



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:09 PM UTC

PDB ID : 4FTE / pdb_00004fte
Title : Crystal structure of the D75N mutant capsid of Flock House virus
Authors : Speir, J.A.; Chen, Z.; Reddy, V.S.; Johnson, J.E.
Deposited on : 2012-06-27
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

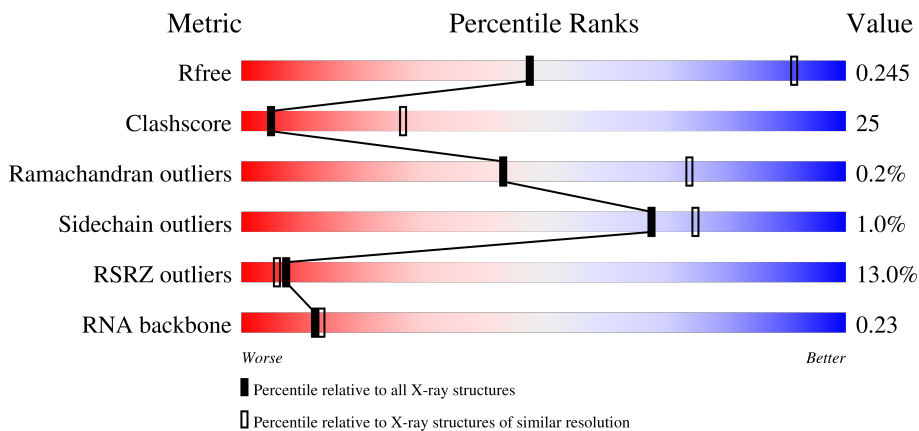
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)
RNA backbone	3983	1010 (3.98-3.02)

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	407	10% (Poor fit) 50% (0 outliers), 29% (1 outlier), 19% (2+ outliers) • (Not modelled)
1	B	407	9% (Poor fit) 55% (0 outliers), 24% (1 outlier), 19% (2+ outliers) • (Not modelled)
1	C	407	9% (Poor fit) 55% (0 outliers), 24% (1 outlier), 19% (2+ outliers) • (Not modelled)
2	R	15	100% (Poor fit) 33% (0 outliers), 53% (1 outlier), 13% (2+ outliers)

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7996 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 Capsid protein alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	328	2456	1563	406	476	11	0	0	0
1	B	330	2466	1570	407	477	12	0	0	0
1	C	329	2461	1566	407	477	11	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	75	ASN	ASP	engineered mutation	UNP P12870
B	75	ASN	ASP	engineered mutation	UNP P12870
C	75	ASN	ASP	engineered mutation	UNP P12870

- Molecule 2 is a RNA chain called Random cellular RNAs.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	R	15	302	136	36	115	15	0	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

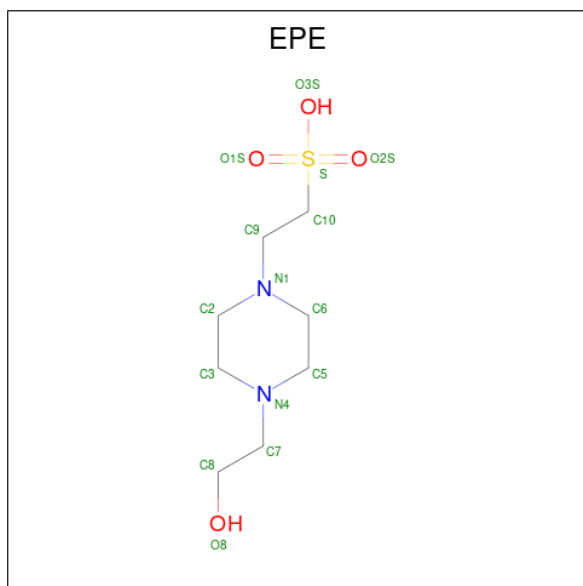
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Ca 2	0	0
3	B	1	Total 1	Ca 1	0	0
3	C	1	Total 1	Ca 1	0	0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

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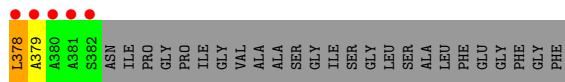
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	C	1	15	8	2	4	1	0	0

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

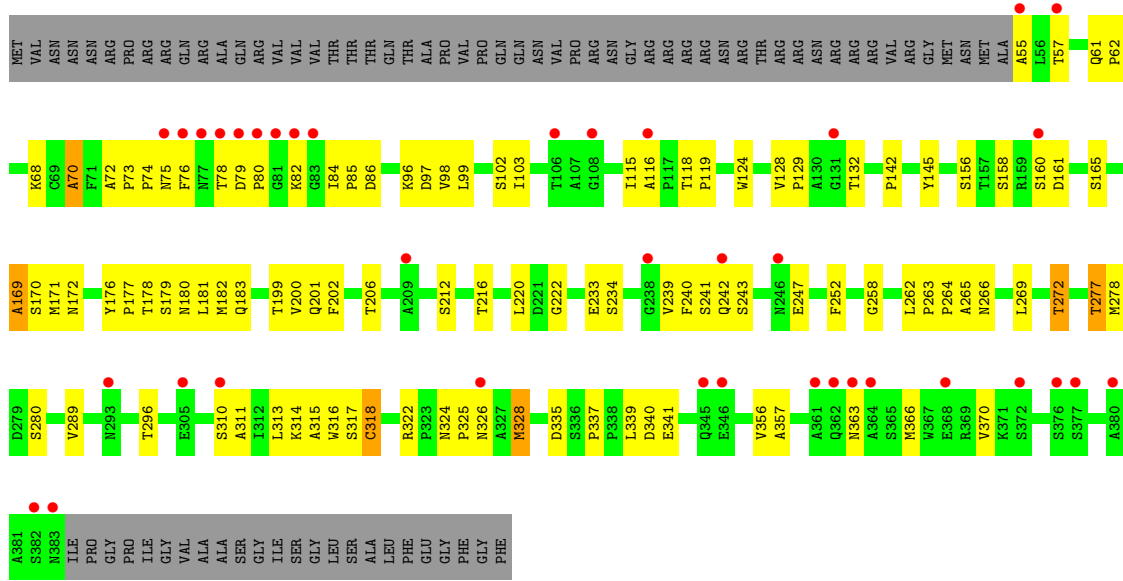
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		

- Molecule 7 is water.

