Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2024 – 09:07 AM EST

PDB ID	:	3NAH
Title	:	Crystal structures and functional analysis of murine norovirus RNA-dependent RNA polymerase
Authors	:	Kim, K.H.; Lee, J.H.; Alam, I.; Park, Y.; Kang, S.
Deposited on	:	2010-06-02
Resolution	:	2.75 Å(reported)

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

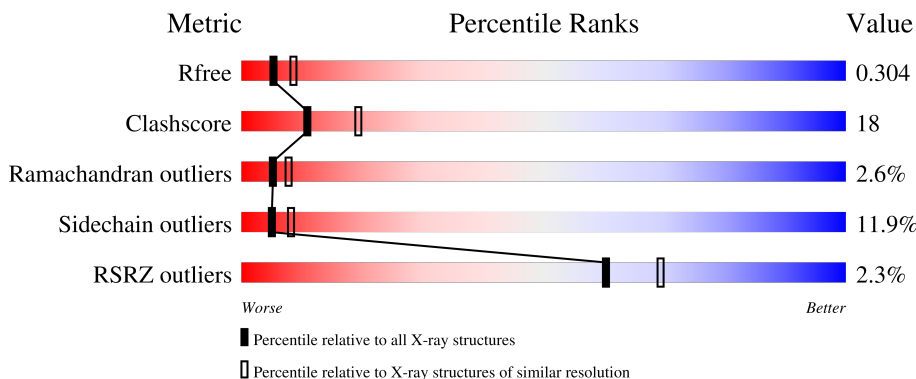|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.304
Clashscore		18
Ramachandran outliers		2.6%
Sidechain outliers		11.9%
RSRZ outliers		2.3%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	517	2% / 56% / 32% / 6% / 6%
1	B	517	2% / 57% / 31% / 5% / 6%
1	C	517	2% / 57% / 30% / 6% / 6%

WORLDWIDE wwPDB PROTEIN DATA BANK

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 11710 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 RNA dependent RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	486	Total	C	N	O	S	0	0	0
			3857	2437	679	716	25			
1	B	485	Total	C	N	O	S	0	0	0
			3846	2431	675	715	25			
1	C	485	Total	C	N	O	S	0	0	0
			3846	2431	675	715	25			

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	510	ALA	-	expression tag	UNP Q80J95
A	511	ALA	-	expression tag	UNP Q80J95
A	512	ALA	-	expression tag	UNP Q80J95
A	513	LEU	-	expression tag	UNP Q80J95
A	514	GLU	-	expression tag	UNP Q80J95
A	515	HIS	-	expression tag	UNP Q80J95
A	516	HIS	-	expression tag	UNP Q80J95
A	517	HIS	-	expression tag	UNP Q80J95
A	518	HIS	-	expression tag	UNP Q80J95
A	519	HIS	-	expression tag	UNP Q80J95
A	520	HIS	-	expression tag	UNP Q80J95
B	510	ALA	-	expression tag	UNP Q80J95
B	511	ALA	-	expression tag	UNP Q80J95
B	512	ALA	-	expression tag	UNP Q80J95
B	513	LEU	-	expression tag	UNP Q80J95
B	514	GLU	-	expression tag	UNP Q80J95
B	515	HIS	-	expression tag	UNP Q80J95
B	516	HIS	-	expression tag	UNP Q80J95
B	517	HIS	-	expression tag	UNP Q80J95
B	518	HIS	-	expression tag	UNP Q80J95
B	519	HIS	-	expression tag	UNP Q80J95
B	520	HIS	-	expression tag	UNP Q80J95
C	510	ALA	-	expression tag	UNP Q80J95

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Chain	Residue	Modelled	Actual	Comment	Reference
C	511	ALA	-	expression tag	UNP Q80J95
C	512	ALA	-	expression tag	UNP Q80J95
C	513	LEU	-	expression tag	UNP Q80J95
C	514	GLU	-	expression tag	UNP Q80J95
C	515	HIS	-	expression tag	UNP Q80J95
C	516	HIS	-	expression tag	UNP Q80J95
C	517	HIS	-	expression tag	UNP Q80J95
C	518	HIS	-	expression tag	UNP Q80J95
C	519	HIS	-	expression tag	UNP Q80J95
C	520	HIS	-	expression tag	UNP Q80J95

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
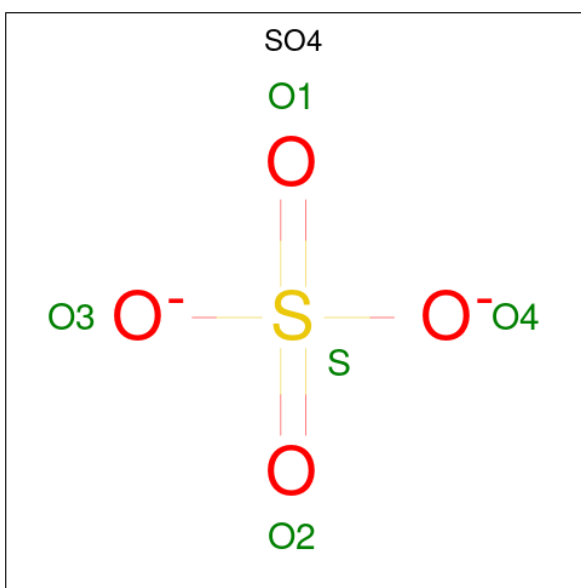
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	49	Total 49	O 49	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	52	Total O 52 52		0	0
3	C	45	Total O 45 45		0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

