Full wwPDB X-ray Structure Validation Report

Aug 9, 2020 – 01:23 PM BST

PDB ID	:	4UYZ
Title	:	STRUCTURE OF THE WNT DEACYLASE NOTUM - CRYSTAL FORM II - 2.8A
Authors	:	Zebisch, M.; Jones, E.Y.
Deposited on	:	2014-09-03
Resolution	:	2.80 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 following versions of software and data (see references) were used in the production of this report:

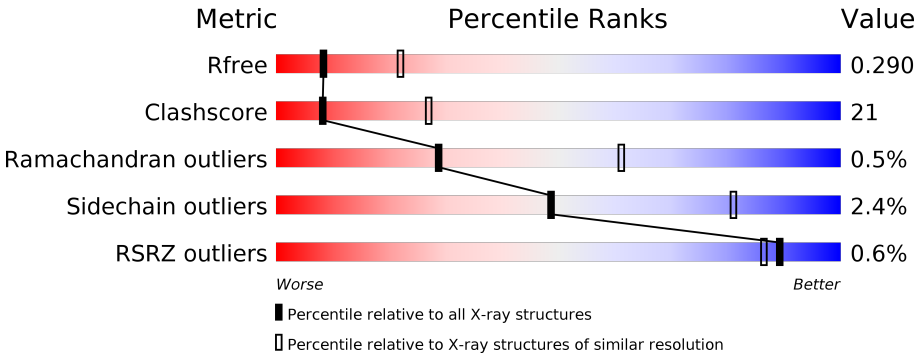
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 on 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	471	50% 22% • 27%
1	B	471	% 49% 21% • 29%
1	C	471	% 42% 28% • 28%
1	D	471	54% 23% • 22%
2	E	10	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	B	1452	X	-	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10991 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 PROTEIN NOTUM HOMOLOG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	345	Total	C	N	O	S	0	0	0
			2730	1728	488	495	19			
1	B	335	Total	C	N	O	S	0	0	0
			2632	1671	468	474	19			
1	C	337	Total	C	N	O	S	0	0	0
			2676	1697	482	478	19			
1	D	369	Total	C	N	O	S	0	0	0
			2888	1828	519	519	22			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	GLU	-	expression tag	UNP Q6P988
A	36	THR	-	expression tag	UNP Q6P988
A	37	GLY	-	expression tag	UNP Q6P988
A	497	GLY	-	expression tag	UNP Q6P988
A	498	THR	-	expression tag	UNP Q6P988
A	499	LYS	-	expression tag	UNP Q6P988
A	500	HIS	-	expression tag	UNP Q6P988
A	501	HIS	-	expression tag	UNP Q6P988
A	502	HIS	-	expression tag	UNP Q6P988
A	503	HIS	-	expression tag	UNP Q6P988
A	504	HIS	-	expression tag	UNP Q6P988
A	505	HIS	-	expression tag	UNP Q6P988
B	35	GLU	-	expression tag	UNP Q6P988
B	36	THR	-	expression tag	UNP Q6P988
B	37	GLY	-	expression tag	UNP Q6P988
B	497	GLY	-	expression tag	UNP Q6P988
B	498	THR	-	expression tag	UNP Q6P988
B	499	LYS	-	expression tag	UNP Q6P988
B	500	HIS	-	expression tag	UNP Q6P988
B	501	HIS	-	expression tag	UNP Q6P988
B	502	HIS	-	expression tag	UNP Q6P988

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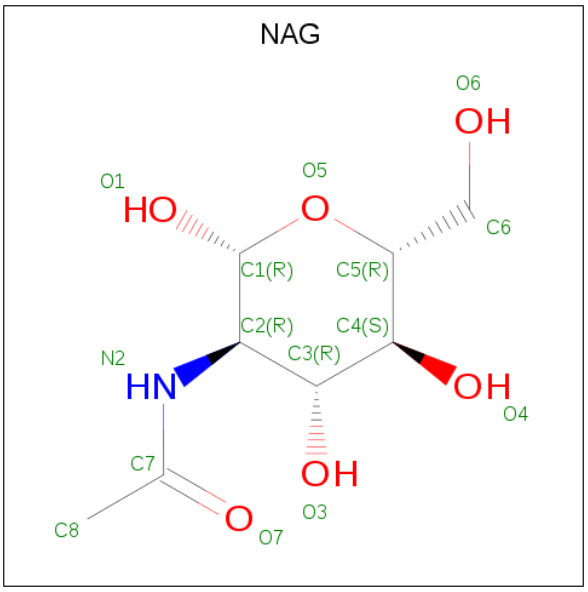
Chain	Residue	Modelled	Actual	Comment	Reference
B	503	HIS	-	expression tag	UNP Q6P988
B	504	HIS	-	expression tag	UNP Q6P988
B	505	HIS	-	expression tag	UNP Q6P988
C	35	GLU	-	expression tag	UNP Q6P988
C	36	THR	-	expression tag	UNP Q6P988
C	37	GLY	-	expression tag	UNP Q6P988
C	497	GLY	-	expression tag	UNP Q6P988
C	498	THR	-	expression tag	UNP Q6P988
C	499	LYS	-	expression tag	UNP Q6P988
C	500	HIS	-	expression tag	UNP Q6P988
C	501	HIS	-	expression tag	UNP Q6P988
C	502	HIS	-	expression tag	UNP Q6P988
C	503	HIS	-	expression tag	UNP Q6P988
C	504	HIS	-	expression tag	UNP Q6P988
C	505	HIS	-	expression tag	UNP Q6P988
D	35	GLU	-	expression tag	UNP Q6P988
D	36	THR	-	expression tag	UNP Q6P988
D	37	GLY	-	expression tag	UNP Q6P988
D	497	GLY	-	expression tag	UNP Q6P988
D	498	THR	-	expression tag	UNP Q6P988
D	499	LYS	-	expression tag	UNP Q6P988
D	500	HIS	-	expression tag	UNP Q6P988
D	501	HIS	-	expression tag	UNP Q6P988
D	502	HIS	-	expression tag	UNP Q6P988
D	503	HIS	-	expression tag	UNP Q6P988
D	504	HIS	-	expression tag	UNP Q6P988
D	505	HIS	-	expression tag	UNP Q6P988