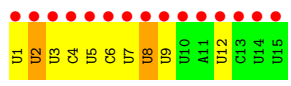
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	93	Total	O	0	0
			93	93		
7	B	90	Total	O	0	0
			90	90		
7	C	70	Total	O	0	0
			70	70		
7	R	3	Total	O	0	0
			3	3		



• Molecule 1: Capsid protein alpha



• Molecule 2: Random cellular RNAs



4 Data and refinement statistics i

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	325.60Å 325.60Å 770.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 3.50 40.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	94.8 (40.00-3.50) 94.8 (40.00-3.50)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 3.48Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.239 , (Not available) 0.243 , 0.245	Depositor DCC
R_{free} test set	18164 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	67.0	Xtrriage
Anisotropy	0.076	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 69.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.000 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k +1/3*l 0.000 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/ 3*k+1/3*l 0.000 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+ 1/3*l,-4/3*h+4/3*k+1/3*l 0.000 for 1/3*h+2/3*k-1/3*l,-k,-8/3*h-4/3* k-1/3*l 0.000 for -1/3*h-2/3*k+1/3*l,-2/3*h-1/3*k- 1/3*l,4/3*h-4/3*k-1/3*l 0.000 for -h,2/3*h+1/3*k+1/3*l,4/3*h+8/3 *k-1/3*l 0.000 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.23	EDS
Total number of atoms	7996	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.30% 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: EPE, CL, CA, SO4

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	1/2520 (0.0%)	1.03	5/3446 (0.1%)
1	B	0.59	0/2530	1.06	7/3459 (0.2%)
1	C	0.57	0/2525	1.06	10/3453 (0.3%)
2	R	0.32	0/332	0.63	0/511
All	All	0.58	1/7907 (0.0%)	1.03	22/10869 (0.2%)

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	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	83	GLY	C-O	5.72	1.27	1.24

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	145	TYR	N-CA-C	-8.56	100.28	110.13
1	B	84	ILE	N-CA-C	8.51	116.35	107.76
1	C	145	TYR	N-CA-C	-6.99	100.99	110.36
1	A	87	ARG	N-CA-C	-6.77	103.90	111.28
1	C	272	THR	N-CA-C	6.44	118.30	111.28
1	C	84	ILE	N-CA-C	5.96	114.44	107.77
1	A	101	GLN	N-CA-C	5.91	118.36	108.02
1	A	277	THR	N-CA-C	5.75	119.10	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	101	GLN	N-CA-C	5.73	117.99	108.13
1	C	179	SER	N-CA-C	5.71	118.11	110.35
1	C	169	ALA	N-CA-C	-5.64	106.32	113.43
1	A	346	GLU	N-CA-C	-5.64	105.05	111.14
1	C	102	SER	N-CA-C	-5.59	101.37	110.20
1	C	277	THR	N-CA-C	5.59	118.84	109.95
1	C	356	VAL	N-CA-C	-5.51	104.57	110.36
1	B	202	PHE	CA-C-N	5.35	125.25	119.85
1	B	202	PHE	C-N-CA	5.35	125.25	119.85
1	C	328	MET	N-CA-C	-5.26	105.60	112.23
1	C	70	ALA	N-CA-C	5.21	116.64	111.07
1	B	378	LEU	N-CA-C	-5.14	107.03	113.15
1	A	103	ILE	N-CA-C	5.06	115.03	108.35
1	B	277	THR	N-CA-C	5.04	117.97	109.95

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	73	PRO	Peptide
1	A	74	PRO	Peptide
1	A	75	ASN	Peptide
1	A	86	ASP	Peptide

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	2456	0	2400	154	0
1	B	2466	0	2413	121	0
1	C	2461	0	2405	111	0
2	R	302	0	155	21	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	5	0	0	0	0
5	A	15	0	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	15	0	18	5	0
5	C	15	0	18	0	0
6	B	1	0	0	0	0
7	A	93	0	0	0	0
7	B	90	0	0	0	0
7	C	70	0	0	1	0
7	R	3	0	0	0	0
All	All	7996	0	7427	383	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 25.

