



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:06 PM UTC

PDB ID : 1FDY / pdb_00001fdy
Title : N-ACETYLNEURAMINATE LYASE IN COMPLEX WITH HYDROX-
YPYRUVATE
Authors : Lawrence, M.C.; Barbosa, J.A.R.G.; Smith, B.J.; Hall, N.E.; Pilling, P.A.;
Ooi, H.C.; Marcuccio, S.M.
Deposited on : 1996-07-08
Resolution : 2.45 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

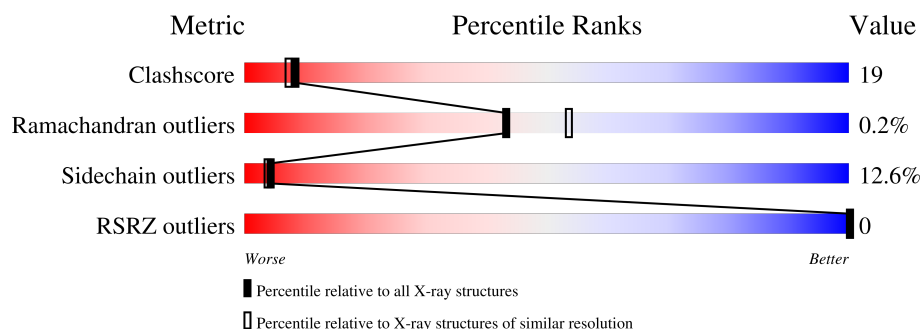
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	297	
1	B	297	
1	C	297	
1	D	297	

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	3PY	A	802	-	X	-	-
2	3PY	C	806	-	X	-	-
2	3PY	D	808	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9190 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.

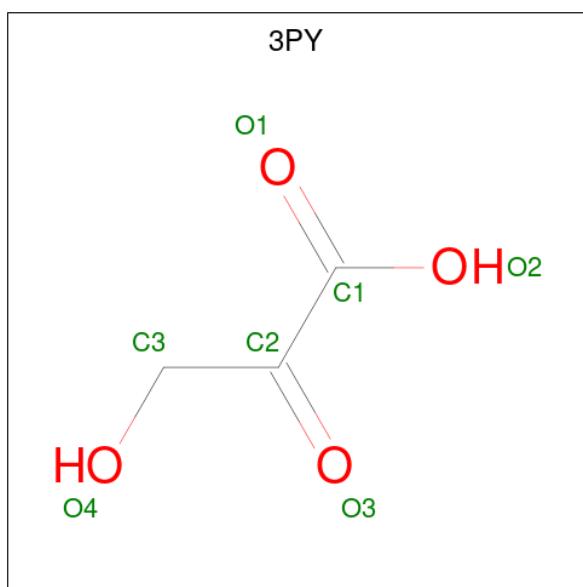
- Molecule 1 is a protein called N-ACETYLNEURAMINATE LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	61	0	0
			2254	1437	380	427	10			
1	B	291	Total	C	N	O	S	50	0	0
			2247	1434	379	424	10			
1	C	291	Total	C	N	O	S	60	0	0
			2247	1434	379	424	10			
1	D	291	Total	C	N	O	S	49	0	0
			2247	1434	379	424	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	70	GLY	ALA	conflict	UNP P0A6L4
A	84	THR	SER	conflict	UNP P0A6L4
B	70	GLY	ALA	conflict	UNP P0A6L4
B	84	THR	SER	conflict	UNP P0A6L4
C	70	GLY	ALA	conflict	UNP P0A6L4
C	84	THR	SER	conflict	UNP P0A6L4
D	70	GLY	ALA	conflict	UNP P0A6L4
D	84	THR	SER	conflict	UNP P0A6L4

- Molecule 2 is 3-HYDROXYPYRUVIC ACID (CCD ID: 3PY) (formula: C₃H₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

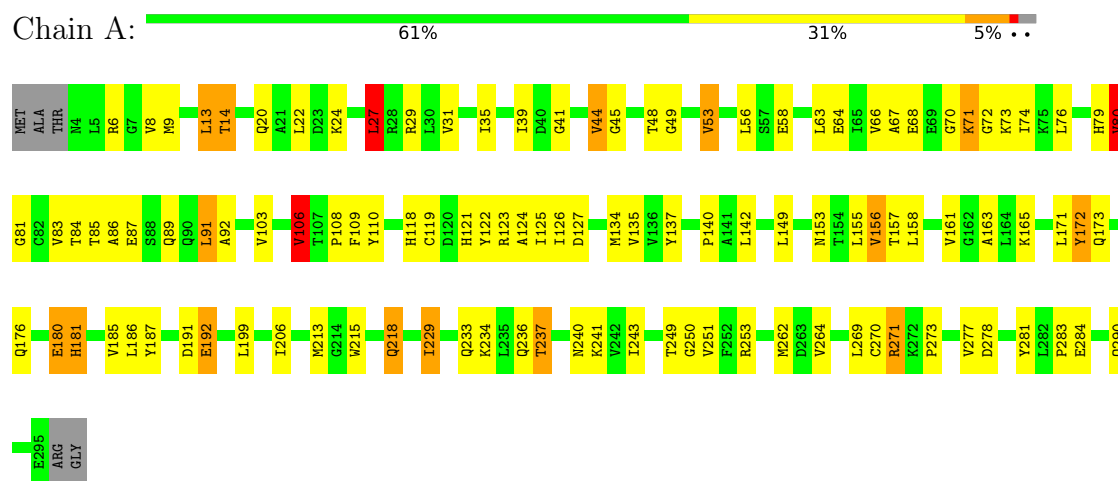
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	53	Total	O	0	0
			53	53		
3	B	38	Total	O	0	0
			38	38		
3	C	29	Total	O	0	0
			29	29		
3	D	51	Total	O	0	0
			51	51		

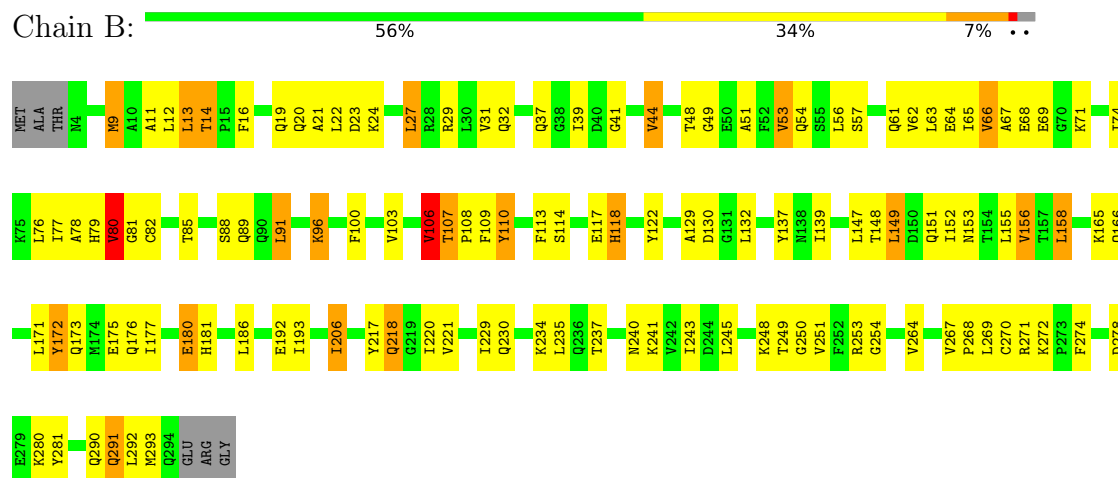
3 Residue-property plots [i](#)

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.

