG2	1:G:192:HIS:HE1	2.21	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:114:LEU:CD1	1:H:200:LEU:HD21	2.44	0.47
1:D:121:VAL:CG2	1:D:192:HIS:CE1	2.93	0.47
1:E:121:VAL:HG13	1:E:192:HIS:HE1	1.73	0.47
1:H:113:ARG:C	1:H:114:LEU:HD12	2.35	0.47
1:A:121:VAL:HG13	1:A:192:HIS:HE1	1.76	0.46
1:C:85[B]:MSE:HB3	1:C:88[B]:VAL:HG12	1.91	0.46
1:B:25:LEU:HD12	1:B:26:LEU:H	1.76	0.46
1:B:91:LEU:HD13	1:B:115:ILE:HG21	1.94	0.46
1:D:91:LEU:HD22	1:D:115:ILE:CG2	2.44	0.46
1:G:117:VAL:HG23	1:G:117:VAL:O	2.14	0.46
1:H:132:LYS:H	3:H:302:PEG:H32	1.81	0.46
1:A:113:ARG:C	1:A:114:LEU:HD12	2.34	0.46
1:C:54:VAL:HG23	1:C:54:VAL:O	2.15	0.46
1:G:114:LEU:CD1	1:G:200:LEU:CD1	2.90	0.46
1:G:114:LEU:HD11	1:G:200:LEU:CG	2.46	0.46
1:A:121:VAL:HG13	1:A:192:HIS:NE2	2.30	0.45
1:A:114:LEU:CD1	1:A:200:LEU:CD1	2.92	0.45
1:A:115:ILE:HD13	1:A:252:VAL:CG2	2.46	0.45
1:G:91:LEU:HD22	1:G:252:VAL:HG21	1.98	0.45
1:C:121:VAL:CG2	1:C:192:HIS:HE1	2.25	0.45
1:C:85[A]:MSE:CB	1:C:88[A]:VAL:HG22	2.47	0.45
1:C:91:LEU:HD12	1:C:115:ILE:O	2.16	0.45
1:C:19:PRO:HB3	1:D:47:LYS:HE2	1.99	0.45
1:C:28:ILE:CD1	1:C:54:VAL:HG21	2.47	0.45
1:D:121:VAL:HG23	1:D:192:HIS:HE2	1.80	0.45
1:H:91:LEU:CD2	1:H:115:ILE:HG22	2.46	0.45
1:D:26:LEU:HD21	1:D:85:MSE:HE1	1.97	0.45
1:F:91:LEU:HD22	1:F:115:ILE:O	2.16	0.45
1:F:196:ALA:HB2	1:F:224:LEU:HD22	1.98	0.45
1:D:105:ARG:CD	1:F:161:ASP:OD1	2.61	0.44
1:D:121:VAL:O	1:D:121:VAL:CG2	2.65	0.44
1:G:28:ILE:HD13	1:G:54:VAL:HG12	1.99	0.44
1:H:91:LEU:HD13	1:H:91:LEU:C	2.38	0.44
1:B:25:LEU:HD12	1:B:89:VAL:O	2.16	0.44
1:E:114:LEU:CD2	1:E:200:LEU:CD2	2.90	0.44
1:H:93:HIS:HD2	1:H:117:VAL:HG13	1.82	0.44
1:A:6[B]:VAL:HG13	1:A:84:ARG:NH1	2.32	0.44
1:C:121:VAL:HG23	1:C:192:HIS:HE2	1.77	0.44
1:G:91:LEU:HD13	1:G:115:ILE:HG22	1.96	0.44
1:H:85:MSE:CB	1:H:88:VAL:HG11	2.48	0.44
1:B:102[B]:ARG:HD2	1:B:105:ARG:NH2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:LEU:HD22	1:D:115:ILE:HG22	2.00	0.43
1:D:114:LEU:CD2	1:D:200:LEU:CG	2.96	0.43
1:F:36:VAL:HG23	4:F:579:HOH:O	2.17	0.43
1:H:85:MSE:CB	1:H:88:VAL:CG1	2.96	0.43
1:H:121:VAL:HG22	4:H:427:HOH:O	2.17	0.43
1:A:91:LEU:HD12	1:A:115:ILE:O	2.18	0.43
1:G:252:VAL:HG22	1:G:252:VAL:O	2.18	0.43
1:B:25:LEU:HD13	1:B:89:VAL:C	2.39	0.43
1:C:85[A]:MSE:CB	1:C:88[A]:VAL:CG2	2.96	0.43