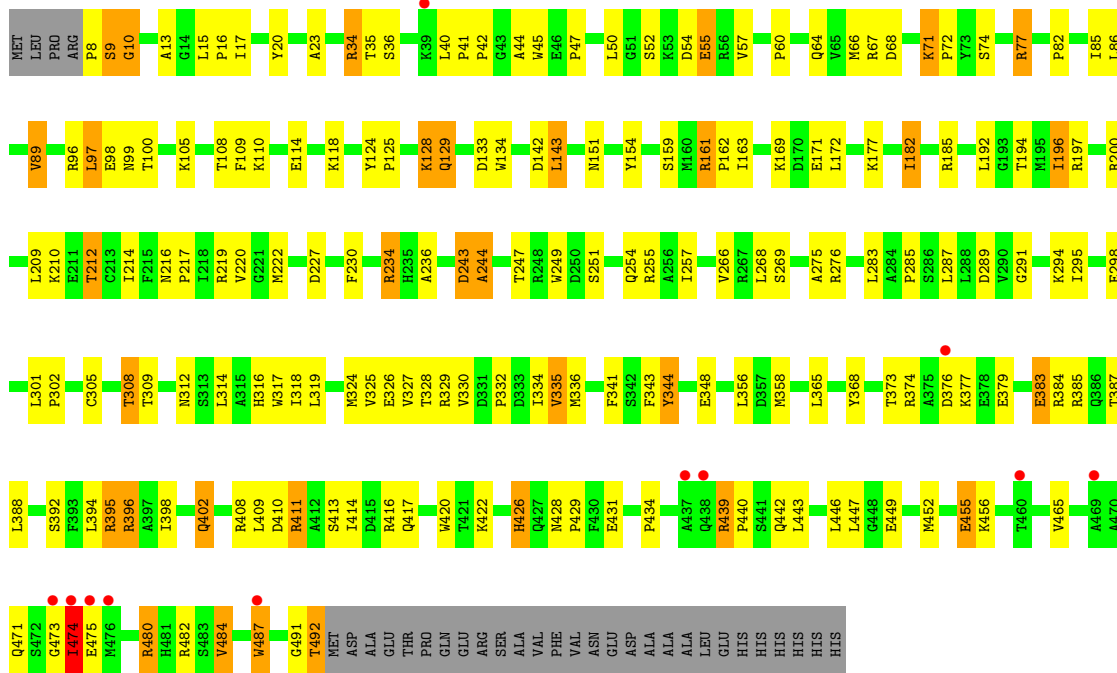• Molecule 1: RNA dependent RNA polymerase
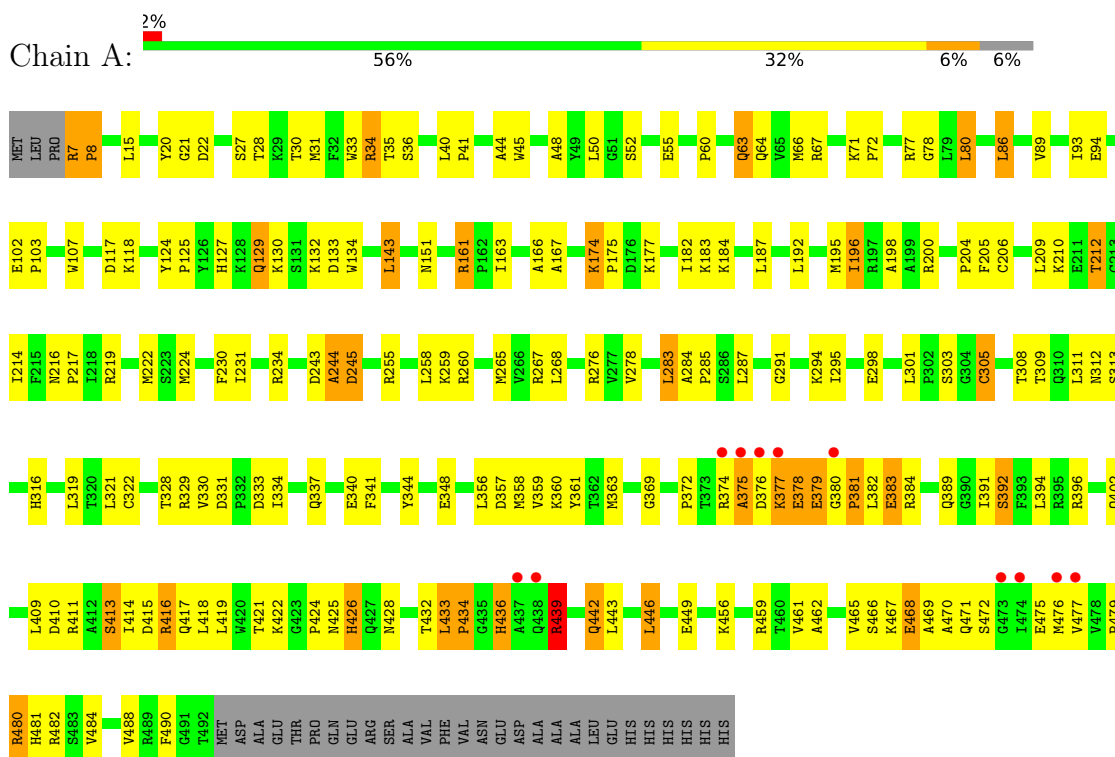
Chain A:

• Molecule 1: RNA dependent RNA polymerase

Chain B:

• Molecule 1: RNA dependent RNA polymerase

Chain C:
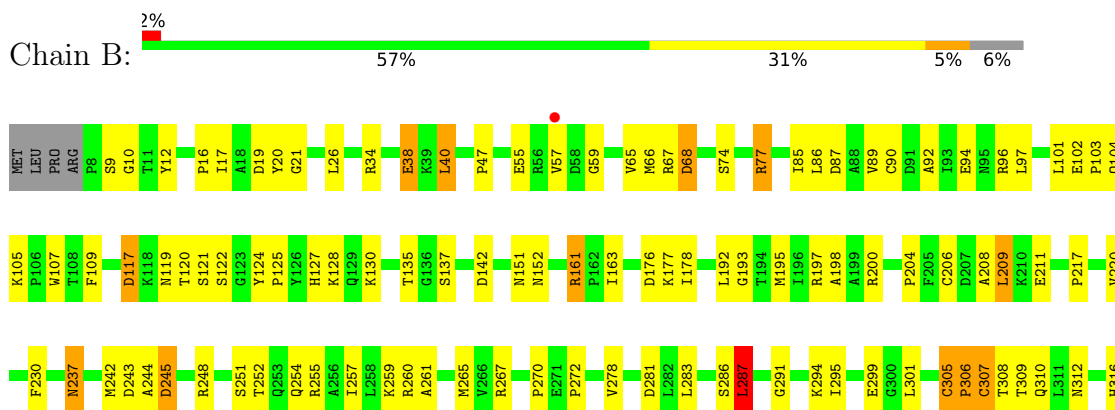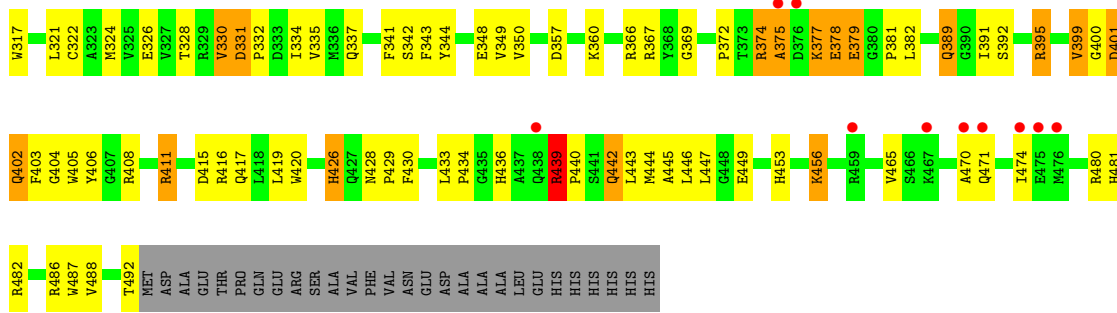
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	120.83Å 196.54Å 109.16Å 90.00° 114.21° 90.00°	Depositor
Resolution (Å)	44.06 – 2.75 44.06 – 2.75	Depositor EDS
% Data completeness (in resolution range)	92.2 (44.06-2.75) 92.2 (44.06-2.75)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.221 , 0.303 0.222 , 0.304	Depositor DCC
R_{free} test set	2824 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	24.3	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 37.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.37, < L^2 > = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	11710	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.37% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \|L\| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.57	0/3952	0.74	0/5355
1	B	0.58	0/3941	0.73	1/5340 (0.0%)
1	C	0.56	0/3941	0.72	0/5340
All	All	0.57	0/11834	0.73	1/16035 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	287	LEU	CA-CB-CG	5.26	127.40	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3857	0	3813	135	0
1	B	3846	0	3801	155	0
1	C	3846	0	3801	134	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0
3	A	49	0	0	7	0
3	B	52	0	0	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	45	0	0	10	0
All	All	11710	0	11415	419	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 18.