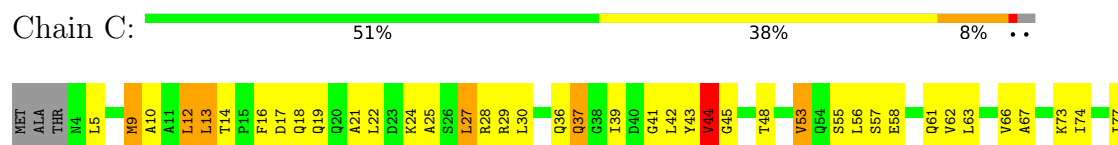
• Molecule 1: N-ACETYLNEURAMINATE LYASE

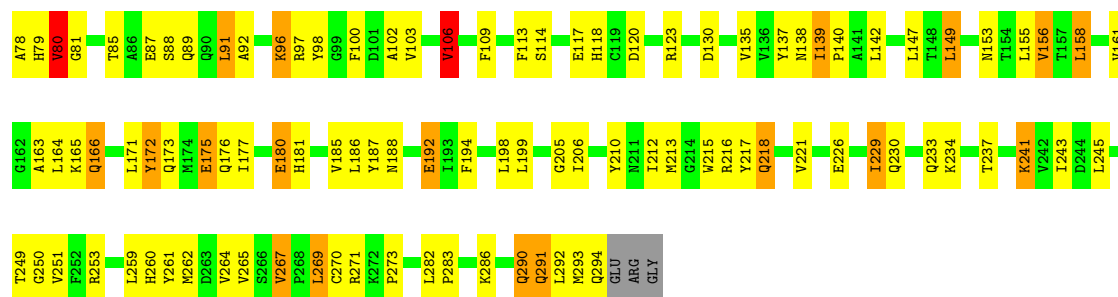


• Molecule 1: N-ACETYLNEURAMINATE LYASE



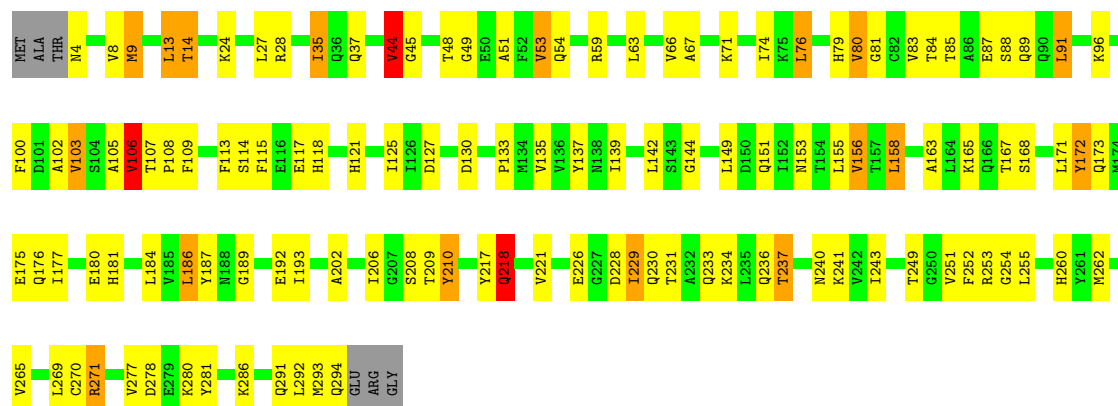
• Molecule 1: N-ACETYLNEURAMINATE LYASE





• Molecule 1: N-ACETYLNEURAMINATE LYASE

Chain D: 57% 35% 6% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	121.00Å 121.00Å 196.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.45 6.00 – 2.45	Depositor EDS
% Data completeness (in resolution range)	93.2 (6.00-2.45) 87.3 (6.00-2.45)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.10 (at 2.39Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.219 , (Not available) 0.213 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 72.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9190	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 3PY

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	0.75	1/2294 (0.0%)	1.17	14/3105 (0.5%)
1	B	0.73	0/2287	1.17	17/3096 (0.5%)
1	C	0.69	1/2287 (0.0%)	1.18	18/3096 (0.6%)
1	D	0.78	1/2287 (0.0%)	1.17	13/3096 (0.4%)
All	All	0.74	3/9155 (0.0%)	1.17	62/12393 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	262	MET	SD-CE	-5.63	1.65	1.79
1	C	44	VAL	CA-CB	5.54	1.61	1.54
1	D	177	ILE	CA-CB	5.23	1.60	1.54