All (383) 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:A:74:PRO:HB3	1:A:316:TRP:CZ2	1.21	1.66
1:A:74:PRO:CB	1:A:316:TRP:HZ2	1.17	1.53
1:C:76:PHE:CE1	1:C:78:THR:HB	1.48	1.47
1:A:74:PRO:CB	1:A:316:TRP:CZ2	1.95	1.34
1:B:74:PRO:CG	1:B:316:TRP:HE1	1.46	1.26
1:A:74:PRO:HB3	1:A:316:TRP:CH2	1.76	1.19
1:C:76:PHE:CD1	1:C:78:THR:HB	1.78	1.17
2:R:1:U:H2'	2:R:2:U:H5''	1.26	1.14
1:A:181:LEU:O	1:A:184:PHE:CE2	2.00	1.13
1:C:128:VAL:HG13	1:C:129:PRO:HD2	1.15	1.11
1:A:74:PRO:CA	1:A:316:TRP:CZ2	2.34	1.10
1:B:74:PRO:HG3	1:B:316:TRP:NE1	1.64	1.10
1:B:218:VAL:HG13	1:C:160:SER:HB2	1.29	1.09
1:C:76:PHE:CE1	1:C:78:THR:CB	2.36	1.09
2:R:7:U:H2'	2:R:8:U:H4'	1.36	1.06
2:R:1:U:C2'	2:R:2:U:H5''	1.86	1.05
1:C:128:VAL:HG13	1:C:129:PRO:CD	1.86	1.05
1:A:181:LEU:O	1:A:184:PHE:CD2	2.11	1.03
1:C:76:PHE:HE1	1:C:78:THR:CB	1.70	1.01
1:B:74:PRO:HG3	1:B:316:TRP:HE1	0.89	1.00
1:B:73:PRO:HB2	1:B:76:PHE:HD2	1.25	0.99
1:C:128:VAL:CG1	1:C:132:THR:OG1	2.11	0.99
1:A:73:PRO:HB2	1:A:76:PHE:HE2	1.26	0.98
1:B:74:PRO:CG	1:B:316:TRP:NE1	2.23	0.95
1:C:178:THR:OG1	1:C:310:SER:C	2.10	0.94
1:C:128:VAL:CG1	1:C:129:PRO:HD2	1.99	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:ALA:O	1:C:74:PRO:HD3	1.67	0.92
2:R:1:U:H2'	2:R:2:U:C5'	2.00	0.92
1:A:68:LYS:O	1:A:72:ALA:CB	2.19	0.91
1:A:74:PRO:HA	1:A:316:TRP:CZ2	2.04	0.89
1:A:326:ASN:HD22	1:C:222:GLY:HA2	1.37	0.89
1:B:55:ALA:CB	1:B:378:LEU:HD13	2.02	0.89
1:A:172:ASN:HB2	1:A:316:TRP:HB2	1.55	0.88
1:B:74:PRO:HD3	1:B:316:TRP:CZ2	2.08	0.88
1:A:365:SER:O	1:A:369:ARG:HG3	1.73	0.88
1:B:218:VAL:HG13	1:C:160:SER:CB	2.03	0.88
1:B:263:PRO:HD2	1:B:277:THR:HG23	1.56	0.87
2:R:7:U:C2'	2:R:8:U:H4'	2.04	0.87
1:B:75:ASN:OD1	1:B:76:PHE:N	2.08	0.86
1:A:84:ILE:HG22	1:A:86:ASP:HB3	1.58	0.85
1:B:55:ALA:HB1	1:B:378:LEU:HD13	1.57	0.85
1:A:155:THR:HG22	1:A:157:THR:H	1.42	0.85
1:A:180:ASN:ND2	1:A:183:GLN:NE2	2.25	0.85
1:A:128:VAL:HB	1:A:129:PRO:CD	2.05	0.85
1:C:74:PRO:HB3	1:C:78:THR:HG22	1.55	0.85
1:C:76:PHE:HE1	1:C:78:THR:HB	1.11	0.84
1:A:71:PHE:O	1:A:73:PRO:HD3	1.75	0.84
1:B:378:LEU:HD23	1:B:378:LEU:O	1.77	0.83
1:B:172:ASN:HB2	1:B:316:TRP:HE3	1.42	0.83
1:A:129:PRO:HD2	1:A:132:THR:OG1	1.78	0.83
1:C:176:TYR:O	1:C:311:ALA:HB1	1.77	0.83
1:B:74:PRO:CB	1:B:316:TRP:HE1	1.92	0.83
1:C:128:VAL:CG1	1:C:129:PRO:CD	2.57	0.83
1:B:172:ASN:HB2	1:B:316:TRP:CE3	2.13	0.82
1:C:178:THR:HG1	1:C:310:SER:C	1.88	0.82
2:R:7:U:H2'	2:R:8:U:C4'	2.09	0.82
1:B:73:PRO:HB2	1:B:76:PHE:CD2	2.13	0.82
1:B:172:ASN:OD1	1:B:242:GLN:HB2	1.82	0.80
1:A:68:LYS:O	1:A:72:ALA:HB2	1.81	0.80
1:A:247:GLU:HG3	1:A:248:PRO:HD2	1.64	0.79
1:A:180:ASN:HD21	1:A:183:GLN:NE2	1.81	0.78
1:C:128:VAL:HG12	1:C:132:THR:OG1	1.84	0.78
1:B:77:ASN:ND2	1:B:79:ASP:O	2.16	0.78
1:B:74:PRO:HD3	1:B:316:TRP:CE2	2.20	0.76
1:A:71:PHE:CD2	1:A:350:VAL:HG11	2.20	0.76
2:R:1:U:O5'	2:R:1:U:H6	1.69	0.76
1:A:128:VAL:HB	1:A:129:PRO:HD3	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ILE:CG2	1:A:86:ASP:HB3	2.16	0.75
1:A:155:THR:HB	1:A:158:SER:OG	1.88	0.74
1:B:352:ARG:HG3	1:C:335:ASP:OD2	1.87	0.74
1:A:73:PRO:O	1:A:76:PHE:HD2	1.69	0.73
1:A:183:GLN:HG3	1:A:308:VAL:HB	1.69	0.73
1:B:204:VAL:HG12	1:B:206:THR:HG23	1.71	0.72
1:C:74:PRO:HB3	1:C:78:THR:CG2	2.19	0.72
2:R:1:U:O2'	2:R:2:U:H5''	1.89	0.72
1:B:263:PRO:HB3	1:B:272:THR:HG21	1.72	0.72
1:A:242:GLN:NE2	1:A:354:LEU:HD13	2.05	0.71
1:C:128:VAL:HG11	1:C:132:THR:OG1	1.91	0.71
1:A:61:GLN:HA	1:A:61:GLN:NE2	2.06	0.70
1:A:73:PRO:HB2	1:A:76:PHE:CE2	2.18	0.70
1:B:53:MET:O	1:B:57:THR:HG23	1.91	0.70
1:A:59:LEU:HD23	1:A:342:VAL:HB	1.73	0.70
1:C:79:ASP:OD2	1:C:80:PRO:HD2	1.91	0.69
2:R:8:U:H5'	2:R:9:U:H5	1.57	0.69
1:B:70:ALA:HA	1:B:170:SER:HB3	1.73	0.69
1:B:75:ASN:OD1	1:B:76:PHE:CD2	2.46	0.69
1:C:263:PRO:HB3	1:C:272:THR:HG21	1.75	0.68
1:C:242:GLN:HE22	1:C:366:MET:HE3	1.58	0.68
1:A:346:GLU:OE2	1:A:346:GLU:HA	1.92	0.68
1:C:180:ASN:HD21	1:C:183:GLN:HG3	1.58	0.68
1:A:188:ILE:HG13	1:A:235:PHE:HA	1.77	0.67
1:B:74:PRO:HB3	1:B:316:TRP:CD1	2.28	0.67
1:B:363:ASN:OD1	1:B:364:ALA:N	2.28	0.67
1:B:74:PRO:CB	1:B:316:TRP:NE1	2.56	0.67
1:A:115:ILE:O	1:A:296:THR:HG23	1.94	0.67
1:B:55:ALA:HB2	1:B:378:LEU:HD22	1.75	0.66