- Molecule 2 is a protein called POLY ALA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	10	50	30	10	10	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

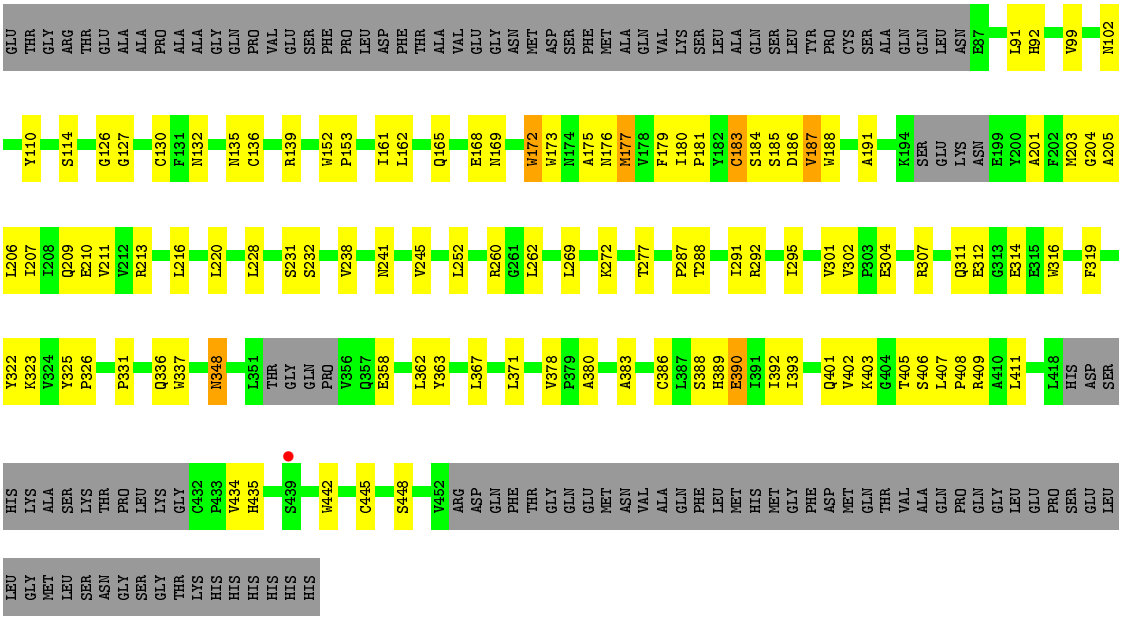
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0

3 Residue-property plots (i)

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

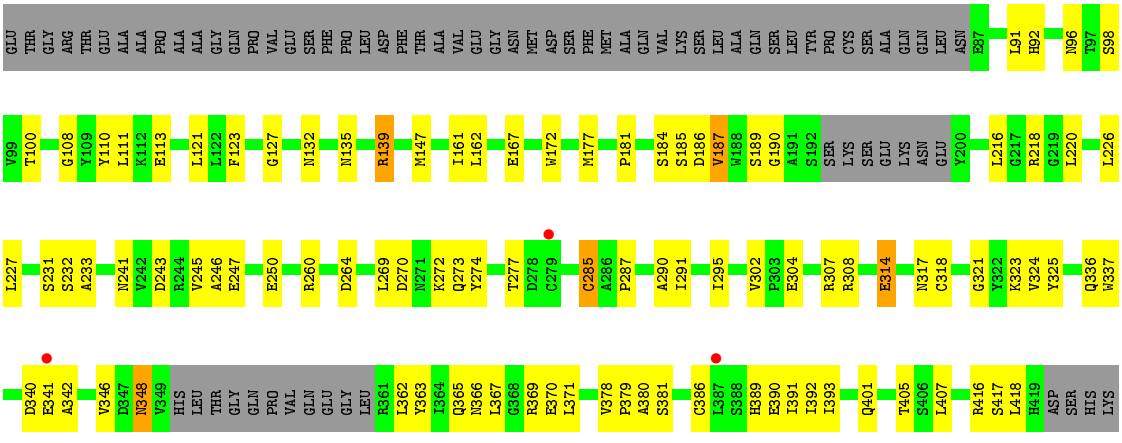
- Molecule 1: PROTEIN NOTUM HOMOLOG

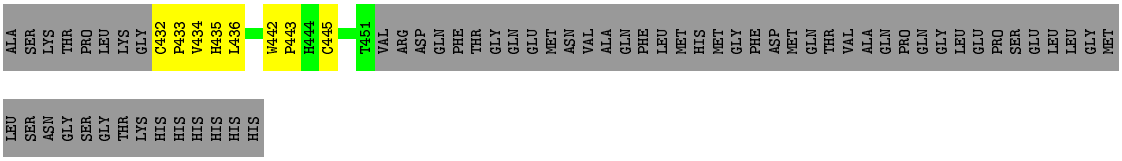
Chain A:



- Molecule 1: PROTEIN NOTUM HOMOLOG

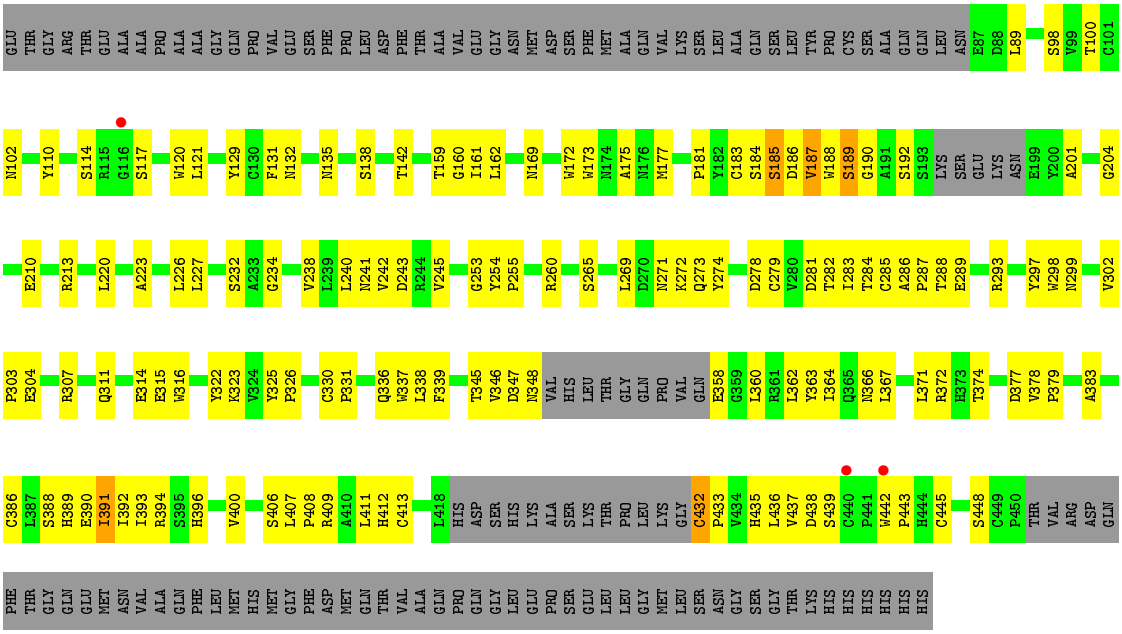
Chain B:





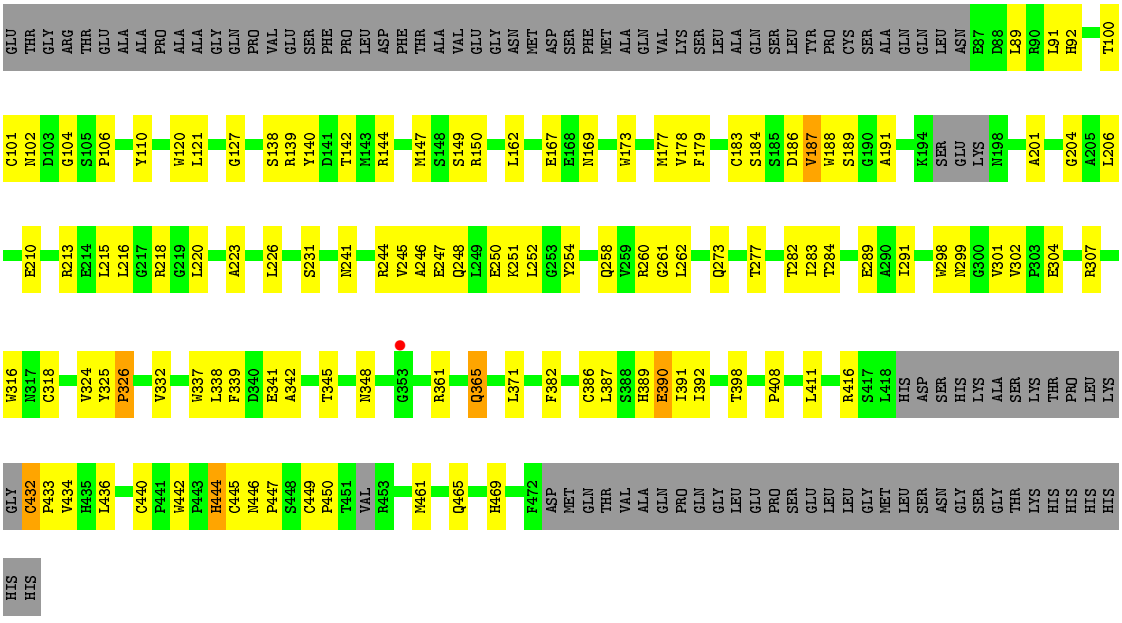
• Molecule 1: PROTEIN NOTUM HOMOLOG

Chain C:

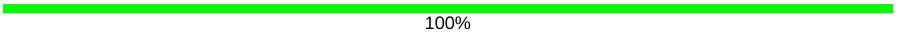


• Molecule 1: PROTEIN NOTUM HOMOLOG

Chain D:



- Molecule 2: POLY ALA

Chain E: 

There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	60.83Å 193.88Å 75.72Å 90.00° 91.88° 90.00°	Depositor
Resolution (Å)	96.94 – 2.80 58.01 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.9 (96.94-2.80) 88.9 (58.01-2.80)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.248 , 0.293 0.244 , 0.290	Depositor DCC
R_{free} test set	1143 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å^2)	38.9	Xtriage
Anisotropy	0.876	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 21.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.069 for h,-k,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	10991	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: NAG, 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	0.43	0/2800	0.64	1/3810 (0.0%)
1	B	0.43	0/2703	0.62	0/3683
1	C	0.42	0/2747	0.62	0/3735
1	D	0.41	0/2963	0.63	0/4029
2	E	0.39	0/49	0.41	0/67
All	All	0.42	0/11262	0.63	1/15324 (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	A	183	CYS	CA-CB-SG	-5.13	104.77	114.00

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	2730	0	2615	83	0
1	B	2632	0	2494	108	0
1	C	2676	0	2565	144	0
1	D	2888	0	2739	118	0
2	E	50	0	49	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	14	0	13	0	0
4	B	1	0	0	0	0
All	All	10991	0	10475	451	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 21.