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	251	VAL	N-CA-C	11.73	121.68	110.30
1	D	106	VAL	CB-CA-C	-10.02	100.22	111.45
1	B	80	VAL	N-CA-CB	-9.71	101.53	112.21
1	B	106	VAL	CB-CA-C	-9.60	100.70	111.45
1	C	67	ALA	N-CA-C	-9.15	100.99	110.97
1	A	172	TYR	N-CA-C	-8.50	101.03	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	VAL	CB-CA-C	-8.36	102.40	111.59
1	C	81	GLY	N-CA-C	8.35	124.75	111.64
1	A	80	VAL	N-CA-CB	-8.19	101.69	112.26
1	C	106	VAL	CB-CA-C	-8.10	100.45	111.63
1	D	172	TYR	N-CA-C	-7.93	101.73	111.40
1	D	80	VAL	N-CA-CB	-7.78	103.66	112.21
1	D	44	VAL	N-CA-C	7.32	119.61	108.71
1	C	139	ILE	CA-C-N	6.90	127.18	119.32
1	C	139	ILE	C-N-CA	6.90	127.18	119.32
1	A	73	LYS	N-CA-C	-6.84	103.93	112.90
1	B	172	TYR	N-CA-C	-6.84	103.28	111.69
1	D	109	PHE	N-CA-C	6.76	120.20	109.65
1	C	12	LEU	N-CA-C	6.76	120.17	110.10
1	D	251	VAL	N-CA-C	6.66	116.81	110.42
1	D	83	VAL	N-CA-C	-6.58	104.08	110.72
1	C	267	VAL	CA-C-N	6.50	127.96	119.84
1	C	267	VAL	C-N-CA	6.50	127.96	119.84
1	A	67	ALA	N-CA-C	-6.48	104.22	111.28
1	C	172	TYR	N-CA-C	-6.44	103.50	112.45
1	B	109	PHE	N-CA-C	6.43	119.21	109.63
1	C	5	LEU	N-CA-C	-6.42	105.19	113.16
1	A	251	VAL	N-CA-C	6.42	116.53	110.30
1	D	144	GLY	N-CA-C	-6.40	106.40	115.30
1	A	81	GLY	N-CA-C	6.36	120.19	111.54
1	A	181	HIS	CA-C-N	6.15	125.83	119.56
1	A	181	HIS	C-N-CA	6.15	125.83	119.56
1	C	80	VAL	N-CA-CB	-6.08	104.20	112.28
1	C	270	CYS	N-CA-C	-6.03	100.79	110.14
1	A	83	VAL	N-CA-C	-5.95	104.71	110.72
1	B	27	LEU	N-CA-C	-5.81	104.85	111.07
1	C	96	LYS	N-CA-C	-5.79	104.66	110.97
1	B	81	GLY	N-CA-C	5.79	118.14	111.36
1	D	81	GLY	N-CA-C	5.76	118.10	111.36
1	B	107	THR	N-CA-C	-5.71	101.11	109.50
1	A	109	PHE	N-CA-C	5.69	118.53	109.65
1	B	270	CYS	N-CA-C	-5.67	100.89	109.85
1	B	139	ILE	CA-C-N	5.64	125.75	119.32
1	B	139	ILE	C-N-CA	5.64	125.75	119.32
1	C	53	VAL	N-CA-C	-5.63	107.50	112.90
1	B	82	CYS	N-CA-C	-5.60	100.61	108.96
1	B	23	ASP	N-CA-C	-5.59	98.13	108.24
1	A	250	GLY	N-CA-C	-5.58	99.96	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	35	ILE	N-CA-C	-5.52	104.94	110.30
1	B	12	LEU	N-CA-C	5.52	118.23	110.23
1	C	251	VAL	N-CA-C	5.51	115.65	110.30
1	B	250	GLY	N-CA-C	-5.45	100.26	113.18
1	C	241	LYS	N-CA-C	-5.45	105.34	111.28
1	C	250	GLY	N-CA-C	-5.43	100.30	113.18
1	B	206	ILE	N-CA-C	-5.30	99.92	107.77
1	C	109	PHE	N-CA-C	5.25	118.19	109.94
1	A	27	LEU	N-CA-C	-5.24	105.26	110.97
1	B	11	ALA	N-CA-C	-5.24	98.77	107.99
1	D	107	THR	N-CA-C	-5.22	100.44	109.58
1	A	270	CYS	N-CA-C	-5.20	101.68	109.95
1	D	218	GLN	N-CA-C	-5.16	105.73	111.36
1	D	270	CYS	N-CA-C	-5.15	102.57	110.14

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	187	TYR	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2254	0	2266	80	0
1	B	2247	0	2267	84	0
1	C	2247	0	2267	98	0
1	D	2247	0	2267	86	0
2	A	6	0	2	0	0
2	B	6	0	2	0	0
2	C	6	0	2	0	0
2	D	6	0	2	0	0
3	A	53	0	0	3	0
3	B	38	0	0	1	0
3	C	29	0	0	0	0
3	D	51	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9190	0	9075	335	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 19.