1:B:264:PRO:HG2	1:B:267:VAL:HG21	1.76	0.66
1:B:74:PRO:HB3	1:B:316:TRP:NE1	2.10	0.66
1:B:363:ASN:OD1	1:B:363:ASN:C	2.39	0.65
1:A:180:ASN:HD21	1:A:183:GLN:HE21	1.43	0.65
2:R:3:U:H3'	2:R:3:U:H6	1.61	0.65
1:A:240:PHE:HE1	1:A:316:TRP:CZ3	2.14	0.65
1:B:196:LYS:HE3	1:C:165:SER:OG	1.96	0.65
1:A:74:PRO:HA	1:A:316:TRP:CE2	2.32	0.65
1:A:128:VAL:HB	1:A:129:PRO:HD2	1.78	0.65
1:A:233:GLU:CG	1:A:237:LYS:HD2	2.27	0.65
1:A:68:LYS:O	1:A:72:ALA:HB3	1.94	0.65
1:B:172:ASN:CB	1:B:316:TRP:HE3	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:GLN:HE22	1:C:366:MET:CE	2.09	0.65
1:B:172:ASN:OD1	1:B:242:GLN:CB	2.45	0.65
1:C:181:LEU:C	1:C:182:MET:HE2	2.22	0.65
1:B:70:ALA:HA	1:B:170:SER:CB	2.26	0.64
1:A:128:VAL:CB	1:A:129:PRO:CD	2.69	0.64
2:R:1:U:C2'	2:R:2:U:C5'	2.68	0.63
1:C:233:GLU:HG3	1:C:234:SER:N	2.14	0.63
1:A:363:ASN:O	1:A:366:MET:HB3	1.99	0.63
1:B:260:GLN:HG3	5:B:503:EPE:H61	1.79	0.63
1:C:181:LEU:O	1:C:182:MET:HE2	2.00	0.62
1:A:61:GLN:N	1:A:62:PRO:HD2	2.14	0.61
1:A:256:LEU:HD12	1:A:290:GLY:HA2	1.83	0.61
1:C:98:VAL:HA	1:C:315:ALA:O	2.00	0.61
1:C:178:THR:OG1	1:C:310:SER:CB	2.49	0.61
1:C:202:PHE:CE1	1:C:212:SER:HB2	2.37	0.60
1:A:203:PRO:HB3	1:B:265:ALA:HB3	1.82	0.60
1:C:76:PHE:CD1	1:C:78:THR:CB	2.72	0.60
1:C:61:GLN:HB3	1:C:62:PRO:HD3	1.84	0.60
1:C:128:VAL:CG1	1:C:129:PRO:N	2.64	0.60
1:A:86:ASP:C	1:A:86:ASP:OD1	2.45	0.59
1:B:74:PRO:HA	1:B:96:LYS:HZ1	1.67	0.59
1:A:78:THR:OG1	1:A:96:LYS:NZ	2.36	0.59
1:B:366:MET:O	1:B:370:VAL:HG23	2.03	0.59
1:C:119:PRO:HB2	1:C:289:VAL:CG2	2.33	0.59
1:B:183:GLN:HB2	1:B:308:VAL:HB	1.85	0.58
1:B:227:GLY:HA3	1:C:325:PRO:HB3	1.85	0.58
1:A:84:ILE:HD13	1:A:250:PHE:CD2	2.40	0.57
1:C:366:MET:O	1:C:370:VAL:HG23	2.04	0.57
2:R:7:U:C3'	2:R:8:U:H4'	2.34	0.57
1:A:180:ASN:CG	1:A:183:GLN:NE2	2.63	0.57
1:B:247:GLU:HG3	1:B:248:PRO:HD2	1.87	0.57
1:A:97:ASP:HB3	1:A:145:TYR:CD1	2.40	0.57
1:C:265:ALA:O	1:C:266:ASN:HB2	2.05	0.56
1:C:322:ARG:HB3	1:C:322:ARG:NH1	2.19	0.56
1:A:85:PRO:O	1:A:344:LEU:HD21	2.04	0.56
1:C:169:ALA:HB3	1:C:318:CYS:HB3	1.86	0.56
1:A:181:LEU:O	1:A:184:PHE:HE2	1.77	0.56
1:B:172:ASN:CB	1:B:316:TRP:CE3	2.86	0.56
1:A:71:PHE:CE2	1:A:350:VAL:CG1	2.89	0.56
1:A:119:PRO:HB2	1:A:289:VAL:CG2	2.36	0.56
1:C:75:ASN:OD1	1:C:76:PHE:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:THR:OG1	1:C:310:SER:HB3	2.05	0.56
1:A:71:PHE:CE2	1:A:350:VAL:HG11	2.41	0.55
2:R:6:C:H2'	2:R:7:U:C6	2.42	0.55
1:B:220:LEU:O	1:B:223:VAL:HG23	2.06	0.55
1:B:352:ARG:CG	1:C:335:ASP:OD2	2.55	0.55
1:B:74:PRO:CD	1:B:316:TRP:NE1	2.69	0.55
1:B:74:PRO:HG3	1:B:316:TRP:CE2	2.38	0.54
1:A:119:PRO:HB2	1:A:289:VAL:HG21	1.90	0.54
1:B:339:LEU:HD12	1:B:340:ASP:H	1.72	0.54
1:A:84:ILE:HG22	1:A:86:ASP:CB	2.35	0.54
1:B:169:ALA:HB3	1:B:318:CYS:HB3	1.88	0.54
1:B:360:ALA:O	1:B:363:ASN:HB3	2.08	0.54
1:A:263:PRO:HG2	1:A:269:LEU:HA	1.90	0.54
1:C:57:THR:HA	7:C:630:HOH:O	2.08	0.54
2:R:7:U:N3	2:R:8:U:O2	2.41	0.54
1:A:180:ASN:O	1:A:180:ASN:OD1	2.26	0.53
1:B:184:PHE:C	1:B:184:PHE:CD2	2.85	0.53
1:C:70:ALA:HA	1:C:170:SER:HB3	1.91	0.53
1:B:336:SER:OG	1:B:337:PRO:HD2	2.09	0.53
1:B:247:GLU:OE1	1:C:252:PHE:HB2	2.08	0.53
1:B:283:GLU:HG2	5:B:503:EPE:H81	1.90	0.53
1:A:74:PRO:CB	1:A:316:TRP:CH2	2.60	0.52
1:B:339:LEU:HD12	1:B:340:ASP:N	2.24	0.52
1:C:98:VAL:HG23	1:C:98:VAL:O	2.09	0.52
1:B:324:ASN:HB3	1:B:326:ASN:OD1	2.10	0.52
1:B:363:ASN:O	1:B:366:MET:HB3	2.09	0.52
1:C:158:SER:HB2	1:C:161:ASP:OD2	2.09	0.52
1:A:99:LEU:O	1:A:314:LYS:HA	2.09	0.52
1:A:233:GLU:HG3	1:A:234:SER:N	2.24	0.52
1:A:180:ASN:OD1	1:A:183:GLN:CG	2.57	0.52
1:A:182:MET:HG3	1:A:183:GLN:N	2.24	0.52
1:B:239:VAL:HG22	1:B:240:PHE:N	2.25	0.52
1:C:128:VAL:HG12	1:C:129:PRO:N	2.24	0.52
1:C:180:ASN:HD21	1:C:183:GLN:CG	2.22	0.52
1:A:57:THR:HG22	1:A:58:ARG:N	2.24	0.51
1:B:61:GLN:HB3	1:B:62:PRO:HD3	1.92	0.51
1:C:68:LYS:O	1:C:72:ALA:HB3	2.09	0.51
1:C:252:PHE:CZ	1:C:322:ARG:HD3	2.45	0.51
1:B:182:MET:O	1:B:182:MET:HG2	2.09	0.51
1:B:262:LEU:HA	1:B:263:PRO:C	2.35	0.51
1:C:76:PHE:HE1	1:C:78:THR:OG1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:PRO:HB2	1:C:340:ASP:HB3	1.92	0.51
1:C:176:TYR:O	1:C:311:ALA:CB	2.54	0.51
1:A:326:ASN:HD22	1:C:222:GLY:CA	2.17	0.51
1:B:95:ARG:NH1	1:B:97:ASP:OD1	2.42	0.51