All (451) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:440:CYS:HB3	1:D:445:CYS:SG	1.57	1.42
1:B:132:ASN:OD1	1:B:135:ASN:HB2	1.32	1.24
1:C:273:GLN:NE2	1:C:286:ALA:HB2	1.54	1.19
1:D:210:GLU:OE2	1:D:213:ARG:NE	1.77	1.18
1:B:416:ARG:NH2	1:B:432:CYS:SG	2.18	1.17
1:D:440:CYS:CB	1:D:445:CYS:SG	2.33	1.16
1:C:271:ASN:HD21	1:C:347:ASP:CG	1.46	1.16
1:C:273:GLN:HE21	1:C:286:ALA:CB	1.59	1.14
1:D:144:ARG:HH21	1:D:150:ARG:HD3	1.07	1.14
1:C:210:GLU:OE2	1:C:213:ARG:NH2	1.81	1.13
1:D:144:ARG:NH2	1:D:150:ARG:HD3	1.64	1.12
1:C:132:ASN:ND2	1:C:135:ASN:OD1	1.82	1.10
1:C:132:ASN:CG	1:C:135:ASN:OD1	1.91	1.09
1:D:444:HIS:CD2	1:D:449:CYS:SG	2.47	1.07
1:B:162:LEU:HA	1:B:177:MET:CE	1.86	1.06
1:B:273:GLN:HE22	1:B:277:THR:HG22	1.21	1.05
1:C:271:ASN:ND2	1:C:347:ASP:OD2	1.91	1.04
1:D:144:ARG:HH22	1:D:150:ARG:HB2	0.92	1.03
1:C:273:GLN:NE2	1:C:286:ALA:CB	2.20	1.02
1:D:144:ARG:NH2	1:D:150:ARG:HB2	1.76	1.01
1:B:433:PRO:O	1:B:436:LEU:HD21	1.61	1.01
1:C:287:PRO:HD3	1:C:346:VAL:HG12	1.40	1.00
1:C:210:GLU:OE2	1:C:213:ARG:CZ	2.10	0.99
1:B:162:LEU:HA	1:B:177:MET:HE3	1.44	0.99
1:C:413:CYS:SG	1:C:432:CYS:N	2.36	0.98
1:B:287:PRO:HD3	1:B:346:VAL:HG22	1.46	0.98
1:B:139:ARG:NH1	1:B:185:SER:OG	1.98	0.97
1:D:144:ARG:HH22	1:D:150:ARG:CB	1.78	0.96
1:D:162:LEU:HA	1:D:177:MET:HE3	1.49	0.94
1:C:339:PHE:CD2	1:C:443:PRO:HG3	2.02	0.93
1:A:311:GLN:HG2	1:A:312:GLU:N	1.83	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:GLU:O	1:C:293:ARG:HG3	1.71	0.90
1:D:140:TYR:CA	1:D:147:MET:HE3	2.02	0.89
1:D:304:GLU:HG3	1:D:307:ARG:HH21	1.37	0.89
1:C:288:THR:HG23	1:C:316:TRP:CZ3	2.07	0.88
1:C:172:TRP:HZ3	1:C:411:LEU:HD23	1.38	0.87
1:A:311:GLN:HG2	1:A:312:GLU:H	1.38	0.85
1:D:162:LEU:HA	1:D:177:MET:CE	2.07	0.85
1:B:132:ASN:OD1	1:B:135:ASN:CB	2.21	0.85
1:C:304:GLU:HG3	1:C:307:ARG:HH21	1.40	0.85
1:B:435:HIS:C	1:B:436:LEU:HD23	1.96	0.85
1:C:186:ASP:O	1:C:189:SER:OG	1.94	0.84
1:A:184:SER:OG	1:A:186:ASP:OD1	1.95	0.84
1:D:440:CYS:CB	1:D:445:CYS:HG	1.85	0.84
1:B:186:ASP:O	1:B:189:SER:OG	1.95	0.84
1:C:132:ASN:OD1	1:C:135:ASN:OD1	1.94	0.84
1:D:138:SER:O	1:D:142:THR:HG22	1.78	0.83
1:D:291:ILE:HG22	1:D:316:TRP:HB2	1.59	0.83
1:B:273:GLN:NE2	1:B:277:THR:HG22	1.92	0.83
1:C:271:ASN:ND2	1:C:347:ASP:CG	2.28	0.82
1:D:444:HIS:NE2	1:D:449:CYS:SG	2.53	0.82
1:D:186:ASP:O	1:D:189:SER:OG	1.98	0.82
1:A:231:SER:HB3	1:A:390:GLU:HG2	1.60	0.82
1:C:271:ASN:ND2	1:C:347:ASP:OD1	2.14	0.81
1:C:432:CYS:HB2	1:C:433:PRO:HD2	1.63	0.80
1:B:162:LEU:CA	1:B:177:MET:CE	2.59	0.80
1:B:272:LYS:O	1:B:363:TYR:OH	1.98	0.80
1:B:366:ASN:O	1:B:370:GLU:HG3	1.81	0.80
1:C:210:GLU:OE2	1:C:213:ARG:NE	2.15	0.79
1:B:186:ASP:OD2	1:B:190:GLY:N	2.16	0.79
1:D:416:ARG:NH2	1:D:432:CYS:N	2.31	0.79
1:C:273:GLN:HE21	1:C:286:ALA:CA	1.95	0.78
1:D:398:THR:HG22	1:D:408:PRO:HG2	1.66	0.78
