



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:19 AM UTC

PDB ID : 4FTS / pdb_00004fts
Title : Crystal structure of the N363T mutant of the Flock House virus capsid
Authors : Speir, J.A.; Chen, Z.; Reddy, V.S.; Johnson, J.E.
Deposited on : 2012-06-28
Resolution : 3.20 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

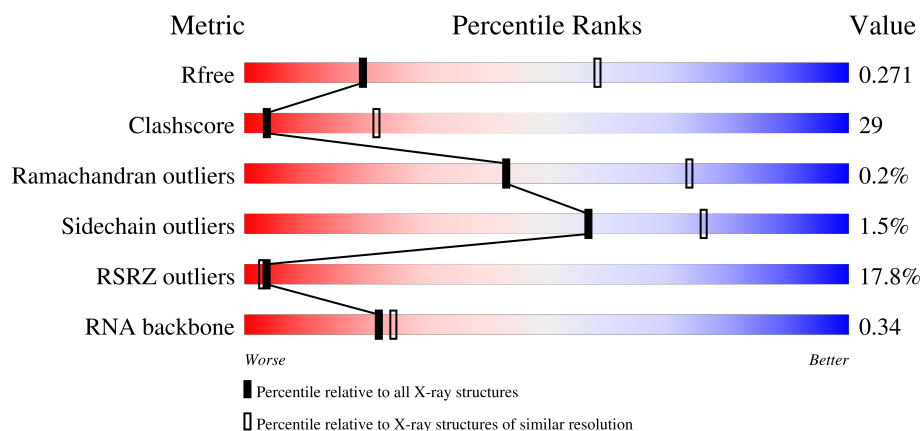
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (3.50-2.90)

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	15% 38% 39% • 19%
1	B	407	13% 49% 30% • 19%
1	C	407	13% 51% 26% • 19%
2	R	15	100% 40% 40% 20%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8001 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
1	A	328	Total	C	N	O	S	0	0	0
			2455	1563	404	477	11			
1	B	329	Total	C	N	O	S	0	0	0
			2459	1567	404	476	12			
1	C	329	Total	C	N	O	S	0	0	0
			2460	1566	405	478	11			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	363	THR	ASN	engineered mutation	UNP P12870
B	363	THR	ASN	engineered mutation	UNP P12870
C	363	THR	ASN	engineered mutation	UNP P12870

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

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

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

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

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

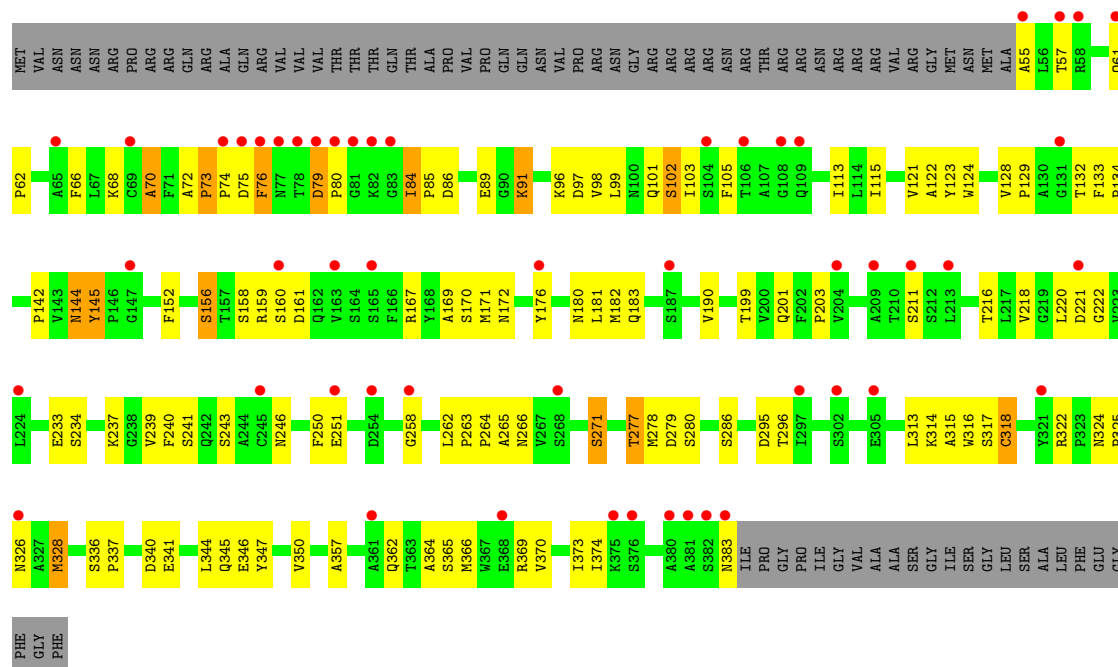


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	S	0	0
			5	4	1		

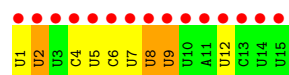
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	74	Total	O	0	0
			74	74		
7	B	101	Total	O	0	0
			101	101		
7	C	92	Total	O	0	0
			92	92		
7	R	3	Total	O	0	0
			3	3		

- Molecule 1: Capsid protein alpha



- Molecule 2: Random cellular RNAs



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	326.04Å 326.04Å 770.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 3.20 40.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	91.8 (40.00-3.20) 91.7 (40.00-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 3.19Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.259 , (Not available) 0.266 , 0.271	Depositor DCC
R_{free} test set	9099 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å ²)	69.4	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 65.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
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	Xtriage
F_o, F_c correlation	0.35	EDS
Total number of atoms	8001	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CA, EPE, CL

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	0.63	0/2519	1.11	19/3445 (0.6%)
1	B	0.62	0/2523	1.06	7/3450 (0.2%)
1	C	0.64	0/2524	1.08	12/3452 (0.3%)
2	R	0.30	0/332	0.57	0/511
All	All	0.62	0/7898	1.06	38/10858 (0.3%)