All (335) 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:D:262:MET:HA	1:D:293:MET:HE3	1.36	1.07
1:C:173:GLN:HA	1:C:176:GLN:HE21	1.25	1.01
1:A:80:VAL:HG22	1:A:91:LEU:HB3	1.44	0.99
1:D:96:LYS:HD2	1:D:130:ASP:HB3	1.51	0.91
1:B:13:LEU:HD13	1:B:48:THR:HG22	1.63	0.81
1:B:153:ASN:OD1	1:B:181:HIS:HE1	1.64	0.80
1:A:108:PRO:HD2	1:A:118:HIS:CD2	2.18	0.78
1:A:108:PRO:HD2	1:A:118:HIS:HD2	1.49	0.76
1:D:217:TYR:O	1:D:221:VAL:HG23	1.87	0.75
1:D:153:ASN:OD1	1:D:181:HIS:HE1	1.70	0.75
1:A:253:ARG:HD3	1:A:277:VAL:HG22	1.68	0.74
1:C:114:SER:OG	1:C:117:GLU:HG3	1.88	0.74
1:A:173:GLN:HA	1:A:176:GLN:HE21	1.51	0.74
1:B:51:ALA:HA	1:B:54:GLN:HE21	1.52	0.74
1:B:148:THR:O	1:B:152:ILE:HG13	1.89	0.73
1:D:291:GLN:O	1:D:294:GLN:HG2	1.88	0.72
1:C:96:LYS:HG3	1:C:130:ASP:HB3	1.70	0.72
1:B:171:LEU:HD12	1:D:171:LEU:HD12	1.71	0.72
1:A:85:THR:O	1:A:89:GLN:HG3	1.89	0.72
1:B:79:HIS:HE1	1:B:106:VAL:H	1.38	0.71
1:A:236:GLN:HE21	1:A:240:ASN:ND2	1.88	0.71
1:A:106:VAL:HG13	1:A:137:TYR:CD2	2.25	0.70
1:D:233:GLN:O	1:D:237:THR:HG23	1.91	0.70
1:D:44:VAL:HG22	1:D:63:LEU:HD23	1.72	0.70
1:D:262:MET:HA	1:D:293:MET:CE	2.17	0.70
1:C:173:GLN:HA	1:C:176:GLN:NE2	2.06	0.69
1:A:44:VAL:HG22	1:A:63:LEU:HD23	1.74	0.69
1:C:106:VAL:HG13	1:C:137:TYR:CD2	2.28	0.68
1:D:237:THR:O	1:D:241:LYS:HG3	1.94	0.68
1:C:22:LEU:HD23	1:C:61:GLN:OE1	1.93	0.68
1:D:153:ASN:OD1	1:D:181:HIS:CE1	2.47	0.67
1:B:108:PRO:HD2	1:B:118:HIS:CD2	2.30	0.67
1:D:249:THR:O	1:D:253:ARG:HD2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ILE:HG12	1:A:74:ILE:HD13	1.77	0.67
1:A:236:GLN:HE21	1:A:240:ASN:HD21	1.41	0.67
1:C:12:LEU:HD13	1:C:42:LEU:HD22	1.76	0.67
1:A:218:GLN:HE21	1:A:218:GLN:HA	1.60	0.66
1:C:173:GLN:O	1:C:177:ILE:HG13	1.96	0.66
1:B:20:GLN:HE22	1:B:271:ARG:HA	1.62	0.64
1:D:9:MET:O	1:D:206:ILE:HA	1.97	0.64
1:A:199:LEU:HD22	1:C:199:LEU:HD22	1.80	0.64
1:A:240:ASN:OD1	1:C:175:GLU:HG2	1.97	0.64
1:C:37:GLN:OE1	1:C:215:TRP:HZ3	1.80	0.63
1:D:293:MET:O	1:D:294:GLN:HB3	1.97	0.63
1:B:108:PRO:HD2	1:B:118:HIS:HD2	1.61	0.63
1:D:192:GLU:HG3	1:D:243:ILE:HG21	1.81	0.63
1:B:79:HIS:HE1	1:B:106:VAL:N	1.96	0.62
1:C:267:VAL:HG12	1:C:269:LEU:HB2	1.80	0.62
1:A:284:GLU:HG3	3:A:530:HOH:O	2.00	0.62
1:C:137:TYR:CD1	1:C:165:LYS:HD3	2.35	0.62
1:A:171:LEU:HD12	1:C:171:LEU:HD12	1.81	0.62
1:C:163:ALA:HB2	1:C:185:VAL:HB	1.82	0.61
1:D:236:GLN:HE21	1:D:240:ASN:ND2	1.98	0.61
1:C:249:THR:O	1:C:253:ARG:HD2	2.00	0.61
1:B:110:TYR:O	1:C:142:LEU:HD12	2.00	0.61
1:C:291:GLN:HG3	1:C:292:LEU:N	2.16	0.61
1:A:14:THR:HG23	1:A:49:GLY:O	2.00	0.61
1:B:137:TYR:CD1	1:B:165:LYS:HD3	2.35	0.60
1:B:13:LEU:HD13	1:B:48:THR:CG2	2.31	0.60
1:C:80:VAL:HG22	1:C:91:LEU:HB3	1.83	0.60
1:D:79:HIS:HE1	1:D:106:VAL:H	1.50	0.60
1:C:192:GLU:HG3	1:C:243:ILE:HG21	1.84	0.60
1:B:249:THR:O	1:B:253:ARG:HD2	2.01	0.60
1:A:249:THR:O	1:A:253:ARG:HD2	2.02	0.59
1:C:55:SER:OG	1:C:58:GLU:HG3	2.02	0.59
1:C:237:THR:O	1:C:241:LYS:HG3	2.02	0.59
1:B:85:THR:O	1:B:89:GLN:HG3	2.02	0.59
1:B:79:HIS:CE1	1:B:106:VAL:HG22	2.38	0.59
1:A:79:HIS:CE1	1:A:106:VAL:HG22	2.38	0.59
1:A:84:THR:HG21	1:A:87:GLU:HG3	1.85	0.59
1:D:218:GLN:HE21	1:D:218:GLN:HA	1.66	0.59
1:B:217:TYR:O	1:B:221:VAL:HG23	2.03	0.59
1:B:20:GLN:NE2	1:B:271:ARG:HA	2.18	0.58
1:B:96:LYS:HG3	1:B:130:ASP:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:VAL:HG13	1:D:137:TYR:CD2	2.38	0.58
1:C:213:MET:HB2	1:C:216:ARG:HD2	1.86	0.58
1:D:96:LYS:HE2	1:D:130:ASP:OD2	2.03	0.58
1:C:153:ASN:OD1	1:C:181:HIS:HE1	1.87	0.58
1:D:14:THR:HG23	1:D:49:GLY:O	2.04	0.58
1:D:173:GLN:HA	1:D:176:GLN:HE21	1.69	0.58
1:B:16:PHE:CE2	1:B:271:ARG:HG3	2.39	0.58
1:D:253:ARG:HD3	1:D:277:VAL:HG22	1.85	0.58
1:C:164:LEU:HD21	1:C:166:GLN:HG2	1.85	0.57
1:D:260:HIS:HD2	1:D:265:VAL:O	1.87	0.57
1:A:79:HIS:HE1	1:A:106:VAL:HG22	1.69	0.57
1:A:9:MET:HE3	1:A:41:GLY:HA3	1.86	0.57
1:A:153:ASN:OD1	1:A:181:HIS:HE1	1.87	0.57
1:C:218:GLN:HE21	1:C:218:GLN:HA	1.69	0.57
1:B:172:TYR:CD1	1:D:192:GLU:HB3	2.39	0.57
1:A:106:VAL:HG13	1:A:137:TYR:CE2	2.40	0.56
1:C:163:ALA:CB	1:C:185:VAL:HB	2.34	0.56
1:B:218:GLN:HE21	1:B:218:GLN:HA	1.69	0.56
1:B:14:THR:CG2	1:B:49:GLY:O	2.54	0.56
1:D:96:LYS:CD	1:D:130:ASP:HB3	2.32	0.56
1:D:13:LEU:HD13	1:D:48:THR:HG22	1.88	0.56
1:A:237:THR:O	1:A:241:LYS:HG3	2.06	0.56
1:C:229:ILE:O	1:C:233:GLN:HG3	2.06	0.55
1:C:56:LEU:HD11	1:C:87:GLU:HG2	1.88	0.55
1:C:85:THR:O	1:C:89:GLN:HG3	2.06	0.55
1:A:80:VAL:HG21	1:A:92:ALA:HA	1.89	0.55
1:D:54:GLN:HG3	1:D:59:ARG:HG3	1.88	0.55
1:A:110:TYR:CE1	1:D:142:LEU:HD13	2.40	0.55
1:B:149:LEU:HD11	1:B:176:GLN:HB3	1.89	0.55
1:A:45:GLY:O	1:A:79:HIS:HD2	1.89	0.55
1:B:29:ARG:NH1	1:B:264:VAL:O	2.39	0.55
1:A:22:LEU:CD2	1:A:24:LYS:HG2	2.37	0.55
1:B:106:VAL:HG13	1:B:137:TYR:CD2	2.42	0.55
1:A:172:TYR:O	1:A:176:GLN:HG3	2.07	0.54
1:B:192:GLU:HG3	1:B:243:ILE:HG21	1.88	0.54
1:D:114:SER:OG	1:D:117:GLU:HG3	2.08	0.54
1:D:291:GLN:HG3	1:D:292:LEU:N	2.23	0.54
1:A:84:THR:OG1	1:D:53:VAL:HG22	2.08	0.54
1:C:43:TYR:CD1	1:C:206:ILE:HD13	2.42	0.54