All (419) 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:7:ARG:CG	1:A:8:PRO:HD2	1.73	1.16
1:A:380:GLY:HA3	1:A:381:PRO:O	1.44	1.12
1:B:480:ARG:HD2	1:B:482:ARG:HG2	1.24	1.11
1:B:395:ARG:HG2	1:B:395:ARG:HH11	0.90	1.07
1:C:374:ARG:HE	1:C:377:LYS:HB2	1.16	1.07
1:A:374:ARG:HD2	1:A:383:GLU:HB2	1.37	1.05
1:B:374:ARG:HG2	1:B:377:LYS:HG3	1.37	1.05
1:B:395:ARG:HG2	1:B:395:ARG:NH1	1.69	1.01
1:C:23:ALA:HB3	1:C:291:GLY:HA2	1.42	0.98
1:C:249:TRP:HE1	1:C:312:ASN:HD21	1.09	0.98
1:A:376:ASP:HB2	3:A:545:HOH:O	1.65	0.95
1:C:45:TRP:HB2	1:C:416:ARG:HD3	1.48	0.94
1:A:7:ARG:CB	1:A:8:PRO:HD2	1.98	0.94
1:A:484:VAL:O	1:A:488:VAL:HG23	1.68	0.93
1:C:491:GLY:CA	1:C:492:THR:HB	1.99	0.92
1:C:428:ASN:HD22	1:C:431:GLU:HG3	1.34	0.91
1:A:480:ARG:HH12	1:A:481:HIS:HB3	1.32	0.91
1:A:303:SER:HA	1:A:308:THR:HG21	1.50	0.91
1:A:433:LEU:HB3	1:A:434:PRO:HD2	1.52	0.90
1:B:411:ARG:CG	1:B:411:ARG:HH11	1.86	0.89
1:C:276:ARG:HD2	3:C:554:HOH:O	1.72	0.87
1:C:374:ARG:NE	1:C:377:LYS:HB2	1.90	0.87
1:A:7:ARG:HG3	1:A:8:PRO:HD2	1.57	0.86
1:B:411:ARG:HH11	1:B:411:ARG:HG3	1.38	0.86
1:C:428:ASN:ND2	1:C:431:GLU:HG3	1.91	0.85
1:C:396:ARG:HE	1:C:409:LEU:HD13	1.42	0.84
1:C:491:GLY:HA2	1:C:492:THR:HB	1.57	0.84
1:C:491:GLY:HA3	1:C:492:THR:HG22	1.57	0.84
1:B:395:ARG:HH11	1:B:395:ARG:CG	1.84	0.83
1:C:374:ARG:HE	1:C:377:LYS:CB	1.91	0.82
1:A:7:ARG:CB	1:A:8:PRO:CD	2.58	0.82
1:C:210:LYS:HG3	3:C:550:HOH:O	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:PRO:HB3	1:B:152:ASN:HD22	1.48	0.79
1:B:374:ARG:HG2	1:B:377:LYS:CG	2.13	0.79
1:B:402:GLN:HE21	1:C:96:ARG:HH11	1.30	0.79
1:B:411:ARG:H	1:B:411:ARG:HD2	1.46	0.79
1:A:161:ARG:NH2	1:A:285:PRO:O	2.16	0.79
1:A:7:ARG:HB2	1:A:8:PRO:CD	2.12	0.78
1:B:357:ASP:HA	3:B:530:HOH:O	1.82	0.78
1:C:491:GLY:HA3	1:C:492:THR:CG2	2.13	0.78
1:A:214:ILE:HG21	1:A:230:PHE:CD2	2.19	0.77
1:A:433:LEU:HB3	1:A:434:PRO:CD	2.13	0.77
1:A:439:ARG:O	1:A:443:LEU:HB2	1.84	0.77
1:A:426:HIS:CE1	1:A:428:ASN:O	2.37	0.77
1:C:192:LEU:O	1:C:196:ILE:HG23	1.84	0.77
1:C:249:TRP:HE1	1:C:312:ASN:ND2	1.81	0.77
1:C:455:GLU:HG2	1:C:456:LYS:H	1.50	0.76
1:C:8:PRO:HD2	3:C:560:HOH:O	1.85	0.75
1:A:30:THR:HG23	1:A:50:LEU:HD21	1.68	0.75
1:B:372:PRO:HB2	1:B:382:LEU:HD11	1.68	0.75
1:B:439:ARG:H	1:B:440:PRO:CD	1.98	0.75
1:B:439:ARG:N	1:B:440:PRO:HD2	2.00	0.75
1:A:243:ASP:HB2	1:A:391:ILE:HG23	1.69	0.74
1:B:94:GLU:OE1	1:B:267:ARG:HD2	1.88	0.74
1:B:439:ARG:H	1:B:440:PRO:HD2	1.53	0.74
1:C:374:ARG:HB2	1:C:379:GLU:O	1.87	0.74
1:A:117:ASP:O	1:A:130:LYS:NZ	2.20	0.74
1:C:491:GLY:CA	1:C:492:THR:CB	2.65	0.74
1:C:422:LYS:HE2	3:C:525:HOH:O	1.88	0.73
1:A:219:ARG:NH1	1:A:231:ILE:HG12	2.04	0.73
1:B:439:ARG:HG2	1:B:443:LEU:HD13	1.70	0.73
1:B:417:GLN:HB2	1:B:446:LEU:HD21	1.70	0.73
1:C:491:GLY:HA3	1:C:492:THR:CB	2.19	0.73
1:A:443:LEU:HG	1:A:465:VAL:HG13	1.70	0.73
1:A:301:LEU:HD22	1:A:312:ASN:ND2	2.03	0.72
1:B:117:ASP:O	1:B:120:THR:HG22	1.90	0.72
1:B:377:LYS:HE2	1:B:378:GLU:H	1.55	0.72
1:B:411:ARG:HD2	1:B:411:ARG:N	2.04	0.71
1:C:8:PRO:CD	3:C:560:HOH:O	2.36	0.71
1:A:183:LYS:HA	3:A:528:HOH:O	1.91	0.71
1:A:7:ARG:HG2	1:A:8:PRO:HD2	1.68	0.71
1:B:374:ARG:CG	1:B:377:LYS:HG3	2.19	0.70
1:A:374:ARG:NH1	1:A:379:GLU:O	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:ARG:HD2	1:B:287:LEU:HD12	1.74	0.69
1:C:163:ILE:CD1	1:C:287:LEU:HD23	2.23	0.68
1:A:34:ARG:HD2	1:A:40:LEU:HD13	1.74	0.68
1:C:23:ALA:HB3	1:C:291:GLY:CA	2.20	0.68
1:C:169:LYS:HD2	1:C:185:ARG:HH21	1.59	0.68
1:C:10:GLY:HA2	1:C:17:ILE:HD12	1.76	0.67
1:A:209:LEU:O	1:A:212:THR:HG22	1.95	0.67
1:C:216:ASN:HB3	1:C:217:PRO:HD2	1.76	0.67
1:C:128:LYS:HE3	1:C:133:ASP:OD2	1.95	0.66
1:C:480:ARG:HH11	1:C:482:ARG:HG2	1.59	0.66
1:A:89:VAL:HG21	1:A:322:CYS:SG	2.34	0.66
1:B:334:ILE:N	1:B:334:ILE:HD12	2.11	0.66
1:C:257:ILE:HD13	1:C:319:LEU:HD21	1.78	0.66
1:B:433:LEU:HD23	1:B:436:HIS:HD2	1.60	0.66
1:B:480:ARG:HD2	1:B:482:ARG:CG	2.15	0.65
1:B:439:ARG:N	1:B:440:PRO:CD	2.58	0.65
1:A:30:THR:CG2	1:A:50:LEU:HD21	2.27	0.64
1:A:480:ARG:NH1	1:A:481:HIS:HB3	2.10	0.64
1:B:217:PRO:HB3	1:B:341:PHE:HB2	1.79	0.64
1:B:480:ARG:HD3	1:B:481:HIS:N	2.13	0.64
1:C:332:PRO:HA	1:C:335:VAL:HG13	1.78	0.64
1:A:217:PRO:HB3	1:A:341:PHE:HB2	1.80	0.64
1:B:59:GLY:HA2	3:B:534:HOH:O	1.98	0.64
1:B:248:ARG:HB3	1:B:251:SER:OG	1.98	0.64
1:B:305:CYS:HB2	1:B:306:PRO:HD2	1.79	0.64
1:C:118:LYS:HE2	1:C:134:TRP:CE2	2.32	0.64
1:A:161:ARG:HD2	1:A:287:LEU:HD22	1.80	0.64
1:C:77:ARG:HG3	1:C:254:GLN:HG2	1.79	0.64
1:C:72:PRO:HB2	1:C:251:SER:HB2	1.80	0.63
1:A:174:LYS:H	1:A:174:LYS:CE	2.10	0.63
1:C:222:MET:O	1:C:222:MET:HG3	1.96	0.63
1:A:378:GLU:O	1:A:379:GLU:HB2	1.98	0.63