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	C	0	1

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	271	SER	N-CA-C	-8.33	102.28	111.36
1	A	80	PRO	N-CA-C	-8.25	102.06	113.53
1	B	83	GLY	N-CA-C	8.05	119.69	111.56
1	A	378	LEU	N-CA-C	-7.78	103.89	113.15
1	C	73	PRO	N-CA-C	-7.22	101.89	110.70
1	A	181	LEU	N-CA-C	6.97	121.80	113.16
1	A	333	GLY	N-CA-C	6.81	119.76	111.93
1	C	70	ALA	N-CA-C	6.61	118.36	111.03
1	B	145	TYR	N-CA-C	-6.59	100.50	110.39
1	A	145	TYR	N-CA-C	-6.47	100.68	110.39
1	C	75	ASP	N-CA-C	-6.37	104.61	112.38
1	A	103	ILE	N-CA-C	6.34	116.72	108.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	84	ILE	N-CA-C	6.27	115.45	108.05
1	A	83	GLY	N-CA-C	6.17	117.63	111.21
1	A	377	SER	N-CA-C	-6.00	106.29	113.97
1	C	145	TYR	N-CA-C	-5.96	100.21	109.87
1	A	70	ALA	N-CA-C	5.94	117.42	111.07
1	B	101	GLN	N-CA-C	5.82	118.14	108.13
1	C	144	ASN	N-CA-C	5.80	118.67	110.50
1	B	144	ASN	N-CA-C	5.70	118.92	110.48
1	C	277	THR	N-CA-C	5.61	118.70	109.72
1	C	102	SER	N-CA-C	-5.61	101.34	110.20
1	A	144	ASN	N-CA-C	5.58	118.37	110.50
1	A	77	ASN	N-CA-C	-5.58	104.21	111.74
1	A	346	GLU	N-CA-C	-5.34	104.88	111.40
1	B	70	ALA	N-CA-C	5.33	117.90	111.40
1	C	190	VAL	N-CA-C	5.32	115.94	108.17
1	A	82	LYS	CA-C-N	-5.29	117.18	122.63
1	A	82	LYS	C-N-CA	-5.29	117.18	122.63
1	A	182	MET	N-CA-C	-5.28	107.39	113.88
1	A	369	ARG	N-CA-C	-5.28	105.61	111.36
1	B	277	THR	N-CA-C	5.28	118.34	109.95
1	A	115	ILE	N-CA-C	-5.27	100.29	107.99
1	A	156	SER	N-CA-C	-5.17	107.04	113.19
1	C	328	MET	N-CA-C	-5.06	105.86	112.23
1	C	337	PRO	O-C-N	5.05	123.63	121.31
1	A	143	VAL	N-CA-C	-5.04	100.39	107.75
1	B	328	MET	N-CA-C	-5.04	107.42	113.21

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	79	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	2455	0	2399	175	0
1	B	2459	0	2407	147	0
1	C	2460	0	2404	139	0
2	R	302	0	155	10	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	15	0	18	0	0
4	B	15	0	18	1	0
4	C	15	0	18	0	0
5	B	1	0	0	0	0
6	C	5	0	0	0	0
7	A	74	0	0	0	0
7	B	101	0	0	1	0
7	C	92	0	0	1	0
7	R	3	0	0	0	0
All	All	8001	0	7419	440	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 29.