1:A:324:ASN:HB3	1:A:326:ASN:ND2	2.25	0.51
1:C:116:ALA:O	1:C:118:THR:N	2.40	0.51
1:C:178:THR:H	1:C:311:ALA:HA	1.75	0.51
1:A:73:PRO:HB3	1:A:363:ASN:OD1	2.10	0.51
1:B:233:GLU:CG	1:B:237:LYS:HD2	2.41	0.50
1:C:339:LEU:HD12	1:C:340:ASP:N	2.26	0.50
1:A:70:ALA:HA	1:A:170:SER:HB3	1.92	0.50
1:A:122:ALA:HA	1:A:145:TYR:CE2	2.47	0.50
1:A:73:PRO:O	1:A:76:PHE:CD2	2.57	0.50
1:A:155:THR:HG22	1:A:157:THR:N	2.21	0.50
1:A:128:VAL:CB	1:A:129:PRO:HD2	2.39	0.50
1:A:204:VAL:HG12	1:A:206:THR:HG23	1.93	0.49
2:R:3:U:H3'	2:R:3:U:C6	2.45	0.49
1:C:172:ASN:HB2	1:C:316:TRP:HE3	1.77	0.49
1:C:269:LEU:O	1:C:272:THR:OG1	2.30	0.49
1:B:55:ALA:HA	1:B:378:LEU:HD11	1.94	0.49
1:B:74:PRO:CD	1:B:75:ASN:H	2.26	0.49
1:B:283:GLU:H	5:B:503:EPE:H82	1.77	0.49
1:C:242:GLN:NE2	1:C:366:MET:HE3	2.25	0.49
1:B:185:ALA:HB3	1:B:307:ALA:CB	2.42	0.49
2:R:2:U:C6	2:R:2:U:H5'	2.47	0.49
1:A:201:GLN:CD	1:B:264:PRO:HB3	2.37	0.49
1:B:363:ASN:O	1:B:366:MET:CB	2.60	0.49
1:B:74:PRO:CD	1:B:316:TRP:CE2	2.93	0.49
1:B:106:THR:HG21	1:B:109:GLN:NE2	2.28	0.49
1:A:241:SER:HB2	1:A:357:ALA:HB2	1.94	0.49
1:C:142:PRO:HG3	1:C:280:SER:HA	1.94	0.49
1:C:156:SER:HB2	1:C:258:GLY:HA2	1.94	0.49
1:A:175:ILE:HB	1:A:239:VAL:HG12	1.94	0.48
1:A:277:THR:HG22	1:A:278:MET:N	2.27	0.48
1:A:172:ASN:HB2	1:A:316:TRP:HE3	1.78	0.48
1:A:184:PHE:CD1	1:A:184:PHE:C	2.89	0.48
1:A:264:PRO:HG2	1:A:267:VAL:HG21	1.95	0.48
1:B:346:GLU:OE2	1:B:346:GLU:HA	2.13	0.48
1:C:313:LEU:C	1:C:313:LEU:HD23	2.38	0.48
1:A:70:ALA:C	1:A:71:PHE:CD1	2.92	0.48
1:A:265:ALA:O	1:A:266:ASN:HB2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:LEU:HD12	1:C:340:ASP:H	1.78	0.48
1:A:61:GLN:HA	1:A:61:GLN:HE21	1.79	0.48
1:A:371:LYS:O	1:A:375:LYS:HG2	2.14	0.48
1:A:162:GLN:HB3	1:A:329:LEU:CD1	2.44	0.48
1:A:383:ASN:O	1:A:384:ILE:HB	2.14	0.48
1:B:188:ILE:HG13	1:B:235:PHE:HA	1.95	0.48
1:B:264:PRO:HG2	1:B:267:VAL:CG2	2.43	0.48
1:A:180:ASN:OD1	1:A:183:GLN:HB3	2.14	0.48
1:B:124:TRP:CE3	1:B:278:MET:HE3	2.48	0.48
1:A:71:PHE:O	1:A:73:PRO:CD	2.56	0.47
1:A:240:PHE:CE1	1:A:316:TRP:CZ3	2.99	0.47
1:A:326:ASN:ND2	1:C:222:GLY:HA2	2.17	0.47
1:C:178:THR:OG1	1:C:311:ALA:N	2.45	0.47
1:B:224:LEU:N	1:B:224:LEU:HD23	2.29	0.47
1:B:217:LEU:HB2	1:B:220:LEU:HD22	1.97	0.47
1:C:80:PRO:HB2	1:C:96:LYS:HB2	1.96	0.47
1:A:181:LEU:C	1:A:184:PHE:CD2	2.90	0.47
1:A:172:ASN:HB2	1:A:316:TRP:CE3	2.50	0.47
1:B:154:THR:O	1:B:284:ALA:HA	2.14	0.47
1:B:233:GLU:HG3	1:B:237:LYS:HD2	1.97	0.47
1:C:239:VAL:HG22	1:C:240:PHE:N	2.30	0.47
1:B:208:PRO:HD2	1:C:206:THR:HG22	1.96	0.47
1:C:171:MET:HE2	1:C:243:SER:HB3	1.97	0.47
2:R:3:U:C6	2:R:3:U:C3'	2.98	0.47
1:B:74:PRO:CD	1:B:316:TRP:CZ2	2.90	0.46
1:A:313:LEU:C	1:A:313:LEU:HD23	2.40	0.46
1:A:264:PRO:HB3	1:C:201:GLN:CD	2.40	0.46
1:C:199:THR:CA	1:C:216:THR:HG22	2.45	0.46
1:A:84:ILE:CD1	1:A:250:PHE:CD2	2.99	0.46
1:C:97:ASP:HB2	1:C:317:SER:HB2	1.98	0.46
1:C:324:ASN:HB3	1:C:326:ASN:OD1	2.14	0.46
1:A:106:THR:O	1:A:109:GLN:HB2	2.16	0.46
1:A:203:PRO:HD3	5:B:503:EPE:O1S	2.15	0.46
1:B:84:ILE:HA	1:B:85:PRO:HD3	1.74	0.46
1:A:71:PHE:HE2	1:A:350:VAL:HB	1.81	0.46
1:C:61:GLN:CB	1:C:62:PRO:HD3	2.46	0.46
1:B:179:SER:HB3	1:B:183:GLN:HG3	1.98	0.46
1:A:126:ALA:HB3	1:A:140:PHE:CE2	2.51	0.46
1:A:180:ASN:OD1	1:A:183:GLN:HG2	2.15	0.45
1:A:86:ASP:O	1:A:87:ARG:C	2.59	0.45
1:A:257:GLU:O	1:C:200:VAL:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:ALA:HB3	1:C:326:ASN:HA	1.98	0.45
1:C:99:LEU:O	1:C:314:LYS:HA	2.17	0.45
1:B:55:ALA:HA	1:B:378:LEU:CD1	2.46	0.45
1:A:155:THR:HG22	1:A:156:SER:N	2.31	0.45
1:C:55:ALA:C	1:C:57:THR:H	2.25	0.45
1:A:162:GLN:HB3	1:A:329:LEU:HD11	1.98	0.45
1:C:70:ALA:HA	1:C:170:SER:CB	2.47	0.45
1:A:185:ALA:HB3	1:A:307:ALA:CB	2.47	0.44
1:A:217:LEU:HB2	1:A:220:LEU:HD11	1.99	0.44
1:C:172:ASN:HB2	1:C:316:TRP:CE3	2.52	0.44
1:A:172:ASN:CB	1:A:316:TRP:HE3	2.31	0.44
1:B:122:ALA:HA	1:B:145:TYR:CE1	2.52	0.44
1:A:252:PHE:HB2	1:C:247:GLU:OE1	2.18	0.44
1:B:358:VAL:HG23	1:B:359:ILE:O	2.17	0.44
1:C:78:THR:O	1:C:79:ASP:C	2.60	0.44
1:A:124:TRP:CE3	1:A:278:MET:HE3	2.53	0.44
1:C:328:MET:HB2	1:C:328:MET:HE2	1.85	0.44
1:B:128:VAL:HB	1:B:129:PRO:CD	2.47	0.44
1:B:365:SER:O	1:B:369:ARG:HB2	2.17	0.44