1:A:380:GLY:HA3	1:A:381:PRO:C	2.17	0.63
1:B:77:ARG:HD2	1:B:299:GLU:CD	2.19	0.63
1:A:396:ARG:HD3	1:A:409:LEU:HB2	1.79	0.63
1:A:414:ILE:HG23	1:A:446:LEU:HD12	1.81	0.63
1:B:306:PRO:O	1:B:308:THR:N	2.32	0.63
1:C:85:ILE:O	1:C:89:VAL:HG13	1.99	0.62
1:B:334:ILE:HA	1:B:337:GLN:HG2	1.82	0.62
1:C:395:ARG:HD3	3:C:541:HOH:O	1.98	0.62
1:B:411:ARG:H	1:B:411:ARG:CD	2.06	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:ASP:HB3	1:B:334:ILE:HD13	1.81	0.61
1:B:447:LEU:HD13	1:B:465:VAL:HG21	1.81	0.61
1:A:224:MET:HG2	1:A:396:ARG:HH11	1.65	0.61
1:A:48:ALA:HB1	1:A:184:LYS:HG3	1.83	0.61
1:B:87:ASP:OD1	1:B:260:ARG:NH2	2.34	0.61
1:A:21:GLY:HA3	1:A:291:GLY:O	2.00	0.61
1:B:307:CYS:HA	3:B:531:HOH:O	2.00	0.61
1:B:401:ASP:HB3	1:B:404:GLY:O	2.01	0.60
1:C:244:ALA:HB3	1:C:348:GLU:OE2	2.00	0.60
1:B:417:GLN:CB	1:B:446:LEU:HD21	2.30	0.60
1:C:217:PRO:HB3	1:C:341:PHE:HB2	1.84	0.59
1:A:380:GLY:CA	1:A:381:PRO:O	2.36	0.59
1:B:244:ALA:HB3	1:B:348:GLU:OE2	2.02	0.59
1:B:38:GLU:HA	3:B:553:HOH:O	2.02	0.59
1:B:193:GLY:O	1:B:197:ARG:HB2	2.02	0.59
1:B:220:VAL:HA	1:B:344:TYR:CE2	2.37	0.59
1:A:192:LEU:HA	1:A:195:MET:HB2	1.84	0.59
1:C:374:ARG:HB3	1:C:379:GLU:H	1.68	0.59
1:C:15:LEU:CD2	1:C:74:SER:HB3	2.33	0.59
1:C:68:ASP:HA	1:C:71:LYS:HD2	1.85	0.59
1:C:15:LEU:HD21	1:C:74:SER:HB3	1.84	0.59
1:A:417:GLN:HE21	1:A:442:GLN:HE21	1.51	0.58
1:B:316:HIS:CE1	1:B:348:GLU:HB3	2.37	0.58
1:B:20:TYR:O	1:B:294:LYS:HE3	2.02	0.58
1:A:417:GLN:HE21	1:A:442:GLN:NE2	2.01	0.58
1:C:255:ARG:HG3	1:C:298:GLU:O	2.02	0.58
1:C:356:LEU:HD23	1:C:358:MET:HE1	1.84	0.58
1:A:402:GLN:HB2	3:A:526:HOH:O	2.02	0.58
1:A:67:ARG:HB3	3:A:530:HOH:O	2.03	0.58
1:C:108:THR:HA	1:C:200:ARG:HH21	1.69	0.58
1:B:206:CYS:SG	3:B:531:HOH:O	2.41	0.58
1:C:162:PRO:HB3	1:C:194:THR:OG1	2.04	0.58
1:A:163:ILE:CD1	1:A:287:LEU:HD23	2.35	0.57
1:B:331:ASP:OD2	1:B:332:PRO:HD2	2.04	0.57
1:B:433:LEU:HD23	1:B:436:HIS:CD2	2.40	0.57
1:B:89:VAL:O	1:B:92:ALA:N	2.38	0.56
1:C:34:ARG:HG2	1:C:420:TRP:CZ3	2.40	0.56
1:A:461:VAL:O	1:A:465:VAL:HG23	2.05	0.56
1:A:259:LYS:HG3	1:A:283:LEU:HD23	1.86	0.56
1:A:334:ILE:HA	1:A:337:GLN:HG2	1.86	0.56
1:A:359:VAL:HG22	1:A:381:PRO:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:PRO:O	1:B:127:HIS:CD2	2.58	0.56
1:B:47:PRO:HG2	1:B:429:PRO:HB3	1.86	0.56
1:A:402:GLN:CB	3:A:526:HOH:O	2.54	0.56
1:B:411:ARG:HG3	1:B:411:ARG:NH1	2.14	0.55
1:B:408:ARG:HD2	1:B:453:HIS:CD2	2.42	0.55
1:A:245:ASP:OD1	1:A:375:ALA:HA	2.07	0.55
1:B:486:ARG:HG3	1:C:99:ASN:O	2.07	0.54
1:B:34:ARG:HG3	1:B:430:PHE:HA	1.89	0.54
1:B:324:MET:O	1:B:328:THR:HG23	2.07	0.54
1:B:192:LEU:HA	1:B:195:MET:HB2	1.89	0.54
1:A:66:MET:HE1	1:A:166:ALA:HB1	1.88	0.54
1:A:86:LEU:HD13	1:A:260:ARG:NH1	2.22	0.54
1:B:377:LYS:HE2	1:B:378:GLU:N	2.21	0.54
1:C:45:TRP:CB	1:C:416:ARG:HD3	2.28	0.54
1:B:378:GLU:OE1	1:B:378:GLU:HA	2.08	0.54
1:C:214:ILE:HD11	1:C:227:ASP:OD1	2.08	0.54
1:C:314:LEU:O	1:C:318:ILE:HG13	2.07	0.53
1:A:125:PRO:O	1:A:127:HIS:CD2	2.61	0.53
1:B:330:VAL:HG22	1:B:335:VAL:CG2	2.39	0.53
1:C:332:PRO:HA	1:C:335:VAL:CG1	2.38	0.53
1:B:480:ARG:HD3	1:B:481:HIS:H	1.74	0.53
1:A:205:PHE:CE2	1:A:265:MET:HG2	2.43	0.53
1:C:77:ARG:HE	1:C:77:ARG:CA	2.22	0.53
1:B:230:PHE:CD1	1:B:230:PHE:O	2.61	0.53
1:C:388:LEU:HG	1:C:398:ILE:HG21	1.90	0.53
1:C:10:GLY:HA3	1:C:17:ILE:HB	1.89	0.53
1:A:7:ARG:HB2	1:A:8:PRO:HD3	1.90	0.53
1:A:410:ASP:OD1	1:A:413:SER:HB2	2.09	0.53
1:B:270:PRO:O	1:B:272:PRO:HD3	2.08	0.52
1:B:401:ASP:HB2	1:B:406:TYR:HE1	1.74	0.52
1:B:487:TRP:CD1	3:B:563:HOH:O	2.53	0.52
1:C:154:TYR:HB2	1:C:197:ARG:HG3	1.90	0.52
1:B:26:LEU:HD21	1:B:66:MET:CE	2.39	0.52
1:B:456:LYS:HB2	3:B:523:HOH:O	2.09	0.52
1:A:417:GLN:NE2	1:A:442:GLN:HE21	2.07	0.52
1:B:65:VAL:O	1:B:68:ASP:HB2	2.10	0.52
1:A:15:LEU:HD12	1:A:295:ILE:HD12	1.92	0.52
1:A:433:LEU:C	3:A:529:HOH:O	2.48	0.52
1:C:410:ASP:O	1:C:414:ILE:HG13	2.10	0.51
1:B:34:ARG:HG2	1:B:420:TRP:CZ3	2.46	0.51
1:C:212:THR:CG2	1:C:216:ASN:OD1	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:CYS:O	1:C:308:THR:HB	2.09	0.51
1:B:77:ARG:HD2	1:B:299:GLU:CG	2.40	0.51
1:C:266:VAL:HG13	1:C:275:ALA:HB3	1.92	0.51
1:B:408:ARG:HH11	1:B:453:HIS:HA	1.76	0.51
1:A:416:ARG:HA	1:A:419:LEU:HD12	1.93	0.51
1:B:379:GLU:HB3	3:B:544:HOH:O	2.11	0.51
1:B:439:ARG:HB2	3:B:554:HOH:O	2.09	0.51
1:A:416:ARG:O	1:A:419:LEU:N	2.39	0.51
1:C:40:LEU:HD12	1:C:41:PRO:HD2	1.93	0.51
1:C:408:ARG:HG3	1:C:452:MET:HE3	1.93	0.51
1:A:471:GLN:O	1:A:471:GLN:HG2	2.11	0.50
1:C:243:ASP:OD2	1:C:243:ASP:N	2.45	0.50
1:A:143:LEU:HG	1:A:192:LEU:HD22	1.93	0.50
1:A:357:ASP:HB3	1:A:360:LYS:HB2	1.93	0.50
1:B:125:PRO:O	1:B:127:HIS:HD2	1.93	0.50