All (440) 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:B:74:PRO:HG3	1:B:316:TRP:CZ2	1.45	1.49
1:A:74:PRO:HG3	1:A:316:TRP:CE2	1.54	1.42
1:B:74:PRO:HB3	1:B:316:TRP:NE1	1.48	1.29
1:B:74:PRO:CB	1:B:316:TRP:HE1	1.50	1.23
1:B:218:VAL:HG13	1:C:160:SER:HB2	1.20	1.19
1:A:328:MET:HA	1:A:328:MET:CE	1.73	1.17
2:R:7:U:H2'	2:R:8:U:H4'	1.17	1.16
1:B:115:ILE:O	1:B:296:THR:HG23	1.45	1.16
1:B:74:PRO:CG	1:B:316:TRP:HZ2	1.60	1.14
1:A:74:PRO:HG3	1:A:316:TRP:CZ2	1.84	1.12
1:A:326:ASN:HD22	1:C:222:GLY:HA2	1.15	1.11
1:A:328:MET:HE2	1:A:328:MET:CA	1.80	1.10
1:A:74:PRO:CG	1:A:316:TRP:CE2	2.35	1.08
1:C:80:PRO:HB3	1:C:96:LYS:HB2	1.32	1.07
1:C:72:ALA:O	1:C:74:PRO:HD3	1.53	1.06
1:A:74:PRO:CG	1:A:316:TRP:CZ2	2.39	1.05
1:C:80:PRO:HB3	1:C:96:LYS:CB	1.86	1.05
2:R:1:U:H2'	2:R:2:U:H5''	1.40	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:VAL:HG13	1:C:160:SER:CB	1.90	1.01
1:B:122:ALA:HA	1:B:145:TYR:CE1	1.96	1.00
1:A:85:PRO:O	1:A:344:LEU:HD21	1.60	1.00
1:C:80:PRO:CB	1:C:96:LYS:HB2	1.94	0.97
1:B:74:PRO:HB3	1:B:316:TRP:HE1	0.81	0.95
1:B:74:PRO:CG	1:B:316:TRP:CZ2	2.40	0.95
1:A:115:ILE:O	1:A:296:THR:HG23	1.68	0.94
1:A:300:ARG:HH11	1:A:300:ARG:HG2	1.33	0.94
2:R:7:U:H2'	2:R:8:U:C4'	1.98	0.94
1:A:73:PRO:O	1:A:76:PHE:HD1	1.53	0.92
2:R:7:U:C2'	2:R:8:U:H4'	1.99	0.91
1:A:74:PRO:CB	1:A:316:TRP:NE1	2.34	0.90
1:A:172:ASN:HB2	1:A:316:TRP:CE3	2.07	0.90
1:A:74:PRO:CG	1:A:316:TRP:NE1	2.35	0.89
1:A:172:ASN:HB2	1:A:316:TRP:HE3	1.34	0.88
1:B:218:VAL:CG1	1:C:160:SER:HB2	2.03	0.88
1:C:85:PRO:O	1:C:344:LEU:HD21	1.75	0.86
1:A:328:MET:HA	1:A:328:MET:HE2	0.88	0.85
1:B:85:PRO:O	1:B:344:LEU:HD21	1.76	0.85
1:C:144:ASN:HD21	1:C:286:SER:HB2	1.41	0.84
1:A:74:PRO:HG3	1:A:316:TRP:NE1	1.91	0.84
1:A:68:LYS:O	1:A:72:ALA:HB3	1.78	0.84
1:C:180:ASN:HD21	1:C:183:GLN:HG3	1.42	0.83
1:B:366:MET:HE1	1:B:369:ARG:HD2	1.61	0.82
1:C:362:GLN:NE2	1:C:369:ARG:HH21	1.76	0.82
1:A:74:PRO:HG2	1:A:316:TRP:CZ2	2.14	0.81
1:A:326:ASN:HD22	1:C:222:GLY:CA	1.93	0.81
1:A:328:MET:CE	1:A:328:MET:CA	2.50	0.81
1:C:72:ALA:O	1:C:74:PRO:CD	2.30	0.80
1:C:362:GLN:HE22	1:C:369:ARG:NH2	1.80	0.80
1:C:128:VAL:HG12	1:C:132:THR:OG1	1.81	0.80
1:B:69:CYS:HA	1:B:77:ASN:ND2	1.98	0.79
1:B:115:ILE:O	1:B:296:THR:CG2	2.30	0.79
1:A:185:ALA:HB3	1:A:307:ALA:CB	2.13	0.78
1:A:84:ILE:HD13	1:A:250:PHE:CD2	2.18	0.78
1:A:74:PRO:HB3	1:A:316:TRP:NE1	1.99	0.77
1:A:74:PRO:CB	1:A:316:TRP:HE1	1.98	0.77
2:R:1:U:C2'	2:R:2:U:H5''	2.14	0.77
1:A:115:ILE:O	1:A:296:THR:CG2	2.32	0.76
1:A:365:SER:O	1:A:369:ARG:HG3	1.86	0.76
1:B:122:ALA:CA	1:B:145:TYR:CE1	2.69	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:GLU:HG3	1:B:248:PRO:HD2	1.68	0.75
1:A:247:GLU:HG3	1:A:248:PRO:HD2	1.69	0.75
1:A:217:LEU:HB2	1:A:220:LEU:HD11	1.68	0.74
1:C:346:GLU:O	1:C:350:VAL:HG23	1.88	0.74
1:C:101:GLN:HG3	1:C:103:ILE:CG2	2.18	0.74
1:A:144:ASN:HD21	1:A:286:SER:HB2	1.54	0.72
1:A:61:GLN:HA	1:A:61:GLN:NE2	2.05	0.72
1:B:172:ASN:OD1	1:B:242:GLN:HB3	1.89	0.72
1:B:115:ILE:HG22	1:B:171:MET:HE3	1.71	0.71
1:C:144:ASN:HD21	1:C:286:SER:CB	2.02	0.71
1:B:172:ASN:HB2	1:B:316:TRP:CE3	2.25	0.71
1:A:78:THR:OG1	1:A:96:LYS:NZ	2.23	0.71
1:A:155:THR:HG22	1:A:157:THR:H	1.55	0.71
1:B:122:ALA:HA	1:B:145:TYR:CZ	2.25	0.71
1:B:74:PRO:CA	1:B:316:TRP:HE1	2.04	0.70
1:B:115:ILE:CD1	1:B:173:VAL:HB	2.21	0.70
1:C:86:ASP:OD2	1:C:167:ARG:NH1	2.25	0.70
1:A:61:GLN:HA	1:A:61:GLN:HE21	1.55	0.69
1:C:142:PRO:HG3	1:C:280:SER:HA	1.73	0.69
1:B:70:ALA:HA	1:B:170:SER:HB3	1.74	0.69
1:A:155:THR:HB	1:A:158:SER:OG	1.91	0.69
1:B:97:ASP:HB3	1:B:145:TYR:CD2	2.28	0.69
1:C:265:ALA:O	1:C:266:ASN:HB2	1.91	0.68
1:A:185:ALA:HB3	1:A:307:ALA:HB2	1.75	0.68
1:C:362:GLN:NE2	1:C:369:ARG:NH2	2.40	0.68
1:A:57:THR:HG22	1:A:58:ARG:H	1.59	0.68
2:R:8:U:H5'	2:R:9:U:H5	1.58	0.68
1:A:57:THR:HG22	1:A:58:ARG:N	2.09	0.67
1:B:169:ALA:HB3	1:B:318:CYS:HB3	1.75	0.67
1:B:229:ASP:OD2	1:C:91:LYS:HE2	1.95	0.67
1:A:61:GLN:N	1:A:62:PRO:HD2	2.10	0.67
1:A:73:PRO:C	1:A:76:PHE:HD1	2.03	0.67
1:A:68:LYS:O	1:A:72:ALA:CB	2.43	0.66
1:A:169:ALA:HB3	1:A:318:CYS:HB3	1.76	0.66
1:B:185:ALA:HB3	1:B:307:ALA:HB1	1.76	0.66
1:B:74:PRO:CB	1:B:316:TRP:NE1	2.28	0.66
1:B:185:ALA:HB3	1:B:307:ALA:CB	2.26	0.66
1:A:84:ILE:C	1:A:337:PRO:HG2	2.21	0.65
1:A:220:LEU:O	1:A:223:VAL:HG23	1.96	0.65
1:A:59:LEU:HD23	1:A:342:VAL:HB	1.79	0.65
1:A:73:PRO:O	1:A:76:PHE:CD1	2.43	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ALA:HB3	1:A:307:ALA:HB1	1.78	0.65
1:A:74:PRO:HB3	1:A:316:TRP:CD1	2.32	0.65
1:A:300:ARG:HG2	1:A:300:ARG:NH1	2.07	0.65
1:B:89:GLU:HA	1:B:336:SER:HB3	1.77	0.65
1:A:263:PRO:HG2	1:A:269:LEU:HA	1.79	0.65
1:C:91:LYS:HB2	1:C:91:LYS:NZ	2.11	0.64
1:A:188:ILE:HG13	1:A:235:PHE:HA	1.78	0.64
1:B:55:ALA:HB2	1:B:378:LEU:HD22	1.80	0.64
1:C:180:ASN:HD21	1:C:183:GLN:CG	2.10	0.64
1:A:185:ALA:O	1:A:309:ASN:ND2	2.31	0.64
1:A:241:SER:HB2	1:A:357:ALA:HB2	1.80	0.64
1:B:74:PRO:HG3	1:B:316:TRP:CE2	2.26	0.63
1:A:326:ASN:ND2	1:C:222:GLY:HA2	2.00	0.63
1:A:352:ARG:HG3	1:B:335:ASP:OD1	1.98	0.63
1:C:76:PHE:CD1	1:C:76:PHE:N	2.62	0.63
1:B:262:LEU:HD23	1:B:264:PRO:HD3	1.80	0.63
1:A:352:ARG:HB3	1:A:352:ARG:NH1	2.14	0.62
1:B:117:PRO:HB2	1:B:292:GLY:CA	2.30	0.62
1:B:220:LEU:O	1:B:223:VAL:HG23	1.99	0.62
1:B:327:ALA:C	1:B:329:LEU:H	2.07	0.62
1:A:256:LEU:HD12	1:A:290:GLY:HA2	1.82	0.61
1:C:124:TRP:CZ3	1:C:142:PRO:HB3	2.35	0.61
1:B:69:CYS:HA	1:B:77:ASN:HD22	1.64	0.61
1:B:264:PRO:HG2	1:B:267:VAL:HG21	1.81	0.61
1:C:113:ILE:HG23	1:C:123:TYR:CD1	2.35	0.61
1:A:84:ILE:O	1:A:337:PRO:HG2	2.01	0.61
1:B:148:PHE:C	1:B:148:PHE:CD2	2.78	0.61
1:A:158:SER:HA	1:A:161:ASP:OD2	1.99	0.61
1:C:102:SER:C	1:C:103:ILE:HG23	2.25	0.60
1:C:79:ASP:OD1	1:C:79:ASP:O	2.19	0.60
1:B:61:GLN:HB3	1:B:62:PRO:HD3	1.83	0.60
1:B:366:MET:HE3	1:B:366:MET:HA	1.81	0.60
1:C:322:ARG:HB3	1:C:322:ARG:NH1	2.16	0.60
1:A:233:GLU:CG	1:A:237:LYS:HD2	2.32	0.60
1:C:181:LEU:C	1:C:182:MET:HE2	2.27	0.60
1:B:70:ALA:HA	1:B:170:SER:CB	2.31	0.59
1:A:74:PRO:HG2	1:A:316:TRP:HZ2	1.64	0.59
1:A:378:LEU:O	1:A:382:SER:HB2	2.02	0.59
1:B:142:PRO:HG3	1:B:280:SER:HA	1.82	0.59
1:A:123:TYR:CZ	1:A:143:VAL:HG21	2.37	0.59
1:B:55:ALA:HB1	1:B:378:LEU:HD13	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:364:ALA:C	1:C:366:MET:H	2.11	0.59
1:B:73:PRO:HB2	1:B:76:PHE:CD1	2.38	0.59
1:A:204:VAL:HG12	1:A:206:THR:HG23	1.84	0.59
1:B:324:ASN:HB3	1:B:326:ASN:OD1	2.03	0.59
1:C:68:LYS:HE2	1:C:76:PHE:HE2	1.66	0.59
1:A:369:ARG:O	1:A:373:ILE:HG13	2.03	0.58
1:B:74:PRO:HB3	1:B:316:TRP:CE2	2.31	0.58