2:R:8:U:H5'	2:R:9:U:C5	2.44	0.44
1:A:73:PRO:HG3	1:A:366:MET:HG2	1.98	0.44
1:A:199:THR:CA	1:A:216:THR:HG22	2.48	0.43
1:B:365:SER:O	1:B:369:ARG:N	2.44	0.43
1:B:74:PRO:HA	1:B:96:LYS:NZ	2.33	0.43
1:B:368:GLU:OE2	1:B:368:GLU:HA	2.18	0.43
1:A:71:PHE:CE2	1:A:350:VAL:HB	2.53	0.43
1:B:75:ASN:OD1	1:B:75:ASN:C	2.61	0.43
1:A:61:GLN:N	1:A:62:PRO:CD	2.81	0.43
1:B:113:ILE:HG23	1:B:123:TYR:CD1	2.54	0.43
1:C:128:VAL:HG12	1:C:132:THR:HG1	1.83	0.43
1:C:115:ILE:O	1:C:296:THR:HG23	2.19	0.43
1:C:277:THR:HG22	1:C:278:MET:N	2.32	0.43
1:A:201:GLN:NE2	1:B:264:PRO:HB3	2.33	0.43
1:B:203:PRO:HB3	1:C:265:ALA:HB3	2.01	0.43
1:C:82:LYS:O	1:C:337:PRO:HG3	2.18	0.43
1:C:72:ALA:C	1:C:74:PRO:HD3	2.41	0.43
1:C:176:TYR:HA	1:C:177:PRO:HD3	1.61	0.43
1:A:71:PHE:CD1	1:A:71:PHE:N	2.83	0.43
1:A:113:ILE:HG23	1:A:123:TYR:CD1	2.54	0.43
1:C:202:PHE:CD1	1:C:202:PHE:C	2.96	0.43
1:B:162:GLN:O	1:B:324:ASN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:GLU:O	1:B:350:VAL:HG23	2.19	0.42
1:A:86:ASP:OD1	1:A:86:ASP:O	2.37	0.42
1:B:220:LEU:HA	1:B:220:LEU:HD12	1.71	0.42
1:C:73:PRO:HG3	1:C:363:ASN:OD1	2.19	0.42
1:C:263:PRO:HD2	1:C:277:THR:HG23	2.01	0.42
1:A:85:PRO:HB2	1:A:340:ASP:HB3	2.00	0.42
1:A:73:PRO:HG3	1:A:366:MET:CG	2.49	0.42
1:A:374:ILE:HG22	1:A:375:LYS:HD3	2.01	0.42
1:B:55:ALA:CB	1:B:378:LEU:CD1	2.86	0.42
2:R:6:C:H2'	2:R:7:U:N1	2.35	0.42
1:A:73:PRO:CG	1:A:366:MET:HB3	2.50	0.42
1:A:121:VAL:HG11	1:A:124:TRP:CE2	2.54	0.42
1:A:102:SER:C	1:A:103:ILE:HG23	2.44	0.42
1:A:170:SER:OG	1:A:318:CYS:HB2	2.19	0.42
1:C:80:PRO:CB	1:C:96:LYS:HB2	2.50	0.42
1:C:85:PRO:HB2	1:C:340:ASP:CB	2.49	0.42
1:A:185:ALA:HB3	1:A:307:ALA:HB2	2.01	0.42
1:A:264:PRO:HG2	1:A:267:VAL:CG2	2.49	0.42
1:B:204:VAL:CG1	1:B:206:THR:HG23	2.44	0.42
1:A:248:PRO:HB3	1:B:86:ASP:OD2	2.20	0.42
1:A:252:PHE:CZ	1:A:322:ARG:HD3	2.55	0.42
1:B:70:ALA:HA	1:B:170:SER:HB2	2.01	0.42
1:B:370:VAL:C	1:B:372:SER:N	2.78	0.42
1:C:220:LEU:HD23	1:C:220:LEU:HA	1.90	0.42
1:A:61:GLN:NE2	1:A:61:GLN:CA	2.75	0.41
1:A:183:GLN:CG	1:A:308:VAL:HB	2.42	0.41
1:B:185:ALA:HB3	1:B:307:ALA:HB1	2.01	0.41
1:B:198:SER:C	1:B:199:THR:HG23	2.44	0.41
1:A:68:LYS:C	1:A:72:ALA:HB2	2.44	0.41
1:A:180:ASN:OD1	1:A:180:ASN:C	2.62	0.41
1:B:218:VAL:CG1	1:C:160:SER:HB2	2.22	0.41
1:A:319:ILE:HG22	1:A:320:GLU:N	2.35	0.41
1:B:242:GLN:NE2	1:B:354:LEU:HD13	2.35	0.41
1:B:283:GLU:HG2	5:B:503:EPE:C8	2.50	0.41
2:R:2:U:H5'	2:R:2:U:H6	1.84	0.41
1:B:84:ILE:C	1:B:337:PRO:HG2	2.46	0.41
1:B:128:VAL:HB	1:B:129:PRO:HD2	2.03	0.41
1:A:85:PRO:HA	1:A:337:PRO:HB2	2.03	0.41
1:A:337:PRO:HA	1:A:338:PRO:HD3	1.97	0.41
1:C:262:LEU:HA	1:C:263:PRO:C	2.46	0.41
1:A:324:ASN:HD22	1:A:324:ASN:HA	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:SER:HB2	1:C:357:ALA:HB2	2.03	0.41
1:A:68:LYS:O	1:A:72:ALA:N	2.51	0.41
1:A:73:PRO:HG3	1:A:366:MET:HB3	2.03	0.41
1:B:245:CYS:HA	1:B:293:ASN:O	2.21	0.41
2:R:8:U:H3'	2:R:9:U:C6	2.55	0.41
1:A:180:ASN:ND2	1:A:183:GLN:HE21	2.02	0.41
1:A:180:ASN:O	1:A:183:GLN:HG2	2.20	0.41
1:A:181:LEU:C	1:A:184:PHE:CE2	2.89	0.41
1:A:369:ARG:O	1:A:373:ILE:HG13	2.21	0.41
1:C:61:GLN:N	1:C:62:PRO:CD	2.84	0.41
1:A:60:SER:HB2	1:A:62:PRO:HD2	2.03	0.41
1:A:92:VAL:HB	1:A:320:GLU:HG2	2.03	0.41
1:A:193:CYS:SG	1:B:325:PRO:HG2	2.61	0.41
1:A:304:PRO:HG2	1:A:307:ALA:HB2	2.02	0.41
1:B:74:PRO:HD2	1:B:75:ASN:H	1.86	0.41
1:A:233:GLU:HG2	1:A:237:LYS:HD2	2.01	0.40
1:B:171:MET:HE2	1:B:243:SER:HB3	2.03	0.40
1:B:324:ASN:HD22	1:B:324:ASN:HA	1.66	0.40
1:A:129:PRO:HG2	1:A:132:THR:HG21	2.02	0.40
1:C:180:ASN:OD1	1:C:183:GLN:HG2	2.22	0.40
1:A:88:PHE:CZ	1:A:90:GLY:HA3	2.56	0.40
1:A:208:PRO:HD2	1:B:206:THR:HG22	2.04	0.40
1:A:71:PHE:CD2	1:A:350:VAL:CG1	2.98	0.40
1:A:383:ASN:N	1:A:383:ASN:HD22	2.19	0.40
1:B:248:PRO:HB3	1:C:86:ASP:OD2	2.22	0.40
1:B:377:SER:C	1:B:379:ALA:H	2.28	0.40
1:C:124:TRP:CH2	1:C:142:PRO:HB3	2.56	0.40
1:C:199:THR:HA	1:C:216:THR:HG22	2.04	0.40
1:C:340:ASP:O	1:C:341:GLU:C	2.64	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	326/407 (80%)	312 (96%)	14 (4%)	0	100	100
1	B	328/407 (81%)	306 (93%)	21 (6%)	1 (0%)	36	67
1	C	327/407 (80%)	302 (92%)	24 (7%)	1 (0%)	36	67
All	All	981/1221 (80%)	920 (94%)	59 (6%)	2 (0%)	43	74