1:B:334:ILE:N	1:B:334:ILE:CD1	2.75	0.50
1:A:177:LYS:O	1:A:182:ILE:HA	2.12	0.50
1:B:480:ARG:HH11	1:B:482:ARG:HG2	1.76	0.50
1:B:305:CYS:HB2	1:B:306:PRO:CD	2.40	0.49
1:C:439:ARG:HG3	1:C:443:LEU:HD13	1.93	0.49
1:A:374:ARG:HH21	1:A:377:LYS:NZ	2.09	0.49
1:A:284:ALA:O	1:A:285:PRO:C	2.49	0.49
1:B:220:VAL:HG11	1:B:310:GLN:NE2	2.26	0.49
1:A:212:THR:O	1:A:212:THR:HG23	2.12	0.49
1:B:135:THR:OG1	1:B:137:SER:HB3	2.12	0.49
1:A:94:GLU:OE1	1:A:267:ARG:HD2	2.11	0.49
1:B:307:CYS:CA	3:B:531:HOH:O	2.58	0.49
1:B:416:ARG:O	1:B:419:LEU:N	2.43	0.49
1:C:96:ARG:HD3	1:C:336:MET:HE3	1.94	0.49
1:A:45:TRP:HA	1:A:175:PRO:HD3	1.95	0.49
1:C:55:GLU:H	1:C:55:GLU:HG2	1.23	0.49
1:C:385:ARG:NE	3:C:563:HOH:O	2.46	0.49
1:B:403:PHE:O	1:C:234:ARG:NH2	2.46	0.48
1:C:212:THR:HG21	1:C:216:ASN:OD1	2.13	0.48
1:A:174:LYS:H	1:A:174:LYS:HE2	1.76	0.48
1:A:372:PRO:HB2	1:A:382:LEU:HD21	1.94	0.48
1:A:468:GLU:HA	1:A:471:GLN:HE22	1.77	0.48
1:A:107:TRP:CD1	1:A:204:PRO:HG3	2.48	0.48
1:B:237:ASN:HD21	1:C:236:ALA:HB1	1.77	0.48
1:A:30:THR:HG23	1:A:50:LEU:CD2	2.41	0.48
1:A:359:VAL:O	1:A:363:MET:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:VAL:HG11	1:C:356:LEU:HD12	1.96	0.48
1:C:289:ASP:HA	1:C:294:LYS:HA	1.96	0.48
1:B:426:HIS:CE1	1:B:428:ASN:O	2.66	0.48
1:A:234:ARG:HD3	1:A:340:GLU:OE2	2.13	0.48
1:A:20:TYR:O	1:A:294:LYS:HE3	2.14	0.47
1:C:172:LEU:HD11	1:C:420:TRP:CD1	2.49	0.47
1:B:408:ARG:NH1	1:B:453:HIS:HA	2.30	0.47
1:A:459:ARG:O	1:A:462:ALA:HB3	2.14	0.47
1:C:163:ILE:HD13	1:C:287:LEU:HD23	1.97	0.47
1:A:415:ASP:HA	1:A:418:LEU:HD12	1.97	0.47
1:A:467:LYS:C	1:A:469:ALA:H	2.18	0.47
1:C:216:ASN:HB3	1:C:217:PRO:CD	2.44	0.47
1:C:230:PHE:CE1	1:C:234:ARG:HD2	2.50	0.47
1:C:417:GLN:NE2	1:C:442:GLN:HE21	2.12	0.47
1:A:167:ALA:HB3	1:A:187:LEU:HB2	1.96	0.47
1:A:219:ARG:HB3	1:A:222:MET:SD	2.55	0.47
1:B:261:ALA:O	1:B:265:MET:HG3	2.14	0.47
1:C:365:LEU:O	1:C:368:TYR:N	2.48	0.47
1:B:197:ARG:NH2	1:B:281:ASP:OD1	2.47	0.47
1:B:366:ARG:O	1:B:369:GLY:N	2.42	0.47
1:C:326:GLU:O	1:C:329:ARG:HG2	2.15	0.47
1:A:443:LEU:HG	1:A:465:VAL:CG1	2.41	0.47
1:C:40:LEU:HB3	3:C:551:HOH:O	2.15	0.46
1:A:244:ALA:CB	1:A:382:LEU:HG	2.45	0.46
1:C:428:ASN:HA	1:C:429:PRO:HD3	1.73	0.46
1:C:324:MET:O	1:C:328:THR:HG23	2.15	0.46
1:C:330:VAL:HG23	1:C:335:VAL:HG12	1.97	0.46
1:C:82:PRO:HG2	1:C:85:ILE:HD12	1.96	0.46
1:A:78:GLY:HA3	1:A:369:GLY:HA3	1.98	0.46
1:B:89:VAL:HG23	1:B:90:CYS:H	1.81	0.46
1:B:326:GLU:OE1	1:B:367:ARG:NH1	2.48	0.46
1:C:9:SER:HA	1:C:10:GLY:HA3	1.49	0.46
1:B:120:THR:HG21	3:B:571:HOH:O	2.16	0.46
1:B:305:CYS:CB	1:B:306:PRO:CD	2.93	0.46
1:C:47:PRO:HG2	1:C:429:PRO:HB3	1.98	0.46
1:C:301:LEU:HA	1:C:302:PRO:HD3	1.77	0.46
1:C:161:ARG:HG2	1:C:161:ARG:HH11	1.81	0.46
1:B:330:VAL:CG2	1:B:335:VAL:HG23	2.45	0.45
1:A:212:THR:HG23	1:A:216:ASN:HB2	1.98	0.45
1:A:244:ALA:HB1	1:A:382:LEU:HG	1.98	0.45
1:B:26:LEU:HD21	1:B:66:MET:HE1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:ARG:HH11	1:B:411:ARG:HG2	1.77	0.45
1:C:402:GLN:CD	1:C:402:GLN:H	2.19	0.45
1:C:409:LEU:HD23	1:C:414:ILE:HG12	1.98	0.45
1:A:41:PRO:O	1:A:44:ALA:HB2	2.16	0.45
1:B:245:ASP:O	1:B:372:PRO:HA	2.16	0.45
1:B:439:ARG:HG3	1:B:442:GLN:HG2	1.98	0.45
1:C:325:VAL:O	1:C:329:ARG:HA	2.16	0.45
1:A:439:ARG:HD3	3:A:539:HOH:O	2.16	0.45
1:C:411:ARG:HG2	3:C:562:HOH:O	2.17	0.45
1:B:120:THR:O	1:B:130:LYS:HE3	2.16	0.45
1:B:433:LEU:CD2	1:B:436:HIS:HD2	2.29	0.45
1:C:8:PRO:HG3	1:C:20:TYR:CE2	2.51	0.45
1:C:100:THR:HG21	1:C:216:ASN:HD21	1.81	0.45
1:C:374:ARG:NH1	1:C:383:GLU:OE2	2.41	0.45
1:B:77:ARG:CG	1:B:254:GLN:HG2	2.46	0.45
1:B:372:PRO:HB2	1:B:382:LEU:CD1	2.44	0.45
1:C:8:PRO:HD3	3:C:560:HOH:O	2.12	0.45
1:C:16:PRO:O	1:C:295:ILE:HB	2.17	0.45
1:C:426:HIS:CE1	1:C:428:ASN:O	2.69	0.45
1:B:334:ILE:HD12	1:B:334:ILE:H	1.82	0.45
1:C:161:ARG:HH11	1:C:161:ARG:CG	2.30	0.45
1:C:344:TYR:CD2	1:C:394:LEU:HD21	2.52	0.45
1:B:10:GLY:HA2	1:B:17:ILE:HB	1.99	0.44
1:B:305:CYS:CB	1:B:306:PRO:HD2	2.47	0.44
1:B:411:ARG:CG	1:B:411:ARG:NH1	2.58	0.44
1:C:143:LEU:HG	1:C:192:LEU:HD22	1.99	0.44
1:A:434:PRO:HG2	1:A:436:HIS:H	1.82	0.44
1:B:259:LYS:HA	1:B:283:LEU:CD2	2.47	0.44
1:B:317:TRP:HA	1:B:343:PHE:CE2	2.52	0.44
1:C:15:LEU:HB2	1:C:295:ILE:HD12	1.98	0.44
1:B:334:ILE:CD1	1:B:334:ILE:H	2.30	0.44
1:A:471:GLN:O	1:A:471:GLN:CG	2.66	0.44
1:A:480:ARG:NH1	1:A:482:ARG:H	2.15	0.44
1:B:330:VAL:HG22	1:B:335:VAL:HG22	2.00	0.44
1:A:63:GLN:O	1:A:66:MET:HB3	2.17	0.44
1:B:374:ARG:CG	1:B:377:LYS:CG	2.86	0.44
1:C:474:ILE:HG22	1:C:475:GLU:H	1.83	0.44
1:B:209:LEU:HD12	1:B:209:LEU:HA	1.90	0.44
1:B:389:GLN:HE22	1:B:400:GLY:HA3	1.82	0.44
1:B:391:ILE:HG22	1:B:392:SER:N	2.33	0.44