1:A:88:PHE:CZ	1:A:90:GLY:HA3	2.39	0.58
1:C:346:GLU:HA	1:C:346:GLU:OE1	2.03	0.58
1:C:263:PRO:HD2	1:C:277:THR:HG23	1.85	0.57
1:A:186:GLY:HA3	1:A:302:SER:O	2.04	0.57
1:A:124:TRP:CE3	1:A:278:MET:HE3	2.39	0.57
1:A:348:ARG:HD2	1:B:87:ARG:O	2.05	0.57
1:B:227:GLY:HA3	1:C:325:PRO:HB3	1.86	0.57
1:A:92:VAL:HG21	1:A:320:GLU:CG	2.35	0.57
1:A:175:ILE:HB	1:A:239:VAL:HG12	1.87	0.57
1:B:117:PRO:HB2	1:B:292:GLY:HA3	1.87	0.57
1:A:116:ALA:HA	1:A:296:THR:HG23	1.86	0.56
1:A:87:ARG:NH1	1:C:341:GLU:OE2	2.38	0.56
1:A:157:THR:HG21	1:C:271:SER:O	2.05	0.56
1:A:142:PRO:HG3	1:A:280:SER:HA	1.88	0.56
1:A:196:LYS:HE3	1:B:165:SER:OG	2.06	0.56
1:C:181:LEU:O	1:C:182:MET:HE2	2.05	0.56
1:A:246:ASN:HB3	1:A:295:ASP:OD1	2.06	0.56
1:A:73:PRO:O	1:A:78:THR:CG2	2.55	0.55
1:A:331:GLN:N	1:A:331:GLN:OE1	2.39	0.55
1:C:102:SER:C	1:C:103:ILE:CG2	2.78	0.55
1:A:99:LEU:O	1:A:314:LYS:HA	2.06	0.55
1:B:346:GLU:OE2	1:B:346:GLU:HA	2.06	0.55
1:B:378:LEU:HD23	1:B:378:LEU:O	2.07	0.55
1:C:341:GLU:HG3	1:C:345:GLN:HE21	1.71	0.55
1:C:85:PRO:HB2	1:C:340:ASP:HB3	1.89	0.55
1:C:96:LYS:NZ	1:C:316:TRP:HB3	2.22	0.55
1:C:172:ASN:HB2	1:C:316:TRP:HE3	1.72	0.55
1:A:233:GLU:HG3	1:A:234:SER:N	2.22	0.55
1:B:115:ILE:C	1:B:296:THR:HG23	2.29	0.55
1:B:115:ILE:HD11	1:B:173:VAL:HG21	1.87	0.54
1:C:73:PRO:O	1:C:73:PRO:HG2	2.06	0.54
1:C:102:SER:O	1:C:103:ILE:CG2	2.55	0.54
1:A:113:ILE:HG23	1:A:123:TYR:CD1	2.43	0.54
1:B:84:ILE:HD13	1:B:250:PHE:CD2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:ILE:HG23	1:C:123:TYR:HD1	1.71	0.54
1:A:183:GLN:HG3	1:A:308:VAL:HB	1.89	0.54
1:B:277:THR:HG22	1:B:278:MET:N	2.22	0.54
1:A:247:GLU:OE1	1:B:251:GLU:HG2	2.08	0.54
1:B:121:VAL:C	1:B:145:TYR:CE1	2.85	0.54
1:B:124:TRP:CH2	1:B:142:PRO:HB3	2.43	0.53
1:C:366:MET:O	1:C:370:VAL:HG23	2.08	0.53
1:B:115:ILE:CD1	1:B:173:VAL:CB	2.87	0.53
1:A:128:VAL:HB	1:A:129:PRO:HD2	1.90	0.53
1:A:366:MET:HA	1:A:366:MET:HE3	1.89	0.53
1:B:204:VAL:HG12	1:B:206:THR:HG23	1.90	0.53
1:C:313:LEU:C	1:C:313:LEU:HD23	2.34	0.53
1:A:196:LYS:HD2	1:B:165:SER:HB3	1.91	0.53
1:B:61:GLN:HE21	1:B:61:GLN:HA	1.73	0.53
1:A:162:GLN:NE2	1:A:327:ALA:HB1	2.24	0.53
1:B:119:PRO:HB2	1:B:289:VAL:CG2	2.38	0.53
1:B:124:TRP:CZ2	1:B:142:PRO:HB3	2.44	0.53
1:A:366:MET:HA	1:A:369:ARG:HD2	1.90	0.53
1:B:75:ASP:OD1	1:B:75:ASP:N	2.42	0.53
1:B:247:GLU:OE1	1:C:251:GLU:HG2	2.09	0.53
1:A:73:PRO:C	1:A:76:PHE:CD1	2.85	0.53
1:B:262:LEU:HA	1:B:263:PRO:C	2.34	0.53
1:B:263:PRO:HB3	1:B:272:THR:HG21	1.91	0.53
1:B:73:PRO:HB2	1:B:76:PHE:HD1	1.73	0.52
1:B:76:PHE:HD1	1:B:76:PHE:H	1.57	0.52
2:R:6:C:H2'	2:R:7:U:C6	2.44	0.52
1:A:70:ALA:HA	1:A:170:SER:HB3	1.90	0.52
1:C:80:PRO:HB2	1:C:96:LYS:HB2	1.84	0.52
1:C:313:LEU:HD23	1:C:314:LYS:N	2.24	0.52
1:A:84:ILE:HD13	1:A:250:PHE:HD2	1.71	0.52
1:A:264:PRO:HG2	1:A:267:VAL:HG21	1.91	0.52
1:C:103:ILE:CD1	1:C:105:PHE:CZ	2.93	0.52
1:C:233:GLU:HG3	1:C:234:SER:N	2.25	0.52
1:A:224:LEU:HD11	1:A:275:PRO:HB2	1.92	0.52
1:A:172:ASN:CB	1:A:316:TRP:HE3	2.17	0.52
1:A:201:GLN:NE2	1:B:264:PRO:HB3	2.25	0.52
1:B:55:ALA:CB	1:B:378:LEU:HD13	2.39	0.52
1:B:97:ASP:HB2	1:B:317:SER:HB2	1.92	0.52
1:C:89:GLU:HA	1:C:336:SER:HB3	1.92	0.52
1:A:242:GLN:NE2	1:A:354:LEU:HD13	2.24	0.51
1:A:184:PHE:CD1	1:A:184:PHE:C	2.88	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:THR:CG2	1:B:278:MET:N	2.72	0.51
1:A:263:PRO:HD2	1:A:277:THR:HG23	1.92	0.51
1:B:121:VAL:O	1:B:145:TYR:HE1	1.93	0.51
1:C:99:LEU:O	1:C:314:LYS:HA	2.11	0.51
1:A:336:SER:OG	1:A:337:PRO:HD2	2.10	0.51
1:B:76:PHE:CD1	1:B:76:PHE:N	2.79	0.51
1:C:246:ASN:HB3	1:C:295:ASP:OD2	2.11	0.51
1:B:182:MET:O	1:B:182:MET:HG2	2.10	0.51
1:A:106:THR:O	1:A:109:GLN:HB2	2.10	0.51
1:A:262:LEU:HA	1:A:263:PRO:C	2.34	0.51
1:A:313:LEU:C	1:A:313:LEU:HD23	2.35	0.51
1:C:98:VAL:HG23	1:C:98:VAL:O	2.10	0.51
1:C:121:VAL:HG22	1:C:144:ASN:OD1	2.11	0.51
1:C:102:SER:O	1:C:103:ILE:HG22	2.11	0.51
1:A:117:PRO:HB2	1:A:292:GLY:H	1.76	0.50
1:C:61:GLN:HB3	1:C:62:PRO:HD3	1.92	0.50
1:C:98:VAL:HA	1:C:315:ALA:O	2.11	0.50
2:R:8:U:H5'	2:R:9:U:C5	2.42	0.50
1:B:342:VAL:O	1:B:346:GLU:HG2	2.11	0.50
1:C:158:SER:HB2	1:C:161:ASP:OD2	2.11	0.50
1:B:179:SER:HB3	1:B:183:GLN:HG3	1.93	0.50
1:C:345:GLN:HB3	7:C:616:HOH:O	2.11	0.50
1:B:260:GLN:HG3	4:B:503:EPE:H61	1.93	0.49
1:C:80:PRO:HB3	1:C:96:LYS:HB3	1.83	0.49
1:B:188:ILE:HG13	1:B:235:PHE:HA	1.93	0.49
1:A:57:THR:CG2	1:A:58:ARG:H	2.23	0.49
1:A:142:PRO:HD3	1:A:279:ASP:O	2.12	0.49
1:A:220:LEU:C	1:A:222:GLY:N	2.70	0.49
1:C:364:ALA:C	1:C:366:MET:N	2.70	0.49
1:C:241:SER:HB2	1:C:357:ALA:HB2	1.94	0.49
2:R:6:C:H2'	2:R:7:U:N1	2.27	0.49
1:C:97:ASP:HB2	1:C:317:SER:HB2	1.94	0.49
1:B:154:THR:O	1:B:284:ALA:HA	2.13	0.49
1:C:172:ASN:HB2	1:C:316:TRP:CE3	2.48	0.49
1:A:116:ALA:HB1	1:A:291:TRP:CH2	2.48	0.49
1:A:197:LEU:HD11	1:A:215:HIS:HB3	1.94	0.49
1:A:241:SER:HB2	1:A:357:ALA:CB	2.42	0.49
1:B:368:GLU:OE2	1:B:368:GLU:HA	2.13	0.49
1:C:277:THR:HG22	1:C:278:MET:N	2.28	0.49
1:C:369:ARG:O	1:C:373:ILE:HG13	2.12	0.49
1:B:119:PRO:HB2	1:B:289:VAL:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:GLU:O	1:B:350:VAL:HG23	2.12	0.48
1:C:103:ILE:HD11	1:C:105:PHE:CZ	2.49	0.48
1:A:377:SER:C	1:A:379:ALA:H	2.21	0.48
1:A:151:MET:SD	1:A:329:LEU:HD11	2.53	0.48
1:C:73:PRO:O	1:C:73:PRO:CG	2.60	0.48
1:A:364:ALA:C	1:A:366:MET:H	2.21	0.48
1:A:352:ARG:HB3	1:A:352:ARG:HH11	1.78	0.48
1:B:61:GLN:HA	1:B:61:GLN:NE2	2.29	0.48
1:A:326:ASN:ND2	1:C:221:ASP:C	2.72	0.48
1:C:70:ALA:HA	1:C:170:SER:HB3	1.95	0.48
1:A:366:MET:HE3	1:A:369:ARG:HB2	1.96	0.48
1:B:122:ALA:N	1:B:145:TYR:CE1	2.82	0.48
1:A:59:LEU:HD22	1:A:343:ALA:HB2	1.95	0.47
1:C:97:ASP:HB3	1:C:145:TYR:CD1	2.49	0.47
1:B:152:PHE:CG	1:B:289:VAL:HG11	2.48	0.47
1:A:200:VAL:HB	1:A:216:THR:HG21	1.96	0.47
1:B:156:SER:HB2	1:B:258:GLY:HA2	1.95	0.47
1:B:218:VAL:HG13	1:C:160:SER:HB3	1.91	0.47
1:B:115:ILE:HD12	1:B:173:VAL:HG11	1.95	0.47
1:B:202:PHE:CE1	1:B:212:SER:HB2	2.49	0.47
1:A:201:GLN:CD	1:B:264:PRO:HB3	2.39	0.47
1:B:117:PRO:HB2	1:B:292:GLY:N	2.29	0.47
1:A:265:ALA:O	1:A:266:ASN:HB2	2.15	0.47
1:B:200:VAL:O	1:B:213:LEU:HA	2.15	0.47
1:A:374:ILE:HG22	1:A:375:LYS:HG3	1.97	0.47
1:B:366:MET:CE	1:B:369:ARG:HD2	2.40	0.47
1:C:124:TRP:CE3	1:C:142:PRO:HB3	2.50	0.47
1:C:199:THR:CA	1:C:216:THR:HG22	2.45	0.47
1:B:369:ARG:O	1:B:373:ILE:HG13	2.15	0.46
1:A:97:ASP:HB2	1:A:317:SER:HB3	1.96	0.46
1:A:264:PRO:HB3	1:C:201:GLN:CD	2.41	0.46
1:C:122:ALA:HB2	1:C:145:TYR:CE2	2.51	0.46
1:C:322:ARG:HB3	1:C:322:ARG:HH11	1.79	0.46
1:A:159:ARG:HG2	1:A:257:GLU:OE1	2.16	0.46