1:B:269:LEU:HD11	1:B:371:LEU:HG	1.64	0.78
1:C:273:GLN:NE2	1:C:286:ALA:CA	2.47	0.78
1:D:416:ARG:HH21	1:D:432:CYS:N	1.83	0.77
1:C:210:GLU:CD	1:C:213:ARG:HH21	1.88	0.76
1:C:162:LEU:HD12	1:C:393:ILE:HD11	1.67	0.76
1:D:140:TYR:N	1:D:147:MET:CE	2.50	0.75
1:A:409:ARG:HB2	1:B:167:GLU:OE2	1.86	0.75
1:C:281:ASP:O	1:C:284:THR:OG1	2.04	0.74
1:C:287:PRO:HD3	1:C:346:VAL:CG1	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:PHE:HD2	1:C:443:PRO:HG3	1.48	0.74
1:A:127:GLY:O	1:A:139:ARG:NH2	2.21	0.74
1:B:162:LEU:HD12	1:B:393:ILE:HD11	1.69	0.73
1:B:435:HIS:O	1:B:436:LEU:HD23	1.87	0.73
1:C:184:SER:HB3	1:C:186:ASP:OD1	1.88	0.73
1:D:139:ARG:HG2	1:D:147:MET:CE	2.19	0.72
1:B:391:ILE:HD13	1:B:407:LEU:CD2	2.20	0.72
1:C:339:PHE:HE2	1:C:443:PRO:CD	2.02	0.72
1:D:140:TYR:CB	1:D:147:MET:HE3	2.19	0.72
1:C:311:GLN:O	1:C:314:GLU:HB2	1.89	0.71
1:D:144:ARG:NH2	1:D:150:ARG:CD	2.50	0.71
1:B:380:ALA:HA	1:B:434:VAL:HG12	1.71	0.71
1:D:120:TRP:CD1	1:D:223:ALA:HB2	2.25	0.71
1:B:342:ALA:O	1:B:346:VAL:HG12	1.90	0.71
1:B:260:ARG:HD3	1:B:418:LEU:HD13	1.74	0.70
1:C:186:ASP:OD2	1:C:190:GLY:N	2.24	0.70
1:A:325:TYR:N	1:A:326:PRO:HD2	2.07	0.69
1:B:273:GLN:HE22	1:B:277:THR:CG2	2.03	0.69
1:D:140:TYR:N	1:D:147:MET:HE3	2.07	0.69
1:C:172:TRP:CZ3	1:C:411:LEU:HD23	2.27	0.69
1:D:184:SER:HB3	1:D:186:ASP:CG	2.13	0.69
1:D:244:ARG:O	1:D:248:GLN:HG3	1.91	0.69
1:A:175:ALA:O	1:A:177:MET:CE	2.40	0.69
1:A:205:ALA:O	1:A:209:GLN:HG3	1.93	0.69
1:C:121:LEU:HD21	1:C:227:LEU:HD23	1.75	0.68
1:D:162:LEU:CA	1:D:177:MET:HE3	2.24	0.68
1:B:162:LEU:HA	1:B:177:MET:HE2	1.72	0.68
1:C:339:PHE:CE2	1:C:443:PRO:HD3	2.29	0.68
1:B:139:ARG:HB3	1:B:147:MET:SD	2.33	0.67
1:A:269:LEU:HD11	1:A:371:LEU:HD12	1.77	0.67
1:D:140:TYR:HB2	1:D:147:MET:HE3	1.75	0.67
1:A:216:LEU:HA	1:A:220:LEU:HB3	1.76	0.67
1:A:389:HIS:O	1:A:390:GLU:HB2	1.95	0.66
1:C:273:GLN:HB3	1:C:347:ASP:O	1.96	0.66
1:D:100:THR:HG22	1:D:101:CYS:O	1.94	0.66
1:B:162:LEU:C	1:B:177:MET:CE	2.65	0.66
1:B:243:ASP:O	1:B:247:GLU:HG3	1.96	0.65
1:D:139:ARG:HG2	1:D:147:MET:HE2	1.76	0.65
1:B:161:ILE:HD11	1:B:172:TRP:CE3	2.31	0.65
1:C:400:VAL:HA	1:C:448:SER:HB3	1.78	0.65
1:C:438:ASP:OD1	1:C:439:SER:N	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:ILE:O	1:B:295:ILE:HG22	1.97	0.65
1:D:100:THR:CG2	1:D:104:GLY:HA2	2.26	0.65
1:C:220:LEU:HD11	1:C:226:LEU:HD12	1.78	0.65
1:C:339:PHE:CE2	1:C:443:PRO:CD	2.80	0.65
1:C:273:GLN:NE2	1:C:286:ALA:HA	2.12	0.65
1:A:162:LEU:HD23	1:A:177:MET:HG2	1.78	0.64
1:D:140:TYR:CA	1:D:147:MET:CE	2.74	0.64
1:D:318:CYS:O	1:D:324:VAL:HG21	1.97	0.64
1:C:121:LEU:HD23	1:C:227:LEU:HB3	1.80	0.64
1:B:184:SER:OG	1:B:186:ASP:OD1	2.10	0.64
1:B:391:ILE:HD13	1:B:407:LEU:HD22	1.80	0.64
1:A:367:LEU:O	1:A:371:LEU:HD13	1.98	0.63
1:C:121:LEU:HD12	1:C:177:MET:CE	2.28	0.63
1:C:121:LEU:HD12	1:C:177:MET:HE2	1.81	0.63