1:C:260:HIS:HD2	1:C:265:VAL:O	1.90	0.54
1:D:260:HIS:CD2	1:D:265:VAL:O	2.61	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:LEU:O	1:A:158:LEU:HB2	2.07	0.54
1:B:9:MET:O	1:B:206:ILE:HA	2.07	0.54
1:D:84:THR:HG22	1:D:87:GLU:H	1.72	0.54
1:B:22:LEU:HD23	1:B:61:GLN:OE1	2.08	0.54
1:B:113:PHE:CZ	1:C:273:PRO:HG2	2.43	0.53
1:C:17:ASP:OD2	1:C:21:ALA:HB3	2.08	0.53
1:A:180:GLU:HB3	1:A:181:HIS:CE1	2.42	0.53
1:B:80:VAL:HG22	1:B:91:LEU:HB3	1.90	0.53
1:C:233:GLN:O	1:C:237:THR:HG23	2.08	0.53
1:A:124:ALA:O	1:A:127:ASP:HB3	2.08	0.53
1:D:121:HIS:O	1:D:125:ILE:HG13	2.09	0.53
1:A:44:VAL:CG2	1:A:63:LEU:HD23	2.37	0.53
1:A:140:PRO:HD2	3:A:591:HOH:O	2.08	0.52
1:C:282:LEU:N	1:C:283:PRO:HD2	2.25	0.52
1:A:135:VAL:HG22	1:A:163:ALA:HB3	1.92	0.52
1:A:14:THR:CG2	1:A:49:GLY:O	2.58	0.52
1:D:278:ASP:HB3	1:D:281:TYR:HD2	1.75	0.52
1:A:84:THR:HG22	1:A:87:GLU:H	1.73	0.52
1:A:27:LEU:O	1:A:31:VAL:HG23	2.09	0.52
1:A:192:GLU:HB3	1:C:172:TYR:CD1	2.45	0.52
1:C:37:GLN:OE1	1:C:215:TRP:CZ3	2.61	0.52
1:C:56:LEU:HD21	1:C:87:GLU:HB3	1.90	0.52
1:C:142:LEU:N	1:C:142:LEU:HD22	2.24	0.52
1:B:114:SER:OG	1:B:117:GLU:HG3	2.10	0.52
1:A:253:ARG:CD	1:A:277:VAL:HG22	2.39	0.51
1:B:9:MET:CE	1:B:77:ILE:HD11	2.40	0.51
1:C:77:ILE:HG12	1:C:102:ALA:HB3	1.92	0.51
1:C:261:TYR:CE2	1:C:286:LYS:HG3	2.46	0.51
1:C:261:TYR:CZ	1:C:286:LYS:HG3	2.45	0.51
1:A:70:GLY:O	1:A:72:GLY:N	2.43	0.51
1:D:118:HIS:HE1	3:D:451:HOH:O	1.92	0.51
1:A:84:THR:CG2	1:A:87:GLU:HG3	2.40	0.51
1:D:135:VAL:HG22	1:D:163:ALA:HB3	1.92	0.51
1:B:96:LYS:HG3	1:B:129:ALA:O	2.10	0.51
1:B:31:VAL:HG11	1:B:69:GLU:HB3	1.93	0.51
1:D:54:GLN:NE2	3:D:453:HOH:O	2.43	0.51
1:D:24:LYS:O	1:D:28:ARG:HG3	2.11	0.50
1:D:85:THR:O	1:D:89:GLN:HG3	2.11	0.50
1:B:237:THR:O	1:B:241:LYS:HG3	2.10	0.50
1:A:119:CYS:O	1:A:123:ARG:HG3	2.11	0.50
1:C:113:PHE:HB2	1:C:118:HIS:CE1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:PHE:CE2	1:C:198:LEU:HD11	2.47	0.50
1:D:278:ASP:HB3	1:D:281:TYR:CD2	2.47	0.50
1:C:13:LEU:HD13	1:C:48:THR:HG22	1.93	0.50
1:D:79:HIS:HE1	1:D:106:VAL:N	2.09	0.50
1:C:192:GLU:CD	1:C:192:GLU:H	2.19	0.50
1:D:35:ILE:HG12	1:D:74:ILE:HD13	1.94	0.50
1:A:213:MET:HA	1:A:215:TRP:CZ3	2.47	0.49
1:C:30:LEU:HD13	1:C:259:LEU:HD13	1.94	0.49
1:A:13:LEU:HD13	1:A:48:THR:CG2	2.42	0.49
1:C:213:MET:HA	1:C:215:TRP:CZ3	2.47	0.49
1:D:108:PRO:HD2	1:D:118:HIS:HD2	1.77	0.49
1:A:29:ARG:HD2	1:A:264:VAL:O	2.12	0.49
1:D:54:GLN:HB3	1:D:271:ARG:HH21	1.76	0.49
1:A:64:GLU:O	1:A:68:GLU:HG3	2.12	0.49
1:B:14:THR:HG21	1:B:49:GLY:O	2.12	0.49
1:B:44:VAL:CG2	1:B:63:LEU:HD23	2.43	0.49
1:D:54:GLN:CB	1:D:271:ARG:HH21	2.24	0.49
1:D:76:LEU:HB3	1:D:100:PHE:CD2	2.48	0.49
1:D:192:GLU:HA	1:D:240:ASN:HD21	1.78	0.49
1:A:233:GLN:O	1:A:237:THR:HG23	2.12	0.49
1:C:155:LEU:O	1:C:158:LEU:HB2	2.13	0.49
1:C:262:MET:O	1:C:264:VAL:HG23	2.13	0.49
1:C:245:LEU:O	1:C:249:THR:HG23	2.13	0.48
1:A:53:VAL:HG11	1:A:271:ARG:HB2	1.95	0.48
1:C:188:ASN:ND2	1:C:194:PHE:HA	2.28	0.48
1:D:79:HIS:CE1	1:D:105:ALA:HA	2.49	0.48
1:C:58:GLU:O	1:C:62:VAL:HG23	2.13	0.48
1:A:192:GLU:HG3	1:A:243:ILE:HG21	1.95	0.48
1:C:164:LEU:CD2	1:C:166:GLN:HG2	2.44	0.48
1:D:44:VAL:CG2	1:D:63:LEU:HD23	2.43	0.48
1:A:9:MET:O	1:A:206:ILE:HA	2.14	0.47
1:C:78:ALA:HB2	1:C:100:PHE:CD2	2.49	0.47
1:D:155:LEU:O	1:D:158:LEU:HB2	2.14	0.47
1:C:16:PHE:CE2	1:C:271:ARG:HG3	2.49	0.47
1:C:79:HIS:CE1	1:C:106:VAL:HG22	2.48	0.47
1:C:164:LEU:HD23	1:C:186:LEU:HD23	1.95	0.47
1:A:122:TYR:O	1:A:126:ILE:HG13	2.14	0.47
1:C:44:VAL:HG21	1:C:66:VAL:HG21	1.97	0.47
1:D:293:MET:O	1:D:294:GLN:CB	2.62	0.47
1:B:269:LEU:HD13	3:B:514:HOH:O	2.13	0.47
1:A:118:HIS:HE1	3:A:409:HOH:O	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:VAL:HA	1:A:161:VAL:HG11	1.97	0.47
1:A:236:GLN:NE2	1:A:240:ASN:HD21	2.12	0.47
1:B:278:ASP:HB3	1:B:281:TYR:CD2	2.49	0.47
1:B:67:ALA:HB2	1:B:100:PHE:CE1	2.50	0.47
1:A:137:TYR:CD1	1:A:165:LYS:HD3	2.49	0.47
1:B:41:GLY:HA2	1:B:74:ILE:HB	1.96	0.47
1:B:96:LYS:NZ	1:B:130:ASP:O	2.43	0.47
1:D:229:ILE:O	1:D:233:GLN:HG3	2.15	0.47
1:C:260:HIS:CD2	1:C:265:VAL:O	2.68	0.46
1:A:273:PRO:HG2	1:D:113:PHE:CZ	2.50	0.46
1:C:80:VAL:HG21	1:C:92:ALA:HA	1.96	0.46
1:C:106:VAL:HA	1:C:137:TYR:HB3	1.96	0.46
1:C:139:ILE:HG23	1:C:139:ILE:O	2.14	0.46
1:B:79:HIS:CE1	1:B:106:VAL:H	2.26	0.46
1:C:262:MET:HA	1:C:293:MET:HE1	1.96	0.46
1:D:8:VAL:HG13	1:D:210:TYR:CE2	2.51	0.46
1:A:253:ARG:HD3	1:A:277:VAL:CG2	2.44	0.46
1:D:102:ALA:HB1	1:D:133:PRO:O	2.15	0.46
1:B:171:LEU:HD21	1:B:193:ILE:HD12	1.97	0.46
1:C:24:LYS:O	1:C:28:ARG:HG3	2.16	0.46
1:A:108:PRO:HG3	1:A:121:HIS:NE2	2.31	0.46
1:A:229:ILE:O	1:A:233:GLN:HG3	2.16	0.46
1:A:79:HIS:HE1	1:A:106:VAL:H	1.64	0.46
1:B:173:GLN:HA	1:B:176:GLN:HE21	1.80	0.46
1:C:9:MET:HE2	1:C:77:ILE:HD11	1.98	0.46
1:C:10:ALA:HB3	1:C:42:LEU:HD23	1.98	0.46
1:C:135:VAL:HG22	1:C:163:ALA:HB3	1.98	0.46
1:C:164:LEU:HD23	1:C:186:LEU:CD2	2.46	0.46
1:D:228:ASP:OD2	1:D:231:THR:HG23	2.16	0.45
1:A:153:ASN:O	1:A:157:THR:HG23	2.15	0.45
1:C:17:ASP:N	1:C:21:ALA:O	2.48	0.45