1:A:228:PRO:HG2	1:B:331:GLN:HE21	1.79	0.46
1:B:115:ILE:HD11	1:B:173:VAL:CG2	2.45	0.46
1:A:304:PRO:HG2	1:A:307:ALA:HB2	1.96	0.46
1:B:74:PRO:CG	1:B:316:TRP:CE2	2.95	0.46
1:B:366:MET:HE3	1:B:369:ARG:HB3	1.97	0.46
1:C:91:LYS:HB2	1:C:91:LYS:HZ3	1.77	0.46
1:C:366:MET:HE2	1:C:366:MET:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ALA:C	1:A:284:ALA:H	2.24	0.46
1:B:197:LEU:HD11	1:B:215:HIS:HB3	1.97	0.46
1:A:220:LEU:C	1:A:222:GLY:H	2.23	0.46
1:A:228:PRO:HD2	1:B:330:TYR:CD2	2.50	0.46
1:A:155:THR:HG22	1:A:156:SER:N	2.31	0.46
1:A:208:PRO:HD2	1:B:206:THR:HG22	1.98	0.46
1:A:342:VAL:O	1:A:346:GLU:HG2	2.16	0.46
1:B:117:PRO:HB2	1:B:292:GLY:H	1.81	0.46
1:A:277:THR:HG22	1:A:278:MET:N	2.30	0.46
1:B:74:PRO:CB	1:B:316:TRP:CE2	2.96	0.46
1:B:264:PRO:HG2	1:B:267:VAL:CG2	2.45	0.46
1:C:103:ILE:HD12	1:C:105:PHE:CZ	2.51	0.46
1:A:57:THR:CG2	1:A:58:ARG:N	2.76	0.45
1:C:239:VAL:HG22	1:C:240:PHE:N	2.31	0.45
1:B:59:LEU:HD23	1:B:342:VAL:HB	1.98	0.45
1:C:101:GLN:HG3	1:C:103:ILE:HG22	1.95	0.45
1:A:224:LEU:HD11	1:A:275:PRO:CB	2.45	0.45
1:C:68:LYS:HE2	1:C:76:PHE:CE2	2.49	0.45
1:C:84:ILE:HD13	1:C:250:PHE:CD2	2.52	0.45
1:C:324:ASN:HB3	1:C:326:ASN:OD1	2.16	0.45
1:A:61:GLN:N	1:A:62:PRO:CD	2.78	0.45
1:A:252:PHE:CZ	1:A:322:ARG:HD3	2.52	0.45
1:C:128:VAL:HG12	1:C:129:PRO:HD2	1.99	0.45
1:B:142:PRO:HD3	1:B:279:ASP:O	2.17	0.45
1:C:128:VAL:HG11	1:C:133:PHE:O	2.17	0.45
1:C:241:SER:HB2	1:C:357:ALA:CB	2.46	0.45
1:C:341:GLU:HG3	1:C:345:GLN:NE2	2.32	0.45
1:A:180:ASN:ND2	1:A:183:GLN:NE2	2.65	0.45
1:A:74:PRO:CG	1:A:316:TRP:HE1	2.23	0.44
1:A:246:ASN:HD22	1:A:294:MET:C	2.26	0.44
1:A:264:PRO:HG2	1:A:267:VAL:CG2	2.47	0.44
1:B:124:TRP:CE3	1:B:278:MET:HE3	2.51	0.44
1:B:324:ASN:HD22	1:B:324:ASN:HA	1.60	0.44
1:C:129:PRO:O	1:C:132:THR:OG1	2.33	0.44
1:C:85:PRO:O	1:C:344:LEU:HD11	2.16	0.44
1:A:217:LEU:CB	1:A:220:LEU:HD11	2.42	0.44
1:A:242:GLN:OE1	1:A:242:GLN:N	2.50	0.44
1:B:222:GLY:HA2	1:C:326:ASN:OD1	2.17	0.44
1:C:124:TRP:CH2	1:C:142:PRO:HB3	2.52	0.44
1:C:80:PRO:CB	1:C:96:LYS:CB	2.68	0.44
1:B:322:ARG:HD2	1:B:322:ARG:HA	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:VAL:HG11	1:C:370:VAL:HG13	1.99	0.44
1:A:366:MET:HE3	1:A:369:ARG:HD2	1.99	0.44
1:A:170:SER:OG	1:A:318:CYS:HB2	2.16	0.44
1:B:245:CYS:HA	1:B:293:ASN:O	2.17	0.44
1:C:156:SER:HB2	1:C:258:GLY:HA2	1.99	0.44
1:C:346:GLU:OE2	1:C:374:ILE:HG23	2.18	0.44
1:C:122:ALA:HB2	1:C:145:TYR:CD2	2.53	0.43
2:R:1:U:C3'	2:R:2:U:H5''	2.47	0.43
1:C:115:ILE:O	1:C:296:THR:HG23	2.18	0.43
1:A:112:PHE:CZ	1:A:300:ARG:HD3	2.53	0.43
1:C:99:LEU:HB2	1:C:145:TYR:HD2	1.82	0.43
1:A:68:LYS:O	1:A:72:ALA:N	2.44	0.43
1:A:126:ALA:HB3	1:A:140:PHE:CE2	2.54	0.43
1:B:62:PRO:HB3	1:B:337:PRO:HB3	2.00	0.43
1:C:61:GLN:N	1:C:62:PRO:CD	2.81	0.43
1:A:177:PRO:HA	1:A:311:ALA:HB2	2.00	0.43
1:A:282:ALA:C	1:A:284:ALA:N	2.77	0.43
1:C:169:ALA:HB3	1:C:318:CYS:HB3	1.99	0.43
1:B:362:GLN:H	1:B:362:GLN:HG2	1.68	0.43
1:C:103:ILE:O	1:C:103:ILE:HG13	2.19	0.43
1:C:128:VAL:CG1	1:C:129:PRO:HD2	2.48	0.43
1:C:142:PRO:HD3	1:C:279:ASP:O	2.19	0.43
1:A:102:SER:C	1:A:103:ILE:HG23	2.43	0.43
1:A:117:PRO:HB2	1:A:292:GLY:N	2.34	0.43
1:C:96:LYS:HZ2	1:C:316:TRP:HB3	1.83	0.43
1:A:160:SER:HB2	1:C:218:VAL:HB	1.99	0.42
1:A:203:PRO:HA	1:A:211:SER:HA	2.01	0.42
1:B:241:SER:HB2	1:B:357:ALA:CB	2.49	0.42
1:C:99:LEU:HB2	1:C:145:TYR:CD2	2.54	0.42
1:C:328:MET:SD	1:C:328:MET:C	3.02	0.42
1:A:322:ARG:NH2	1:C:295:ASP:OD1	2.51	0.42
1:A:339:LEU:HD12	1:A:340:ASP:N	2.34	0.42
1:B:220:LEU:HD12	1:B:220:LEU:HA	1.66	0.42
1:B:371:LYS:HA	1:B:374:ILE:HD12	2.01	0.42
1:B:115:ILE:HD11	1:B:173:VAL:CB	2.49	0.42
1:C:346:GLU:O	1:C:347:TYR:C	2.61	0.42
1:B:184:PHE:CD2	1:B:184:PHE:C	2.97	0.42
1:B:241:SER:HB2	1:B:357:ALA:HB2	2.02	0.42
1:B:174:GLY:O	1:B:313:LEU:HD12	2.19	0.42
1:C:233:GLU:CG	1:C:237:LYS:HD2	2.50	0.42
1:C:55:ALA:C	1:C:57:THR:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:PRO:HA	1:C:264:PRO:HD3	1.89	0.42
1:A:234:SER:OG	1:A:236:ILE:HG22	2.19	0.42
1:A:359:ILE:CD1	1:A:361:ALA:HB3	2.49	0.42
1:A:91:LYS:C	1:A:92:VAL:HG13	2.45	0.42
1:A:203:PRO:HB3	1:B:265:ALA:HB3	2.01	0.42
1:B:124:TRP:CE2	1:B:142:PRO:HB3	2.55	0.42
1:B:183:GLN:HB2	1:B:308:VAL:HB	2.02	0.42
1:B:355:PRO:O	1:B:356:VAL:C	2.63	0.42
1:C:133:PHE:HB3	1:C:134:PRO:CD	2.49	0.41
1:B:366:MET:O	1:B:370:VAL:HG23	2.20	0.41
1:A:102:SER:O	1:A:103:ILE:CG2	2.68	0.41
1:A:193:CYS:SG	1:B:325:PRO:HG2	2.60	0.41
1:B:216:THR:HG21	1:B:272:THR:O	2.21	0.41
1:C:99:LEU:HD22	1:C:122:ALA:HB3	2.01	0.41
1:C:203:PRO:HA	1:C:211:SER:HA	2.02	0.41
1:A:91:LYS:C	1:A:92:VAL:CG1	2.93	0.41
1:A:218:VAL:HB	1:B:160:SER:HB2	2.01	0.41
1:A:374:ILE:O	1:A:378:LEU:HB2	2.20	0.41
1:C:91:LYS:HB2	1:C:91:LYS:HZ2	1.84	0.41
1:B:186:GLY:HA3	1:B:302:SER:O	2.20	0.41
1:A:182:MET:HG3	1:A:183:GLN:N	2.35	0.41
1:A:239:VAL:HG22	1:A:240:PHE:N	2.35	0.41
1:B:184:PHE:CD2	1:B:236:ILE:HB	2.56	0.41
1:C:171:MET:HE2	1:C:243:SER:HB3	2.03	0.41
1:A:246:ASN:ND2	1:A:294:MET:N	2.68	0.41
1:A:346:GLU:O	1:A:347:TYR:C	2.63	0.41
1:A:337:PRO:HA	1:A:338:PRO:HD3	1.88	0.41
1:B:119:PRO:HB2	1:B:289:VAL:HG23	2.03	0.41
1:B:172:ASN:CB	1:B:316:TRP:CE3	3.02	0.41
1:B:322:ARG:HG3	1:B:322:ARG:HH11	1.86	0.41
1:C:79:ASP:HA	1:C:80:PRO:HD3	1.72	0.41
1:C:133:PHE:HB3	1:C:134:PRO:HD2	2.02	0.41
1:C:265:ALA:O	1:C:266:ASN:CB	2.64	0.41
1:B:223:VAL:O	1:B:223:VAL:HG12	2.21	0.41
1:A:115:ILE:HB	1:A:297:ILE:HB	2.03	0.40
1:B:144:ASN:HD21	1:B:286:SER:CB	2.34	0.40
1:B:202:PHE:CD1	1:B:202:PHE:C	3.00	0.40
1:B:224:LEU:HB3	7:B:607:HOH:O	2.21	0.40
1:C:364:ALA:O	1:C:366:MET:N	2.54	0.40
1:A:289:VAL:H	1:A:289:VAL:HG22	1.66	0.40
1:C:66:PHE:CD1	1:C:85:PRO:HD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:PHE:HB3	1:C:159:ARG:HD2	2.03	0.40
1:C:176:TYR:CD1	1:C:176:TYR:N	2.89	0.40
1:A:172:ASN:OD1	1:A:242:GLN:HB2	2.22	0.40
1:A:366:MET:HE3	1:A:369:ARG:CD	2.51	0.40
1:B:231:PHE:CE2	1:B:239:VAL:HG23	2.57	0.40
1:B:239:VAL:HG22	1:B:240:PHE:N	2.36	0.40
1:C:220:LEU:HA	1:C:220:LEU:HD23	1.90	0.40
1:C:262:LEU:HA	1:C:263:PRO:C	2.46	0.40
1:A:157:THR:CG2	1:C:271:SER:O	2.68	0.40
1:B:352:ARG:HG2	1:B:352:ARG:HH11	1.87	0.40
1:C:128:VAL:CG1	1:C:132:THR:OG1	2.61	0.40
1:C:383:ASN:N	1:C:383:ASN:HD22	2.20	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	326/407 (80%)	306 (94%)	20 (6%)	0	100	100
1	B	327/407 (80%)	299 (91%)	28 (9%)	0	100	100
1	C	327/407 (80%)	300 (92%)	25 (8%)	2 (1%)	21	56
All	All	980/1221 (80%)	905 (92%)	73 (7%)	2 (0%)	43	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	365	SER
1	C	156	SER