1:C:169:LYS:HD3	1:C:171:GLU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:SER:O	1:A:469:ALA:HB3	2.18	0.43
1:A:118:LYS:HE2	1:A:134:TRP:CE2	2.53	0.43
1:C:209:LEU:O	1:C:212:THR:HG22	2.18	0.43
1:C:439:ARG:N	1:C:440:PRO:HD2	2.33	0.43
1:A:22:ASP:OD2	1:A:124:TYR:HE1	2.02	0.43
1:B:102:GLU:HA	1:B:103:PRO:HD3	1.87	0.43
1:B:267:ARG:HD3	3:B:527:HOH:O	2.17	0.43
1:C:439:ARG:HD2	1:C:439:ARG:HA	1.92	0.43
1:A:102:GLU:O	1:A:103:PRO:C	2.57	0.43
1:B:101:LEU:HD22	1:B:208:ALA:HB1	2.01	0.43
1:A:89:VAL:O	1:A:93:ILE:HG13	2.17	0.43
1:B:124:TYR:HA	1:B:125:PRO:HA	1.76	0.43
1:B:415:ASP:O	1:B:419:LEU:HG	2.18	0.43
1:B:474:ILE:HG23	3:B:555:HOH:O	2.18	0.43
1:C:317:TRP:HA	1:C:343:PHE:CZ	2.54	0.43
1:B:161:ARG:HH11	1:B:287:LEU:HD12	1.83	0.43
1:C:169:LYS:CD	1:C:185:ARG:HH21	2.31	0.43
1:C:449:GLU:HA	1:C:452:MET:HE2	2.01	0.43
1:A:133:ASP:HB2	1:A:143:LEU:HD22	2.01	0.42
1:A:433:LEU:HD13	1:A:436:HIS:CD2	2.54	0.42
1:B:401:ASP:OD2	1:B:403:PHE:HB2	2.19	0.42
1:C:41:PRO:O	1:C:44:ALA:HB2	2.19	0.42
1:C:77:ARG:HA	1:C:77:ARG:NE	2.34	0.42
1:A:151:ASN:HD21	1:A:200:ARG:HH11	1.66	0.42
1:A:196:ILE:HD12	1:A:196:ILE:C	2.39	0.42
1:B:104:GLN:HB2	1:B:204:PRO:HB3	2.01	0.42
1:B:176:ASP:C	1:B:178:ILE:H	2.22	0.42
1:C:41:PRO:HA	1:C:42:PRO:HD2	1.78	0.42
1:C:411:ARG:HG2	1:C:411:ARG:H	1.59	0.42
1:A:60:PRO:HB2	1:A:64:GLN:HB3	2.01	0.42
1:C:108:THR:HA	1:C:200:ARG:NH2	2.33	0.42
1:A:316:HIS:CE1	1:A:348:GLU:HB3	2.54	0.42
1:C:64:GLN:O	1:C:67:ARG:N	2.53	0.42
1:A:71:LYS:HB2	1:A:72:PRO:HD3	2.01	0.42
1:A:198:ALA:HA	1:A:278:VAL:HG11	2.02	0.42
1:B:21:GLY:HA3	1:B:291:GLY:O	2.19	0.42
1:A:28:THR:O	1:A:50:LEU:HB3	2.20	0.42
1:B:151:ASN:HD21	1:B:200:ARG:HD2	1.85	0.42
1:A:7:ARG:HG3	1:A:8:PRO:CD	2.40	0.42
1:A:35:THR:HG22	1:A:421:THR:HG22	2.02	0.42
1:A:206:CYS:O	1:A:210:LYS:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:ARG:NE	1:B:77:ARG:HA	2.35	0.42
1:B:399:VAL:O	1:B:405:TRP:HA	2.19	0.42
1:A:48:ALA:CB	1:A:184:LYS:HG3	2.49	0.42
1:B:395:ARG:NH1	1:B:395:ARG:CG	2.53	0.42
1:C:332:PRO:O	1:C:335:VAL:HG13	2.20	0.42
1:C:480:ARG:CG	1:C:482:ARG:HG2	2.50	0.42
1:A:449:GLU:OE1	1:A:449:GLU:HA	2.20	0.41
1:B:12:TYR:CE2	1:B:67:ARG:HG2	2.55	0.41
1:B:122:SER:N	1:B:128:LYS:O	2.49	0.41
1:B:341:PHE:HD1	1:B:350:VAL:HG22	1.85	0.41
1:A:216:ASN:HD22	1:A:216:ASN:HA	1.63	0.41
1:B:21:GLY:HA2	1:B:294:LYS:HG3	2.03	0.41
1:B:405:TRP:HH2	3:B:535:HOH:O	2.04	0.41
1:A:129:GLN:O	1:A:132:LYS:HG2	2.20	0.41
1:A:477:VAL:O	1:A:479:PRO:HD3	2.20	0.41
1:B:255:ARG:NH2	1:B:286:SER:OG	2.54	0.41
1:C:316:HIS:NE2	1:C:348:GLU:HB3	2.34	0.41
1:A:31:MET:SD	1:A:422:LYS:HD3	2.61	0.41
1:A:80:LEU:HD12	1:A:80:LEU:HA	1.86	0.41
1:C:109:PHE:HB2	1:C:151:ASN:OD1	2.21	0.41
1:B:34:ARG:CZ	1:B:40:LEU:HD13	2.51	0.41
1:B:85:ILE:HD12	1:B:326:GLU:CG	2.50	0.41
1:B:257:ILE:O	1:B:260:ARG:N	2.54	0.41
1:B:348:GLU:O	1:B:349:VAL:HG23	2.20	0.41
1:B:377:LYS:HE2	1:B:378:GLU:O	2.21	0.41
1:C:124:TYR:HA	1:C:125:PRO:HA	1.74	0.41
1:C:219:ARG:O	1:C:222:MET:HB3	2.20	0.41
1:A:86:LEU:HD23	1:A:86:LEU:HA	1.97	0.41
1:B:439:ARG:O	1:B:443:LEU:HB2	2.20	0.41
1:B:445:ALA:O	1:B:449:GLU:HG2	2.20	0.41
1:C:50:LEU:HB2	1:C:54:ASP:HB2	2.01	0.41
1:A:260:ARG:HD3	1:A:260:ARG:HA	1.91	0.41
1:A:328:THR:O	1:A:329:ARG:HB2	2.20	0.41
1:A:392:SER:HB3	1:A:396:ARG:O	2.21	0.41
1:B:16:PRO:O	1:B:295:ILE:HB	2.21	0.41
1:B:85:ILE:HD12	1:B:326:GLU:HG2	2.02	0.41
1:B:198:ALA:HA	1:B:278:VAL:HG11	2.02	0.41
1:C:13:ALA:HB2	1:C:67:ARG:HG2	2.03	0.41
1:A:30:THR:O	1:A:425:ASN:HA	2.21	0.40
1:A:358:MET:HE3	1:A:384:ARG:HB3	2.02	0.40
1:C:220:VAL:HG22	1:C:344:TYR:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:484:VAL:O	1:C:487:TRP:N	2.55	0.40
1:A:151:ASN:HD21	1:A:200:ARG:NH1	2.19	0.40
1:A:356:LEU:HD21	1:A:361:TYR:CD1	2.55	0.40
1:B:330:VAL:CG2	1:B:335:VAL:CG2	2.99	0.40
1:C:129:GLN:HE21	1:C:129:GLN:HB2	1.68	0.40
1:A:7:ARG:CZ	1:A:7:ARG:N	2.84	0.40
1:B:243:ASP:OD2	1:B:375:ALA:HB1	2.22	0.40
1:B:252:THR:HB	1:B:369:GLY:O	2.20	0.40
1:B:342:SER:O	1:B:348:GLU:HA	2.21	0.40
1:C:97:LEU:O	1:C:98:GLU:C	2.59	0.40
1:A:33:TRP:CD1	1:A:33:TRP:N	2.89	0.40
1:A:64:GLN:NE2	1:A:67:ARG:HB2	2.36	0.40
1:A:255:ARG:HA	1:A:258:LEU:HB2	2.02	0.40
1:B:242:MET:HE2	1:B:242:MET:HB2	1.92	0.40
1:B:89:VAL:HG21	1:B:322:CYS:SG	2.61	0.40
1:B:109:PHE:CD1	1:B:151:ASN:ND2	2.90	0.40
1:C:177:LYS:O	1:C:182:ILE:HA	2.20	0.40
1:C:447:LEU:HD13	1:C:465:VAL:HG21	2.03	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	484/517 (94%)	422 (87%)	48 (10%)	14 (3%)	4	6
1	B	483/517 (93%)	424 (88%)	44 (9%)	15 (3%)	4	6
1	C	483/517 (93%)	413 (86%)	61 (13%)	9 (2%)	8	14
All	All	1450/1551 (94%)	1259 (87%)	153 (11%)	38 (3%)	5	8