1:C:156:VAL:HA	1:C:161:VAL:HG11	1.98	0.45
1:D:67:ALA:O	1:D:71:LYS:HB2	2.16	0.45
1:B:280:LYS:HE3	1:B:281:TYR:CZ	2.52	0.45
1:C:27:LEU:HD11	1:C:62:VAL:HG13	1.97	0.45
1:B:291:GLN:HG3	1:B:292:LEU:N	2.26	0.45
1:B:9:MET:HG3	1:B:41:GLY:C	2.41	0.45
1:B:80:VAL:HG13	1:B:88:SER:O	2.17	0.45
1:D:80:VAL:HG21	1:D:103:VAL:CG2	2.47	0.45
1:B:155:LEU:O	1:B:158:LEU:HB2	2.17	0.45
1:D:139:ILE:O	1:D:139:ILE:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:GLN:NE2	1:A:271:ARG:HA	2.32	0.45
1:C:213:MET:HA	1:C:215:TRP:CH2	2.51	0.45
1:C:41:GLY:HA2	1:C:74:ILE:HB	1.98	0.45
1:C:45:GLY:O	1:C:79:HIS:HD2	2.01	0.44
1:A:249:THR:HG22	1:A:281:TYR:CG	2.53	0.44
1:B:21:ALA:O	1:B:22:LEU:C	2.61	0.44
1:B:64:GLU:O	1:B:68:GLU:HG3	2.18	0.44
1:C:165:LYS:HA	1:C:187:TYR:HB2	1.98	0.44
1:A:180:GLU:HB3	1:A:181:HIS:ND1	2.33	0.44
1:B:253:ARG:HG3	1:B:254:GLY:N	2.32	0.44
1:D:186:LEU:HB3	1:D:202:ALA:HA	1.98	0.44
1:D:48:THR:HA	1:D:252:PHE:CE1	2.52	0.44
1:B:53:VAL:O	1:B:53:VAL:HG13	2.18	0.44
1:D:156:VAL:HG21	1:D:184:LEU:HD21	1.98	0.44
1:A:39:ILE:HD12	1:A:39:ILE:HA	1.72	0.44
1:B:180:GLU:HB3	1:B:181:HIS:CE1	2.53	0.44
1:B:278:ASP:OD1	1:B:280:LYS:HG2	2.18	0.44
1:B:292:LEU:HD23	1:B:292:LEU:HA	1.89	0.44
1:B:9:MET:HE2	1:B:77:ILE:HD11	1.99	0.43
1:C:217:TYR:O	1:C:221:VAL:HG23	2.17	0.43
1:D:14:THR:CG2	1:D:49:GLY:O	2.66	0.43
1:A:278:ASP:HB3	1:A:281:TYR:CD2	2.52	0.43
1:D:13:LEU:HD13	1:D:48:THR:CG2	2.48	0.43
1:D:106:VAL:HG13	1:D:137:TYR:CE2	2.53	0.43
1:B:152:ILE:O	1:B:156:VAL:HB	2.18	0.43
1:A:22:LEU:HD21	1:A:24:LYS:HG2	1.99	0.43
1:A:58:GLU:CD	1:A:271:ARG:HH22	2.26	0.43
1:B:62:VAL:O	1:B:66:VAL:HG12	2.18	0.43
1:C:290:GLN:O	1:C:293:MET:HG2	2.18	0.43
1:B:245:LEU:O	1:B:248:LYS:HB2	2.17	0.43
1:C:39:ILE:HD12	1:C:39:ILE:HA	1.86	0.43
1:B:148:THR:OG1	1:B:151:GLN:HG3	2.18	0.43
1:C:120:ASP:O	1:C:123:ARG:HB2	2.19	0.43
1:C:137:TYR:CE1	1:C:165:LYS:HD3	2.53	0.43
1:D:51:ALA:HA	1:D:54:GLN:HE21	1.83	0.43
1:C:180:GLU:HB3	1:C:181:HIS:ND1	2.33	0.43
1:B:39:ILE:HD12	1:B:39:ILE:HA	1.78	0.43
1:C:212:ILE:O	1:C:292:LEU:HD13	2.19	0.43
1:D:115:PHE:CE1	1:D:151:GLN:HB3	2.54	0.43
1:D:210:TYR:CD1	1:D:210:TYR:N	2.87	0.43
1:B:172:TYR:CG	1:D:192:GLU:HB3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:TYR:CD1	1:D:165:LYS:HD3	2.54	0.43
1:B:19:GLN:O	1:B:20:GLN:HB2	2.18	0.42
1:C:19:GLN:CD	1:C:19:GLN:N	2.77	0.42
1:B:65:ILE:O	1:B:69:GLU:HG2	2.18	0.42
1:C:80:VAL:HG13	1:C:88:SER:O	2.18	0.42
1:D:167:THR:HA	1:D:189:GLY:HA3	2.01	0.42
1:D:262:MET:CA	1:D:293:MET:HE3	2.27	0.42
1:B:106:VAL:HG13	1:B:137:TYR:CE2	2.54	0.42
1:C:97:ARG:HD2	1:C:98:TYR:CE1	2.54	0.42
1:D:45:GLY:HA2	3:D:453:HOH:O	2.18	0.42
1:D:165:LYS:HA	1:D:187:TYR:HB2	2.02	0.42
1:B:9:MET:HE3	1:B:77:ILE:HD11	2.01	0.42
1:B:192:GLU:HA	1:B:240:ASN:HD21	1.85	0.42
1:C:180:GLU:HA	1:C:180:GLU:OE1	2.19	0.42
1:D:209:THR:HA	1:D:255:LEU:HD21	2.01	0.42
1:A:6:ARG:HA	1:A:185:VAL:HG13	2.00	0.42
1:B:78:ALA:HB2	1:B:100:PHE:CD2	2.55	0.42
1:D:171:LEU:HD21	1:D:193:ILE:HD12	2.00	0.42
1:B:249:THR:HG22	1:B:281:TYR:CG	2.55	0.42
1:C:25:ALA:HB1	1:C:29:ARG:HH21	1.85	0.42
1:B:56:LEU:HD22	1:B:91:LEU:HD22	2.02	0.42
1:B:118:HIS:O	1:B:122:TYR:HD2	2.02	0.42
1:C:44:VAL:HG22	1:C:63:LEU:HD23	2.02	0.42
1:C:149:LEU:HD23	1:C:149:LEU:HA	1.86	0.42
1:D:278:ASP:OD1	1:D:280:LYS:HG2	2.20	0.42
1:A:125:ILE:HG21	1:A:134:MET:HE1	2.01	0.41
1:A:192:GLU:HG3	1:A:243:ILE:HD13	2.02	0.41
1:C:16:PHE:CZ	1:C:271:ARG:HG3	2.55	0.41
1:C:293:MET:O	1:C:294:GLN:HB3	2.20	0.41
1:D:48:THR:CG2	1:D:208:SER:HB3	2.49	0.41
1:B:220:ILE:HG13	1:B:235:LEU:CB	2.50	0.41
1:C:292:LEU:HD23	1:C:292:LEU:HA	1.92	0.41
1:A:22:LEU:HD23	1:A:24:LYS:HG2	2.02	0.41
1:A:45:GLY:O	1:A:79:HIS:CD2	2.70	0.41
1:B:192:GLU:HB3	1:D:172:TYR:CD1	2.55	0.41
1:D:80:VAL:HG13	1:D:88:SER:O	2.21	0.41
1:B:67:ALA:O	1:B:71:LYS:HB2	2.21	0.41
1:C:138:ASN:HD21	1:C:140:PRO:HG3	1.85	0.41
1:A:9:MET:HG2	1:A:41:GLY:N	2.36	0.41
1:B:272:LYS:NZ	1:B:274:PHE:O	2.43	0.41
1:D:80:VAL:HG22	1:D:91:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:VAL:HG12	1:A:39:ILE:HD11	2.03	0.41
1:B:267:VAL:HA	1:B:268:PRO:HD3	1.89	0.41
1:C:205:GLY:O	1:C:210:TYR:HE2	2.04	0.41
1:A:153:ASN:O	1:A:156:VAL:HG12	2.21	0.41
1:B:173:GLN:O	1:B:177:ILE:HG13	2.21	0.41
1:B:66:VAL:HA	1:B:69:GLU:HB2	2.02	0.40
1:B:220:ILE:HG13	1:B:235:LEU:HB2	2.04	0.40
1:D:48:THR:HG21	1:D:208:SER:HB3	2.02	0.40
1:A:84:THR:HG22	1:A:86:ALA:N	2.37	0.40
1:B:22:LEU:CD2	1:B:24:LYS:HG2	2.51	0.40
1:B:107:THR:HG21	1:B:147:LEU:HD11	2.04	0.40
1:C:147:LEU:HD13	1:C:155:LEU:HD12	2.04	0.40
1:C:215:TRP:CZ2	1:C:292:LEU:HD22	2.57	0.40
1:D:253:ARG:HD3	1:D:277:VAL:CG2	2.49	0.40
1:D:253:ARG:HG3	1:D:254:GLY:N	2.37	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	290/297 (98%)	283 (98%)	6 (2%)	1 (0%)	36	45
1	B	289/297 (97%)	276 (96%)	12 (4%)	1 (0%)	36	45
1	C	289/297 (97%)	277 (96%)	12 (4%)	0	100	100
1	D	289/297 (97%)	279 (96%)	10 (4%)	0	100	100
All	All	1157/1188 (97%)	1115 (96%)	40 (4%)	2 (0%)	43	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	LYS
1	B	110	TYR