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	264	PRO
1	B	239	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	272/336 (81%)	270 (99%)	2 (1%)	76	78
1	B	272/336 (81%)	268 (98%)	4 (2%)	57	71
1	C	272/336 (81%)	270 (99%)	2 (1%)	76	78
All	All	816/1008 (81%)	808 (99%)	8 (1%)	68	75

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	318	CYS
1	A	342	VAL
1	B	165	SER
1	B	318	CYS
1	B	358	VAL
1	B	363	ASN
1	C	103	ILE
1	C	318	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	141	ASN
1	A	183	GLN
1	A	215	HIS
1	A	266	ASN
1	A	326	ASN
1	A	345	GLN
1	A	383	ASN
1	B	77	ASN
1	B	215	HIS
1	B	246	ASN
1	B	324	ASN
1	B	331	GLN
1	B	345	GLN
1	B	362	GLN
1	C	77	ASN
1	C	100	ASN
1	C	215	HIS
1	C	242	GLN
1	C	266	ASN
1	C	334	HIS
1	C	383	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	R	14/15 (93%)	5 (35%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	R	2	U
2	R	4	C
2	R	5	U
2	R	8	U
2	R	12	U

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 5 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	A	503	-	4,4,4	0.40	0	6,6,6	0.09	0
5	EPE	C	502	-	15,15,15	1.51	1 (6%)	19,20,20	1.37	2 (10%)
5	EPE	A	504	-	15,15,15	1.45	1 (6%)	19,20,20	1.33	3 (15%)
5	EPE	B	503	-	15,15,15	1.29	1 (6%)	19,20,20	1.38	3 (15%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EPE	C	502	-	-	0/9/19/19	0/1/1/1
5	EPE	A	504	-	-	0/9/19/19	0/1/1/1
5	EPE	B	503	-	-	1/9/19/19	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	502	EPE	C10-S	4.14	1.83	1.77
5	A	504	EPE	C10-S	3.60	1.82	1.77
5	B	503	EPE	C10-S	3.08	1.81	1.77