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	PRO
1	A	375	ALA
1	A	379	GLU
1	A	381	PRO
1	B	245	ASP
1	B	306	PRO
1	B	307	CYS
1	B	375	ALA
1	B	381	PRO
1	B	401	ASP
1	C	244	ALA
1	C	434	PRO
1	C	455	GLU
1	A	244	ALA
1	A	305	CYS
1	A	433	LEU
1	A	468	GLU
1	B	121	SER
1	B	439	ARG
1	B	470	ALA
1	C	9	SER
1	C	474	ILE
1	A	394	LEU
1	A	434	PRO
1	A	436	HIS
1	A	470	ALA
1	B	177	LYS
1	B	40	LEU
1	B	142	ASP
1	B	471	GLN
1	C	285	PRO
1	A	378	GLU
1	A	439	ARG
1	B	117	ASP
1	B	434	PRO
1	C	10	GLY
1	C	60	PRO
1	C	473	GLY

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	414/440 (94%)	365 (88%)	49 (12%)	5	8
1	B	413/440 (94%)	369 (89%)	44 (11%)	6	11
1	C	413/440 (94%)	358 (87%)	55 (13%)	4	6
All	All	1240/1320 (94%)	1092 (88%)	148 (12%)	5	8

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	27	SER
1	A	34	ARG
1	A	36	SER
1	A	52	SER
1	A	55	GLU
1	A	63	GLN
1	A	77	ARG
1	A	80	LEU
1	A	86	LEU
1	A	129	GLN
1	A	143	LEU
1	A	161	ARG
1	A	174	LYS
1	A	196	ILE
1	A	212	THR
1	A	245	ASP
1	A	268	LEU
1	A	276	ARG
1	A	283	LEU
1	A	298	GLU
1	A	305	CYS
1	A	309	THR
1	A	311	LEU
1	A	313	SER
1	A	319	LEU
1	A	321	LEU
1	A	330	VAL
1	A	331	ASP
1	A	333	ASP