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	240/244 (98%)	212 (88%)	28 (12%)	5	4
1	B	240/244 (98%)	208 (87%)	32 (13%)	4	3
1	C	240/244 (98%)	210 (88%)	30 (12%)	4	4
1	D	240/244 (98%)	209 (87%)	31 (13%)	4	3
All	All	960/976 (98%)	839 (87%)	121 (13%)	4	4

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	14	THR
1	A	27	LEU
1	A	44	VAL
1	A	53	VAL
1	A	56	LEU
1	A	66	VAL
1	A	71	LYS
1	A	76	LEU
1	A	80	VAL
1	A	91	LEU
1	A	103	VAL
1	A	106	VAL
1	A	142	LEU
1	A	149	LEU
1	A	156	VAL
1	A	180	GLU
1	A	186	LEU
1	A	191	ASP
1	A	192	GLU

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Mol	Chain	Res	Type
1	A	218	GLN
1	A	229	ILE
1	A	234	LYS
1	A	237	THR
1	A	269	LEU
1	A	271	ARG
1	A	283	PRO
1	A	290	GLN
1	B	9	MET
1	B	13	LEU
1	B	14	THR
1	B	27	LEU
1	B	32	GLN
1	B	37	GLN
1	B	44	VAL
1	B	53	VAL
1	B	57	SER
1	B	66	VAL
1	B	76	LEU
1	B	80	VAL
1	B	91	LEU
1	B	96	LYS
1	B	103	VAL
1	B	106	VAL
1	B	118	HIS
1	B	132	LEU
1	B	149	LEU
1	B	156	VAL
1	B	158	LEU
1	B	166	GLN
1	B	175	GLU
1	B	180	GLU
1	B	186	LEU
1	B	218	GLN
1	B	229	ILE
1	B	230	GLN
1	B	234	LYS
1	B	290	GLN
1	B	291	GLN
1	B	293	MET
1	C	9	MET
1	C	13	LEU