1:E:114:LEU:HD23	1:E:200:LEU:HD21	1.97	0.43
1:C:85[B]:MSE:HB2	1:C:88[B]:VAL:HG11	1.98	0.43
1:E:121:VAL:HG11	4:E:570:HOH:O	2.19	0.43
1:F:114:LEU:CD1	1:F:200:LEU:HD21	2.49	0.43
1:G:121:VAL:CG2	1:G:192:HIS:NE2	2.76	0.43
1:D:114:LEU:HD22	1:D:200:LEU:HD11	1.99	0.43
1:F:204:LEU:HD22	1:F:230:THR:HG23	1.99	0.43
1:C:196:ALA:HB2	1:C:224:LEU:HD22	2.00	0.42
1:E:114:LEU:HD21	1:E:200:LEU:CD2	2.40	0.42
1:H:91:LEU:HD23	1:H:115:ILE:CB	2.48	0.42
1:G:114:LEU:HD11	1:G:200:LEU:CD2	2.46	0.42
1:H:114:LEU:CD1	1:H:200:LEU:HD11	2.43	0.42
1:D:115:ILE:HG21	1:D:252:VAL:CG2	2.46	0.42
1:G:25:LEU:HD13	1:G:89:VAL:O	2.20	0.42
1:F:2:LYS:HG3	1:F:2:LYS:O	2.19	0.42
1:F:2:LYS:O	1:F:17:HIS:HB3	2.19	0.42
1:F:91:LEU:HD21	1:F:115:ILE:CG2	2.45	0.42
1:H:93:HIS:CD2	1:H:117:VAL:HG13	2.55	0.42
1:D:114:LEU:CD2	1:D:200:LEU:CD2	2.95	0.41
1:G:114:LEU:CD1	1:G:200:LEU:CG	2.98	0.41
1:C:6:VAL:CG2	1:C:84:ARG:CZ	2.96	0.41
1:D:45:LEU:N	1:D:45:LEU:HD22	2.35	0.41
1:E:6:VAL:HG23	1:E:84:ARG:NH2	2.36	0.41
1:G:79:VAL:O	1:G:83:GLN:HG2	2.21	0.41
1:H:83:GLN:HG2	1:H:110:VAL:HG11	2.03	0.41
1:C:121:VAL:CG2	1:C:121:VAL:O	2.68	0.40
1:H:85:MSE:HB3	1:H:88:VAL:HG13	2.04	0.40
1:G:91:LEU:HD11	1:G:117:VAL:CG1	2.52	0.40
1:H:117:VAL:CG1	1:H:117:VAL:O	2.68	0.40
1:D:93:HIS:CA	1:D:117:VAL:HG22	2.31	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	258/255 (101%)	254 (98%)	4 (2%)	0	100	100
1	B	259/255 (102%)	252 (97%)	7 (3%)	0	100	100
1	C	254/255 (100%)	248 (98%)	6 (2%)	0	100	100
1	D	255/255 (100%)	252 (99%)	3 (1%)	0	100	100
1	E	255/255 (100%)	250 (98%)	5 (2%)	0	100	100
1	F	250/255 (98%)	245 (98%)	5 (2%)	0	100	100
1	G	250/255 (98%)	246 (98%)	4 (2%)	0	100	100
1	H	258/255 (101%)	251 (97%)	7 (3%)	0	100	100
All	All	2039/2040 (100%)	1998 (98%)	41 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	211/201 (105%)	208 (99%)	3 (1%)	62	43
1	B	216/201 (108%)	212 (98%)	4 (2%)	52	30
1	C	208/201 (104%)	206 (99%)	2 (1%)	73	59
1	D	209/201 (104%)	208 (100%)	1 (0%)	86	80
1	E	210/201 (104%)	204 (97%)	6 (3%)	37	14
1	F	206/201 (102%)	202 (98%)	4 (2%)	52	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	205/201 (102%)	201 (98%)	4 (2%)	50	28
1	H	213/201 (106%)	211 (99%)	2 (1%)	75	63
All	All	1678/1608 (104%)	1652 (98%)	26 (2%)	60	41