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Mol	Chain	Res	Type
1	A	344	TYR
1	A	377	LYS
1	A	383	GLU
1	A	389	GLN
1	A	392	SER
1	A	411	ARG
1	A	413	SER
1	A	416	ARG
1	A	426	HIS
1	A	432	THR
1	A	439	ARG
1	A	442	GLN
1	A	446	LEU
1	A	456	LYS
1	A	472	SER
1	A	475	GLU
1	A	476	MET
1	A	480	ARG
1	A	490	PHE
1	B	9	SER
1	B	19	ASP
1	B	38	GLU
1	B	55	GLU
1	B	57	VAL
1	B	68	ASP
1	B	74	SER
1	B	77	ARG
1	B	86	LEU
1	B	96	ARG
1	B	97	LEU
1	B	105	LYS
1	B	107	TRP
1	B	119	ASN
1	B	161	ARG
1	B	163	ILE
1	B	209	LEU
1	B	211	GLU
1	B	237	ASN
1	B	287	LEU
1	B	301	LEU
1	B	305	CYS
1	B	309	THR

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Mol	Chain	Res	Type
1	B	312	ASN
1	B	321	LEU
1	B	330	VAL
1	B	331	ASP
1	B	360	LYS
1	B	374	ARG
1	B	377	LYS
1	B	378	GLU
1	B	379	GLU
1	B	389	GLN
1	B	395	ARG
1	B	399	VAL
1	B	402	GLN
1	B	411	ARG
1	B	426	HIS
1	B	439	ARG
1	B	442	GLN
1	B	444	MET
1	B	456	LYS
1	B	488	VAL
1	B	492	THR
1	C	34	ARG
1	C	35	THR
1	C	36	SER
1	C	52	SER
1	C	55	GLU
1	C	57	VAL
1	C	66	MET
1	C	71	LYS
1	C	77	ARG
1	C	86	LEU
1	C	89	VAL
1	C	97	LEU
1	C	105	LYS
1	C	110	LYS
1	C	114	GLU
1	C	128	LYS
1	C	129	GLN
1	C	142	ASP
1	C	143	LEU
1	C	159	SER
1	C	161	ARG

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Mol	Chain	Res	Type
1	C	182	ILE
1	C	196	ILE
1	C	212	THR
1	C	234	ARG
1	C	243	ASP
1	C	247	THR
1	C	268	LEU
1	C	269	SER
1	C	283	LEU
1	C	308	THR
1	C	309	THR
1	C	334	ILE
1	C	335	VAL
1	C	344	TYR
1	C	373	THR
1	C	376	ASP
1	C	383	GLU
1	C	384	ARG
1	C	387	THR
1	C	392	SER
1	C	395	ARG
1	C	396	ARG
1	C	402	GLN
1	C	411	ARG
1	C	413	SER
1	C	426	HIS
1	C	439	ARG
1	C	446	LEU
1	C	471	GLN
1	C	474	ILE
1	C	480	ARG
1	C	484	VAL
1	C	487	TRP
1	C	492	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	64	GLN
1	A	127	HIS
1	A	146	GLN

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Mol	Chain	Res	Type
1	A	151	ASN
1	A	152	ASN
1	A	216	ASN
1	A	254	GLN
1	A	312	ASN
1	A	417	GLN
1	A	426	HIS
1	A	427	GLN
1	A	481	HIS
1	B	69	GLN
1	B	127	HIS
1	B	151	ASN
1	B	152	ASN
1	B	237	ASN
1	B	254	GLN
1	B	312	ASN
1	B	389	GLN
1	B	402	GLN
1	C	69	GLN
1	C	104	GLN
1	C	129	GLN
1	C	146	GLN
1	C	151	ASN
1	C	152	ASN
1	C	237	ASN
1	C	254	GLN
1	C	312	ASN
1	C	402	GLN
1	C	417	GLN
1	C	428	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 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	SO4	A	3	-	4,4,4	0.17	0	6,6,6	0.18	0
2	SO4	B	2	-	4,4,4	0.14	0	6,6,6	0.14	0
2	SO4	B	1	-	4,4,4	0.16	0	6,6,6	0.24	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

WORLDWIDE
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PROTEIN DATA BANK

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	486/517 (94%)	-0.29	11 (2%)	60	69	7, 18, 44, 59	0
1	B	485/517 (93%)	-0.20	11 (2%)	60	69	6, 22, 45, 60	0
1	C	485/517 (93%)	-0.22	11 (2%)	60	69	8, 22, 48, 58	0
All	All	1456/1551 (93%)	-0.24	33 (2%)	60	69	6, 21, 47, 60	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	376	ASP	4.1
1	C	437	ALA	4.0
1	A	376	ASP	3.9
1	C	438	GLN	3.8
1	B	476	MET	3.8
1	A	476	MET	3.6
1	A	438	GLN	3.3
1	B	375	ALA	3.1
1	A	437	ALA	3.1
1	A	375	ALA	3.0
1	B	470	ALA	3.0
1	A	473	GLY	2.9
1	B	438	GLN	2.8
1	C	474	ILE	2.8
1	B	376	ASP	2.7
1	A	380	GLY	2.6
1	C	473	GLY	2.6
1	B	467	LYS	2.6
1	A	377	LYS	2.5
1	B	459	ARG	2.4
1	C	475	GLU	2.4
1	C	39	LYS	2.4
1	A	474	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	471	GLN	2.3
1	C	476	MET	2.3
1	B	475	GLU	2.2
1	A	477	VAL	2.2
1	C	469	ALA	2.1
1	B	57	VAL	2.1
1	C	487	TRP	2.1
1	B	474	ILE	2.0
1	A	374	ARG	2.0
1	C	460	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	B	2	5/5	0.90	0.30	82,82,82,83	0
2	SO4	B	1	5/5	0.97	0.20	47,48,49,49	0
2	SO4	A	3	5/5	0.98	0.12	49,50,50,50	0

6.5 Other polymers ⓘ

There are no such residues in this entry.