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Mol	Chain	Res	Type
1	C	14	THR
1	C	18	GLN
1	C	27	LEU
1	C	36	GLN
1	C	37	GLN
1	C	44	VAL
1	C	53	VAL
1	C	57	SER
1	C	73	LYS
1	C	80	VAL
1	C	91	LEU
1	C	103	VAL
1	C	106	VAL
1	C	149	LEU
1	C	156	VAL
1	C	158	LEU
1	C	166	GLN
1	C	175	GLU
1	C	180	GLU
1	C	192	GLU
1	C	218	GLN
1	C	226	GLU
1	C	229	ILE
1	C	230	GLN
1	C	234	LYS
1	C	269	LEU
1	C	290	GLN
1	C	291	GLN
1	D	4	ASN
1	D	9	MET
1	D	13	LEU
1	D	14	THR
1	D	27	LEU
1	D	37	GLN
1	D	44	VAL
1	D	53	VAL
1	D	66	VAL
1	D	76	LEU
1	D	91	LEU
1	D	103	VAL
1	D	106	VAL
1	D	127	ASP

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Mol	Chain	Res	Type
1	D	149	LEU
1	D	156	VAL
1	D	158	LEU
1	D	168	SER
1	D	175	GLU
1	D	180	GLU
1	D	186	LEU
1	D	210	TYR
1	D	218	GLN
1	D	226	GLU
1	D	229	ILE
1	D	230	GLN
1	D	234	LYS
1	D	237	THR
1	D	269	LEU
1	D	271	ARG
1	D	286	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	20	GLN
1	A	54	GLN
1	A	61	GLN
1	A	79	HIS
1	A	118	HIS
1	A	138	ASN
1	A	166	GLN
1	A	173	GLN
1	A	176	GLN
1	A	181	HIS
1	A	218	GLN
1	A	240	ASN
1	A	260	HIS
1	B	20	GLN
1	B	32	GLN
1	B	54	GLN
1	B	79	HIS
1	B	90	GLN
1	B	138	ASN
1	B	166	GLN

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Mol	Chain	Res	Type
1	B	176	GLN
1	B	181	HIS
1	B	188	ASN
1	B	211	ASN
1	B	218	GLN
1	C	4	ASN
1	C	18	GLN
1	C	20	GLN
1	C	79	HIS
1	C	90	GLN
1	C	118	HIS
1	C	138	ASN
1	C	166	GLN
1	C	176	GLN
1	C	181	HIS
1	C	188	ASN
1	C	218	GLN
1	C	240	ASN
1	C	260	HIS
1	C	294	GLN
1	D	20	GLN
1	D	37	GLN
1	D	54	GLN
1	D	79	HIS
1	D	90	GLN
1	D	118	HIS
1	D	138	ASN
1	D	166	GLN
1	D	176	GLN
1	D	181	HIS
1	D	218	GLN
1	D	240	ASN
1	D	260	HIS
1	D	294	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	3PY	B	804	1	5,5,6	2.40	2 (40%)	5,5,7	2.38	1 (20%)
2	3PY	C	806	1	5,5,6	2.01	2 (40%)	5,5,7	5.77	4 (80%)
2	3PY	A	802	1	5,5,6	1.91	1 (20%)	5,5,7	6.67	5 (100%)
2	3PY	D	808	1	5,5,6	1.74	1 (20%)	5,5,7	4.64	3 (60%)

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
2	3PY	B	804	1	-	2/3/3/6	-
2	3PY	C	806	1	-	3/3/3/6	-
2	3PY	A	802	1	-	2/3/3/6	-
2	3PY	D	808	1	-	2/3/3/6	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	802	3PY	O4-C3	-3.55	1.24	1.42
2	B	804	3PY	C2-C1	3.55	1.58	1.50
2	C	806	3PY	O4-C3	-3.49	1.24	1.42
2	D	808	3PY	O4-C3	-3.45	1.24	1.42
2	B	804	3PY	O4-C3	-3.41	1.24	1.42
2	C	806	3PY	C2-C1	2.02	1.55	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	802	3PY	C3-C2-C1	9.02	125.49	113.11
2	A	802	3PY	O2-C1-C2	8.45	140.69	114.00
2	A	802	3PY	O2-C1-O1	-7.73	103.45	123.33
2	C	806	3PY	O2-C1-O1	-7.53	103.97	123.33
2	D	808	3PY	C3-C2-C1	7.17	122.96	113.11
2	C	806	3PY	O4-C3-C2	7.12	137.63	110.96
2	C	806	3PY	O2-C1-C2	6.90	135.81	114.00
2	D	808	3PY	O2-C1-C2	5.68	131.96	114.00
2	B	804	3PY	O4-C3-C2	5.08	129.99	110.96
2	D	808	3PY	O1-C1-C2	-4.60	108.49	123.09
2	C	806	3PY	C3-C2-C1	-3.26	108.64	113.11
2	A	802	3PY	O1-C1-C2	-2.30	115.79	123.09
2	A	802	3PY	O4-C3-C2	-2.19	102.77	110.96

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	806	3PY	C1-C2-C3-O4
2	B	804	3PY	O2-C1-C2-C3
2	C	806	3PY	O2-C1-C2-C3
2	B	804	3PY	O1-C1-C2-C3
2	C	806	3PY	O1-C1-C2-C3
2	A	802	3PY	O2-C1-C2-C3
2	D	808	3PY	O2-C1-C2-C3
2	A	802	3PY	O1-C1-C2-C3
2	D	808	3PY	O1-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	292/297 (98%)	-0.97	0 100 100	14, 27, 45, 76	15 (5%)
1	B	291/297 (97%)	-0.91	0 100 100	15, 31, 51, 79	13 (4%)
1	C	291/297 (97%)	-0.68	0 100 100	22, 36, 55, 87	17 (5%)
1	D	291/297 (97%)	-1.03	0 100 100	13, 26, 42, 67	13 (4%)
All	All	1165/1188 (98%)	-0.90	0 100 100	13, 30, 49, 87	58 (4%)

There are no RSRZ outliers to report.

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	3PY	B	804	6/7	0.90	0.07	29,36,50,54	0
2	3PY	A	802	6/7	0.94	0.06	30,34,53,68	0
2	3PY	C	806	6/7	0.94	0.05	44,46,54,56	0
2	3PY	D	808	6/7	0.94	0.07	23,24,43,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.