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	272/336 (81%)	267 (98%)	5 (2%)	51	74
1	B	271/336 (81%)	267 (98%)	4 (2%)	57	76
1	C	272/336 (81%)	269 (99%)	3 (1%)	65	79
All	All	815/1008 (81%)	803 (98%)	12 (2%)	57	76

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	THR
1	A	300	ARG
1	A	318	CYS
1	A	328	MET
1	A	374	ILE
1	B	103	ILE
1	B	310	SER
1	B	318	CYS
1	B	342	VAL
1	C	76	PHE
1	C	91	LYS
1	C	318	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	109	GLN
1	A	144	ASN
1	A	162	GLN
1	A	183	GLN
1	A	215	HIS
1	A	246	ASN
1	A	266	ASN
1	A	324	ASN

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Mol	Chain	Res	Type
1	A	326	ASN
1	A	362	GLN
1	A	383	ASN
1	B	61	GLN
1	B	144	ASN
1	B	246	ASN
1	B	253	ASN
1	B	293	ASN
1	B	331	GLN
1	B	345	GLN
1	B	362	GLN
1	C	77	ASN
1	C	100	ASN
1	C	144	ASN
1	C	215	HIS
1	C	266	ASN
1	C	345	GLN
1	C	362	GLN
1	C	383	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	R	14/15 (93%)	6 (42%)	0