1:D:184:SER:CB	1:D:186:ASP:OD1	2.46	0.63
1:A:337:TRP:CE3	1:A:386:CYS:HB2	2.34	0.63
1:A:295:ILE:CD1	1:A:316:TRP:HA	2.30	0.62
1:C:364:ILE:HD13	1:C:364:ILE:N	2.15	0.62
1:A:162:LEU:HD12	1:A:393:ILE:CD1	2.29	0.62
1:D:342:ALA:HB2	1:D:389:HIS:CE1	2.34	0.62
1:B:401:GLN:HA	1:B:405:THR:O	1.98	0.62
1:C:409:ARG:HG2	1:D:167:GLU:OE2	2.00	0.62
1:B:162:LEU:O	1:B:177:MET:HE2	2.00	0.61
1:A:287:PRO:O	1:A:291:ILE:HG12	2.00	0.61
1:C:272:LYS:O	1:C:363:TYR:OH	2.18	0.61
1:A:367:LEU:HD23	1:A:367:LEU:C	2.21	0.61
1:A:241:ASN:O	1:A:245:VAL:HG23	2.01	0.61
1:A:91:LEU:HB2	1:A:110:TYR:CE1	2.35	0.61
1:A:277:THR:HG21	1:A:348:ASN:OD1	2.01	0.60
1:D:461:MET:HE2	1:D:465:GLN:CB	2.31	0.60
1:C:242:VAL:HG13	1:C:243:ASP:N	2.15	0.60
1:C:339:PHE:HE2	1:C:443:PRO:HD3	1.64	0.60
1:D:140:TYR:HA	1:D:147:MET:HE3	1.81	0.60
1:D:100:THR:HG21	1:D:104:GLY:HA2	1.82	0.60
1:D:231:SER:HB3	1:D:390:GLU:HG2	1.83	0.60
1:B:273:GLN:HE21	1:B:348:ASN:HB2	1.65	0.60
1:C:339:PHE:CE2	1:C:443:PRO:HG3	2.37	0.60
1:B:162:LEU:CA	1:B:177:MET:HE2	2.30	0.59
1:D:102:ASN:ND2	1:D:201:ALA:O	2.35	0.59
1:B:348:ASN:ND2	1:B:348:ASN:O	2.29	0.59
1:C:325:TYR:HB3	1:C:326:PRO:HD3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:LEU:HD12	1:A:393:ILE:HD12	1.83	0.59
1:D:337:TRP:HZ2	1:D:391:ILE:HD13	1.68	0.59
1:A:402:VAL:HG12	1:A:403:LYS:HG3	1.84	0.59
1:C:315:GLU:OE1	1:C:315:GLU:N	2.35	0.59
1:D:187:VAL:O	1:D:187:VAL:HG12	2.03	0.59
1:D:283:ILE:HG23	1:D:345:THR:CG2	2.32	0.59
1:C:432:CYS:HB2	1:C:433:PRO:CD	2.30	0.59
1:C:232:SER:HA	1:C:265:SER:O	2.03	0.59
1:C:391:ILE:HG23	1:C:392:ILE:N	2.17	0.58
1:D:432:CYS:HB2	1:D:433:PRO:HD2	1.83	0.58
1:A:191:ALA:HB2	1:A:301:VAL:CG2	2.33	0.58
1:A:311:GLN:CG	1:A:312:GLU:H	2.14	0.58
1:B:127:GLY:O	1:B:139:ARG:NH2	2.36	0.58
1:D:184:SER:HB2	1:D:186:ASP:OD1	2.03	0.58
1:D:210:GLU:OE2	1:D:213:ARG:CD	2.49	0.58
1:A:161:ILE:O	1:A:169:ASN:ND2	2.37	0.58
1:C:186:ASP:OD2	1:C:190:GLY:HA3	2.04	0.58
1:C:120:TRP:CD1	1:C:223:ALA:HB2	2.39	0.58
1:B:161:ILE:HD11	1:B:172:TRP:CZ3	2.39	0.58
1:B:274:TYR:HD1	1:B:363:TYR:CD2	2.21	0.57
1:C:367:LEU:C	1:C:367:LEU:HD23	2.25	0.57
1:D:337:TRP:CZ2	1:D:391:ILE:HD13	2.39	0.57
1:C:406:SER:HB3	1:C:408:PRO:HD2	1.86	0.57
1:B:216:LEU:HD23	1:B:220:LEU:HD23	1.86	0.57
1:D:140:TYR:HA	1:D:147:MET:CE	2.34	0.57
1:B:314:GLU:HG3	1:B:317:ASN:HD21	1.70	0.56
1:A:175:ALA:O	1:A:177:MET:HE2	2.04	0.56
1:C:273:GLN:HE21	1:C:286:ALA:HA	1.65	0.56
1:C:188:TRP:HA	1:C:204:GLY:HA3	1.86	0.56
1:B:287:PRO:O	1:B:291:ILE:HG12	2.05	0.56
1:C:184:SER:O	1:C:185:SER:HB2	2.04	0.56
1:C:377:ASP:OD1	1:C:377:ASP:N	2.39	0.56
1:B:391:ILE:HD13	1:B:407:LEU:HD23	1.87	0.56
1:A:311:GLN:CG	1:A:312:GLU:N	2.62	0.56
1:A:304:GLU:HA	1:A:307:ARG:HB2	1.88	0.56
1:A:295:ILE:HD11	1:A:316:TRP:HA	1.87	0.55
1:C:260:ARG:HG2	1:C:331:PRO:HG2	1.87	0.55