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	GLN
1	A	114	LEU
1	A	118	ASP
1	B	25	LEU
1	B	86	GLU
1	B	114	LEU
1	B	118	ASP
1	C	1	MSE
1	C	118	ASP
1	D	118	ASP
1	E	1	MSE
1	E	25	LEU
1	E	102	ARG
1	E	118	ASP
1	E	204[A]	LEU
1	E	204[B]	LEU
1	F	2	LYS
1	F	114	LEU
1	F	118	ASP
1	F	204	LEU
1	G	25	LEU
1	G	102	ARG
1	G	114	LEU
1	G	118	ASP
1	H	114	LEU
1	H	118	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	B	14	HIS
1	B	214	GLN

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Mol	Chain	Res	Type
1	C	14	HIS
1	D	14	HIS
1	D	83	GLN
1	D	214	GLN
1	E	14	HIS
1	E	83	GLN
1	F	187	HIS
1	F	214	GLN
1	G	14	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 ⓘ

11 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	ACY	A	301	-	3,3,3	0.67	0	3,3,3	0.94	0
2	ACY	C	301	-	3,3,3	1.03	0	3,3,3	0.30	0
2	ACY	G	302	-	3,3,3	0.86	0	3,3,3	0.75	0
2	ACY	B	301	-	3,3,3	0.39	0	3,3,3	1.36	0
2	ACY	A	302	-	3,3,3	0.96	0	3,3,3	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	ACY	H	301	-	3,3,3	1.07	0	3,3,3	0.38	0
2	ACY	F	301	-	3,3,3	0.71	0	3,3,3	0.87	0
2	ACY	D	301	-	3,3,3	0.85	0	3,3,3	0.66	0
3	PEG	H	302	-	6,6,6	0.53	0	5,5,5	0.31	0
2	ACY	G	301	-	3,3,3	0.92	0	3,3,3	0.46	0
2	ACY	E	301	-	3,3,3	1.10	0	3,3,3	0.43	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	H	302	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	302	PEG	C4-C3-O2-C2
3	H	302	PEG	O2-C3-C4-O4

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	ACY	1	0
2	B	301	ACY	2	0
2	A	302	ACY	3	0
3	H	302	PEG	2	0

5.7 Other polymers ⓘ

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	248/255 (97%)	-0.22	3 (1%)	76	80	6, 10, 16, 30	14 (5%)
1	B	248/255 (97%)	-0.08	7 (2%)	55	59	7, 12, 18, 29	19 (7%)
1	C	246/255 (96%)	0.28	7 (2%)	55	59	8, 15, 25, 37	13 (5%)
1	D	246/255 (96%)	0.19	12 (4%)	36	38	5, 14, 23, 33	21 (8%)
1	E	248/255 (97%)	-0.03	6 (2%)	59	63	6, 12, 19, 24	15 (6%)
1	F	246/255 (96%)	0.43	14 (5%)	30	33	7, 16, 24, 33	18 (7%)
1	G	246/255 (96%)	0.06	11 (4%)	39	42	7, 13, 22, 33	10 (4%)
1	H	248/255 (97%)	-0.16	4 (1%)	70	74	6, 11, 17, 23	16 (6%)
All	All	1976/2040 (96%)	0.06	64 (3%)	50	54	5, 12, 22, 37	126 (6%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	86	GLU	5.4
1	F	125	GLY	4.6
1	D	108	SER	4.3
1	G	25	LEU	4.3
1	G	235	GLU	4.2
1	F	2	LYS	4.1
1	D	252	VAL	4.0
1	A	87	GLY	3.9
1	C	252	VAL	3.5
1	D	45	LEU	3.4
1	D	235	GLU	3.4
1	B	87	GLY	3.3
1	G	87	GLY	3.3
1	C	235	GLU	3.2
1	B	21	THR	3.2
1	F	21	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	23	SER	3.1
1	D	21	THR	3.0
1	E	86	GLU	3.0
1	E	21	THR	3.0
1	F	204	LEU	3.0
1	F	20	GLY	3.0
1	G	231	TYR	2.9
1	D	87	GLY	2.9
1	H	86	GLU	2.8
1	C	209	GLY	2.8
1	D	249	ILE	2.7
1	G	252	VAL	2.7
1	C	253	SER	2.7
1	D	231	TYR	2.6
1	F	47	LYS	2.6
1	D	236	ALA	2.6
1	B	252	VAL	2.6
1	F	88	VAL	2.6
1	F	109	GLN	2.6
1	H	145	ARG	2.5
1	D	86	GLU	2.5
1	H	88	VAL	2.5
1	F	108	SER	2.4
1	D	66[A]	ASP	2.4
1	F	107	ASP	2.4
1	B	117	VAL	2.4
1	F	89	VAL	2.4
1	E	117	VAL	2.3
1	G	86	GLU	2.3
1	A	22	GLY	2.3
1	F	87	GLY	2.3
1	H	21	THR	2.3
1	A	86	GLU	2.2
1	C	86	GLU	2.2
1	B	66[A]	ASP	2.2
1	B	83	GLN	2.2
1	C	117	VAL	2.2
1	E	88	VAL	2.2
1	G	54	VAL	2.2
1	D	234	GLU	2.1
1	E	252	VAL	2.1
1	F	215	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	234	GLU	2.1
1	G	108	SER	2.1
1	G	21	THR	2.0
1	E	87	GLY	2.0
1	C	108	SER	2.0
1	G	84	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
3	PEG	H	302	7/7	0.79	0.14	34,36,38,39	0
2	ACY	A	302	4/4	0.82	0.14	20,21,23,26	0
2	ACY	A	301	4/4	0.85	0.13	13,14,14,16	0
2	ACY	C	301	4/4	0.88	0.12	15,16,17,19	0
2	ACY	B	301	4/4	0.91	0.11	15,15,17,18	0
2	ACY	E	301	4/4	0.93	0.08	13,14,14,14	0
2	ACY	H	301	4/4	0.93	0.07	13,14,14,15	0
2	ACY	D	301	4/4	0.93	0.10	16,17,17,18	0
2	ACY	G	302	4/4	0.94	0.10	25,27,27,29	0
2	ACY	F	301	4/4	0.94	0.08	16,17,17,19	0
2	ACY	G	301	4/4	0.94	0.10	13,14,14,14	0

6.5 Other polymers ⓘ

There are no such residues in this entry.