All (6) 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	9	U
2	R	12	U

There are no RNA pucker outliers to report.

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](#)

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	EPE	A	503	-	15,15,15	1.27	1 (6%)	19,20,20	1.33	2 (10%)
6	SO4	C	502	-	4,4,4	0.46	0	6,6,6	0.12	0
4	EPE	C	503	-	15,15,15	1.41	1 (6%)	19,20,20	1.41	2 (10%)
4	EPE	B	503	-	15,15,15	1.44	1 (6%)	19,20,20	1.53	2 (10%)

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
4	EPE	A	503	-	-	0/9/19/19	0/1/1/1
4	EPE	C	503	-	-	0/9/19/19	0/1/1/1
4	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)
4	C	503	EPE	C10-S	3.55	1.82	1.77
4	B	503	EPE	C10-S	3.39	1.82	1.77
4	A	503	EPE	C10-S	2.23	1.80	1.77

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	503	EPE	O1S-S-C10	5.07	114.39	106.73
4	C	503	EPE	O1S-S-C10	3.72	112.35	106.73
4	A	503	EPE	O1S-S-C10	3.54	112.07	106.73
4	C	503	EPE	O3S-S-O2S	-3.28	103.18	111.40
4	A	503	EPE	O3S-S-O2S	-3.05	103.78	111.40
4	B	503	EPE	O3S-S-O1S	-2.59	104.93	111.40