1:C:102:ASN:ND2	1:C:201:ALA:O	2.39	0.55
1:D:461:MET:HE1	1:D:469:HIS:HD2	1.71	0.55
1:A:126:GLY:HA3	1:A:232:SER:HB3	1.88	0.55
1:D:184:SER:HB3	1:D:186:ASP:OD1	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:LEU:CA	1:D:177:MET:CE	2.81	0.55
1:B:186:ASP:OD2	1:B:190:GLY:CA	2.56	0.54
1:C:186:ASP:OD2	1:C:190:GLY:CA	2.56	0.54
1:C:187:VAL:O	1:C:187:VAL:HG12	2.07	0.54
1:A:191:ALA:HB2	1:A:301:VAL:HG22	1.89	0.54
1:A:152:TRP:CZ2	1:A:181:PRO:HB2	2.43	0.54
1:A:358:GLU:O	1:A:362:LEU:HD13	2.07	0.54
1:B:442:TRP:O	1:B:445:CYS:SG	2.66	0.54
1:B:187:VAL:HG12	1:B:187:VAL:O	2.09	0.53
1:B:365:GLN:O	1:B:369:ARG:HG3	2.08	0.53
1:C:132:ASN:OD1	1:C:135:ASN:CG	2.47	0.53
1:C:442:TRP:O	1:C:445:CYS:SG	2.66	0.53
1:D:461:MET:CE	1:D:469:HIS:CD2	2.92	0.53
1:D:461:MET:HE1	1:D:469:HIS:CD2	2.44	0.53
1:B:162:LEU:C	1:B:177:MET:HE2	2.28	0.53
1:B:340:ASP:OD1	1:B:389:HIS:ND1	2.40	0.53
1:C:254:TYR:N	1:C:255:PRO:HD3	2.23	0.53
1:A:228:LEU:HG	1:A:238:VAL:HG22	1.89	0.53
1:A:442:TRP:O	1:A:445:CYS:SG	2.66	0.53
1:B:337:TRP:CE3	1:B:386:CYS:HB2	2.44	0.53
1:A:367:LEU:HD23	1:A:367:LEU:O	2.09	0.53
1:C:389:HIS:O	1:C:390:GLU:HB2	2.08	0.53
1:D:186:ASP:OD2	1:D:204:GLY:N	2.41	0.53
1:A:260:ARG:HG2	1:A:331:PRO:HG2	1.91	0.53
1:B:220:LEU:HD11	1:B:226:LEU:HD12	1.90	0.53
1:C:407:LEU:HD12	1:C:407:LEU:O	2.09	0.53
1:B:260:ARG:CD	1:B:418:LEU:HD13	2.39	0.52
1:C:98:SER:O	1:C:100:THR:HG23	2.10	0.52
1:D:442:TRP:O	1:D:445:CYS:SG	2.67	0.52
1:C:169:ASN:O	1:C:173:TRP:HB3	2.09	0.52
1:D:169:ASN:HB3	1:D:173:TRP:HB3	1.92	0.52
1:B:121:LEU:HD13	1:B:227:LEU:HD23	1.92	0.52
1:C:210:GLU:CD	1:C:213:ARG:NH2	2.50	0.52
1:D:92:HIS:NE2	1:D:218:ARG:NH1	2.58	0.52
1:C:337:TRP:CZ3	1:C:386:CYS:HB2	2.45	0.52
1:C:358:GLU:O	1:C:362:LEU:HG	2.09	0.52
1:A:207:ILE:O	1:A:211:VAL:HG23	2.09	0.52
1:B:321:GLY:HA2	1:B:324:VAL:HG12	1.92	0.52
1:B:321:GLY:HA2	1:B:324:VAL:CG1	2.40	0.52
1:A:187:VAL:HG12	1:A:187:VAL:O	2.10	0.51
1:C:432:CYS:CB	1:C:433:PRO:HD2	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:ASP:OD2	1:B:190:GLY:HA3	2.10	0.51
1:B:231:SER:HA	1:B:264:ASP:O	2.10	0.51
1:C:121:LEU:CD2	1:C:227:LEU:HD23	2.41	0.51
1:C:242:VAL:CG1	1:C:243:ASP:N	2.73	0.51
1:B:274:TYR:CD1	1:B:363:TYR:CD2	2.98	0.51
1:D:139:ARG:HG2	1:D:147:MET:HE1	1.93	0.51
1:D:298:TRP:O	1:D:299:ASN:HB2	2.10	0.51
1:B:91:LEU:HB2	1:B:110:TYR:CE2	2.46	0.51
1:B:162:LEU:HD12	1:B:393:ILE:CD1	2.40	0.51
1:D:241:ASN:O	1:D:245:VAL:HG23	2.11	0.51
1:D:342:ALA:CB	1:D:389:HIS:CE1	2.94	0.50
1:C:172:TRP:CZ3	1:C:411:LEU:HB3	2.47	0.50
1:C:435:HIS:C	1:C:436:LEU:HD22	2.31	0.50
1:D:139:ARG:CB	1:D:147:MET:HE1	2.41	0.50
1:D:341:GLU:HB2	1:D:389:HIS:HB2	1.94	0.50
1:B:270:ASP:OD1	1:B:270:ASP:N	2.35	0.50
1:D:318:CYS:HA	1:D:324:VAL:HG22	1.93	0.50
1:D:391:ILE:HG23	1:D:392:ILE:N	2.27	0.50
1:B:184:SER:O	1:B:185:SER:HB2	2.11	0.50