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	503	EPE	O1S-S-C10	4.12	112.96	106.73
5	C	502	EPE	O1S-S-C10	4.06	112.87	106.73
5	A	504	EPE	O1S-S-C10	3.81	112.48	106.73
5	A	504	EPE	O3S-S-O2S	-2.67	104.72	111.40
5	C	502	EPE	O3S-S-O2S	-2.63	104.82	111.40
5	B	503	EPE	O3S-S-O1S	-2.45	105.28	111.40
5	B	503	EPE	O3S-S-O2S	-2.13	106.07	111.40
5	A	504	EPE	O3S-S-O1S	-2.07	106.22	111.40

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	503	EPE	N4-C7-C8-O8

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	503	EPE	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	328/407 (80%)	1.06	41 (12%) 8 6	42, 66, 151, 266	0
1	B	330/407 (81%)	1.07	37 (11%) 10 7	43, 66, 153, 224	0
1	C	329/407 (80%)	1.07	37 (11%) 10 7	40, 65, 124, 222	0
2	R	15/15 (100%)	6.08	15 (100%) 0 0	210, 278, 328, 345	0
All	All	1002/1236 (81%)	1.15	130 (12%) 7 6	40, 66, 160, 345	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	R	14	U	9.4
1	B	382	SER	9.3
1	A	384	ILE	8.2
2	R	15	U	8.2
2	R	4	C	7.4
1	A	383	ASN	7.2
2	R	11	A	6.9
2	R	3	U	6.6
1	C	77	ASN	6.5
2	R	8	U	6.2
2	R	6	C	6.0
2	R	2	U	5.7
1	B	381	ALA	5.6
2	R	1	U	5.5
2	R	12	U	5.5
1	C	383	ASN	5.5
2	R	5	U	5.4
1	B	379	ALA	5.3
1	A	381	ALA	5.2
1	B	54	ALA	5.2
1	C	376	SER	5.2

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Mol	Chain	Res	Type	RSRZ
2	R	7	U	5.0
1	B	53	MET	4.9
1	A	74	PRO	4.8
2	R	9	U	4.7
1	C	79	ASP	4.6
1	C	78	THR	4.6
1	A	382	SER	4.5
1	A	376	SER	4.4
1	A	379	ALA	4.4
1	C	131	GLY	4.4
1	A	380	ALA	4.3
2	R	10	U	4.3
2	R	13	C	4.2
1	C	382	SER	4.2
1	B	79	ASP	4.2
1	B	377	SER	4.2
1	A	57	THR	4.2
1	A	372	SER	3.9
1	C	380	ALA	3.8
1	B	380	ALA	3.7
1	B	306	GLY	3.7
1	C	76	PHE	3.7
1	C	80	PRO	3.7
1	C	83	GLY	3.5
1	B	368	GLU	3.5
1	A	377	SER	3.5
1	A	361	ALA	3.5
1	C	55	ALA	3.4
1	A	77	ASN	3.4
1	C	81	GLY	3.3
1	A	364	ALA	3.3
1	B	74	PRO	3.3
1	C	75	ASN	3.2
1	A	75	ASN	3.1
1	B	80	PRO	3.1
1	A	80	PRO	3.1
1	A	94	SER	3.0
1	A	266	ASN	3.0
1	A	58	ARG	3.0
1	B	376	SER	3.0
1	A	302	SER	2.9
1	A	368	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	305	GLU	2.8
1	B	238	GLY	2.8
1	C	361	ALA	2.8
1	A	61	GLN	2.7
1	A	378	LEU	2.7
1	C	293	ASN	2.7
1	B	251	GLU	2.7
1	A	79	ASP	2.6
1	B	75	ASN	2.6
1	A	365	SER	2.6
1	C	246	ASN	2.6
1	B	78	THR	2.6
1	A	369	ARG	2.5
1	C	362	GLN	2.5
1	A	72	ALA	2.5
1	B	242	GLN	2.5
1	A	81	GLY	2.5
1	A	73	PRO	2.5
1	B	131	GLY	2.5
1	B	357	ALA	2.4
1	B	369	ARG	2.4
1	A	251	GLU	2.4
1	B	373	ILE	2.4
1	C	364	ALA	2.4
1	A	375	LYS	2.4
1	B	225	ALA	2.4
1	C	377	SER	2.3
1	C	363	ASN	2.3
1	B	254	ASP	2.3
1	A	100	ASN	2.3
1	C	57	THR	2.3
1	C	82	LYS	2.3
1	B	364	ALA	2.3
1	C	345	GLN	2.3
1	B	57	THR	2.3
1	C	106	THR	2.3
1	A	303	ALA	2.3
1	A	305	GLU	2.2
1	B	90	GLY	2.2
1	C	108	GLY	2.2
1	B	120	GLY	2.2
1	A	318	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	372	SER	2.2
1	B	378	LEU	2.2
1	B	81	GLY	2.2
1	B	362	GLN	2.1
1	A	63	GLY	2.1
1	A	257	GLU	2.1
1	A	78	THR	2.1
1	C	160	SER	2.1
1	B	375	LYS	2.1
1	A	87	ARG	2.1
1	A	279	ASP	2.1
1	B	215	HIS	2.1
1	C	116	ALA	2.1
1	C	209	ALA	2.1
1	C	310	SER	2.1
1	C	238	GLY	2.1
1	C	346	GLU	2.1
1	A	293	ASN	2.1
1	B	76	PHE	2.1
1	C	242	GLN	2.1
1	C	326	ASN	2.0
1	B	58	ARG	2.0
1	B	207	ASP	2.0
1	B	334	HIS	2.0
1	C	368	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	A	503	5/5	0.83	0.37	131,136,151,180	0
3	CA	A	502	1/1	0.90	0.09	105,105,105,105	0
3	CA	A	501	1/1	0.91	0.20	63,63,63,63	0
5	EPE	A	504	15/15	0.93	0.22	50,83,162,169	0
6	CL	B	502	1/1	0.93	0.13	75,75,75,75	0
5	EPE	B	503	15/15	0.95	0.17	43,86,141,160	0
5	EPE	C	502	15/15	0.95	0.18	46,105,165,173	0
3	CA	B	501	1/1	0.95	0.15	60,60,60,60	0
3	CA	C	501	1/1	0.96	0.09	61,61,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.