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	503	EPE	1	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%)	1.34	60 (18%) 3 3	46, 70, 136, 236	0
1	B	329/407 (80%)	1.27	52 (15%) 5 4	46, 71, 135, 216	0
1	C	329/407 (80%)	1.26	51 (15%) 5 4	45, 70, 115, 196	0
2	R	15/15 (100%)	5.02	15 (100%) 0 0	213, 289, 331, 334	0
All	All	1001/1236 (80%)	1.35	178 (17%) 4 3	45, 71, 146, 334	0

All (178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	54	ALA	13.4
1	A	383	ASN	11.1
1	A	381	ALA	10.4
1	C	383	ASN	10.0
1	C	382	SER	10.0
1	A	382	SER	8.9
1	B	381	ALA	8.2
1	A	380	ALA	8.1
1	A	57	THR	7.7
2	R	1	U	7.6
1	C	81	GLY	6.9
2	R	15	U	6.9
1	B	379	ALA	6.8
1	C	77	ASN	6.7
1	A	384	ILE	6.7
1	C	79	ASP	6.7
2	R	14	U	6.3
2	R	11	A	6.0
2	R	12	U	5.7
1	C	376	SER	5.6
2	R	4	C	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	80	PRO	5.5
1	A	376	SER	5.5
2	R	3	U	5.4
1	B	53	MET	5.3
1	B	251	GLU	5.2
1	B	380	ALA	5.2
1	C	380	ALA	5.1
2	R	8	U	4.9
1	A	58	ARG	4.5
1	B	57	THR	4.5
2	R	2	U	4.5
1	A	379	ALA	4.4
1	A	81	GLY	4.3
2	R	5	U	4.2
2	R	9	U	4.2
1	C	76	PHE	4.2
1	A	74	PRO	4.2
2	R	10	U	4.1
1	B	254	ASP	4.1
1	B	377	SER	4.1
1	B	81	GLY	4.1
1	C	381	ALA	4.0
1	C	78	THR	3.8
1	A	266	ASN	3.8
1	A	75	ASP	3.7
1	A	94	SER	3.6
1	A	377	SER	3.6
1	B	376	SER	3.6
1	A	61	GLN	3.6
2	R	7	U	3.5
1	C	326	ASN	3.4
1	B	90	GLY	3.4
1	B	74	PRO	3.4
1	A	365	SER	3.4
2	R	6	C	3.3
1	A	78	THR	3.3
1	C	305	GLU	3.3
1	B	302	SER	3.3
1	C	163	VAL	3.3
1	B	328	MET	3.3
1	B	306	GLY	3.3
1	A	80	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	369	ARG	3.2
1	A	174	GLY	3.1
1	C	55	ALA	3.1
1	A	368	GLU	3.1
1	C	375	LYS	3.1
1	C	61	GLN	3.1
1	A	257	GLU	3.1
1	B	75	ASP	3.1
2	R	13	C	3.0
1	C	204	VAL	3.0
1	A	198	SER	3.0
1	B	212	SER	2.9
1	C	160	SER	2.9
1	C	211	SER	2.9
1	C	75	ASP	2.9
1	C	131	GLY	2.9
1	A	211	SER	2.9
1	B	78	THR	2.9
1	C	69	CYS	2.9
1	B	308	VAL	2.8
1	A	378	LEU	2.8
1	C	83	GLY	2.8
1	C	58	ARG	2.8
1	B	76	PHE	2.8
1	A	87	ARG	2.8
1	C	302	SER	2.8
1	C	258	GLY	2.7
1	C	106	THR	2.7
1	A	82	LYS	2.7
1	B	335	ASP	2.7
1	A	361	ALA	2.7
1	B	225	ALA	2.7
1	B	165	SER	2.7
1	C	209	ALA	2.7
1	C	80	PRO	2.7
1	A	221	ASP	2.7
1	A	229	ASP	2.7
1	B	82	LYS	2.6
1	A	238	GLY	2.6
1	C	57	THR	2.6
1	A	372	SER	2.6
1	A	88	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	333	GLY	2.6
1	A	364	ALA	2.6
1	C	104	SER	2.6
1	A	251	GLU	2.6
1	A	63	GLY	2.6
1	A	77	ASN	2.5
1	A	79	ASP	2.5
1	B	161	ASP	2.5
1	C	82	LYS	2.5
1	C	321	TYR	2.5
1	A	145	TYR	2.5
1	A	125	SER	2.4
1	A	139	THR	2.4
1	B	330	TYR	2.4
1	C	221	ASP	2.4
1	B	61	GLN	2.4
1	B	242	GLN	2.4
1	B	58	ARG	2.4
1	C	268	SER	2.4
1	A	332	PHE	2.4
1	C	251	GLU	2.4
1	A	302	SER	2.4
1	A	303	ALA	2.3
1	A	161	ASP	2.3
1	A	375	LYS	2.3
1	B	333	GLY	2.3
1	C	187	SER	2.3
1	B	171	MET	2.3
1	B	79	ASP	2.3
1	B	365	SER	2.3
1	C	213	LEU	2.3
1	B	77	ASN	2.3
1	C	147	GLY	2.3
1	C	224	LEU	2.3
1	A	186	GLY	2.2
1	B	141	ASN	2.2
1	B	368	GLU	2.2
1	A	86	ASP	2.2
1	A	306	GLY	2.2
1	B	125	SER	2.2
1	C	368	GLU	2.2
1	B	248	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	160	SER	2.2
1	B	362	GLN	2.2
1	C	108	GLY	2.2
1	C	254	ASP	2.2
1	C	176	TYR	2.1
1	C	109	GLN	2.1
1	A	104	SER	2.1
1	B	179	SER	2.1
1	C	165	SER	2.1
1	A	147	GLY	2.1
1	A	254	ASP	2.1
1	B	89	GLU	2.1
1	B	257	GLU	2.1
1	A	100	ASN	2.1
1	B	100	ASN	2.1
1	B	196	LYS	2.1
1	A	369	ARG	2.1
1	B	184	PHE	2.1
1	A	196	LYS	2.1
1	C	297	ILE	2.1
1	A	193	CYS	2.1
1	B	69	CYS	2.1
1	C	245	CYS	2.1
1	B	55	ALA	2.1
1	C	361	ALA	2.1
1	A	345	GLN	2.1
1	B	326	ASN	2.0
1	A	316	TRP	2.0
1	B	153	GLY	2.0
1	C	65	ALA	2.0
1	C	74	PRO	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 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
3	CA	A	502	1/1	0.67	0.34	112,112,112,112	0
5	CL	B	502	1/1	0.86	0.17	95,95,95,95	0
6	SO4	C	502	5/5	0.92	0.22	124,128,150,190	0
3	CA	C	501	1/1	0.93	0.09	61,61,61,61	0
4	EPE	A	503	15/15	0.93	0.21	56,86,162,162	0
4	EPE	B	503	15/15	0.94	0.20	55,98,145,156	0
4	EPE	C	503	15/15	0.95	0.17	51,102,157,161	0
3	CA	B	501	1/1	0.96	0.12	58,58,58,58	0
3	CA	A	501	1/1	0.98	0.08	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.