1:D:139:ARG:HB3	1:D:147:MET:HE1	1.93	0.50
1:B:391:ILE:HG23	1:B:392:ILE:N	2.27	0.50
1:C:138:SER:O	1:C:142:THR:HG22	2.11	0.50
1:D:277:THR:HB	1:D:348:ASN:ND2	2.26	0.50
1:B:321:GLY:CA	1:B:324:VAL:HG12	2.42	0.50
1:C:367:LEU:HD23	1:C:367:LEU:O	2.12	0.49
1:B:389:HIS:O	1:B:390:GLU:HB2	2.12	0.49
1:C:304:GLU:HG3	1:C:307:ARG:NH2	2.19	0.49
1:C:337:TRP:CD1	1:C:388:SER:O	2.65	0.49
1:C:339:PHE:HE2	1:C:443:PRO:N	2.10	0.49
1:C:161:ILE:O	1:C:169:ASN:ND2	2.46	0.49
1:B:270:ASP:OD2	1:B:323:LYS:NZ	2.44	0.49
1:B:121:LEU:HD12	1:B:227:LEU:O	2.13	0.49
1:D:220:LEU:HD11	1:D:226:LEU:HD12	1.94	0.49
1:A:272:LYS:O	1:A:363:TYR:OH	2.23	0.49
1:C:131:PHE:O	1:C:297:TYR:CD2	2.66	0.49
1:C:339:PHE:CE2	1:C:443:PRO:CG	2.96	0.49
1:B:139:ARG:HH11	1:B:185:SER:HG	1.56	0.49
1:C:241:ASN:O	1:C:245:VAL:HG23	2.12	0.49
1:D:289:GLU:HA	1:D:289:GLU:OE1	2.11	0.49
1:C:302:VAL:O	1:C:307:ARG:NH2	2.46	0.49
1:B:442:TRP:HD1	1:B:443:PRO:O	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:ILE:CG2	1:C:392:ILE:N	2.76	0.48
1:D:144:ARG:NH2	1:D:150:ARG:CB	2.55	0.48
1:B:435:HIS:O	1:B:436:LEU:CD2	2.61	0.48
1:C:253:GLY:C	1:C:255:PRO:HD3	2.34	0.48
1:D:273:GLN:HE22	1:D:277:THR:HG22	1.78	0.48
1:A:380:ALA:HA	1:A:434:VAL:HG12	1.95	0.48
1:C:102:ASN:OD1	1:C:185:SER:HB2	2.13	0.48
1:C:274:TYR:CE2	1:C:360:LEU:HD13	2.48	0.48
1:A:186:ASP:O	1:A:187:VAL:HB	2.13	0.48
1:A:392:ILE:HD13	1:A:407:LEU:HD21	1.96	0.48
1:B:314:GLU:HG3	1:B:317:ASN:ND2	2.28	0.48
1:C:269:LEU:HD21	1:C:374:THR:HG21	1.95	0.48
1:C:184:SER:CB	1:C:186:ASP:OD1	2.58	0.48
1:D:382:PHE:HA	1:D:436:LEU:O	2.14	0.48
1:A:102:ASN:ND2	1:A:201:ALA:O	2.47	0.48
1:B:232:SER:OG	1:B:233:ALA:N	2.46	0.48
1:D:361:ARG:O	1:D:365:GLN:HG2	2.14	0.48
1:C:121:LEU:HB2	1:C:177:MET:HE2	1.95	0.47
1:C:394:ARG:CG	1:C:396:HIS:NE2	2.76	0.47
1:D:291:ILE:CG2	1:D:316:TRP:HB2	2.40	0.47
1:A:99:VAL:HG21	1:A:210:GLU:CG	2.44	0.47
1:B:216:LEU:CD2	1:B:220:LEU:HD23	2.44	0.47
1:C:192:SER:HB2	1:C:299:ASN:HB2	1.95	0.47
1:A:187:VAL:O	1:A:188:TRP:HB2	2.15	0.47
1:C:175:ALA:HB3	1:C:177:MET:CE	2.45	0.47
1:A:130:CYS:SG	1:A:136:CYS:N	2.87	0.47
1:A:188:TRP:HA	1:A:204:GLY:HA3	1.97	0.47
1:A:406:SER:HB3	1:A:408:PRO:HD2	1.95	0.47
1:D:261:GLY:HA3	1:D:332:VAL:HG22	1.97	0.47
1:B:393:ILE:HD12	1:B:393:ILE:HA	1.75	0.47
1:B:325:TYR:CE2	1:B:378:VAL:HG13	2.50	0.47
1:C:336:GLN:HG3	1:C:337:TRP:O	2.14	0.47
1:D:186:ASP:O	1:D:187:VAL:HB	2.14	0.47
1:D:461:MET:CE	1:D:469:HIS:HD2	2.28	0.47
1:B:362:LEU:O	1:B:366:ASN:HB2	2.15	0.46
1:B:442:TRP:CD1	1:B:443:PRO:O	2.69	0.46
1:C:159:THR:HG23	1:C:393:ILE:HG13	1.97	0.46
1:B:123:PHE:HE1	1:B:392:ILE:HD11	1.78	0.46
1:D:139:ARG:CG	1:D:147:MET:HE1	2.45	0.46
1:D:162:LEU:C	1:D:177:MET:CE	2.83	0.46
1:B:336:GLN:NE2	1:B:340:ASP:OD2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:GLU:HB2	1:B:389:HIS:HB2	1.96	0.46
1:D:244:ARG:O	1:D:247:GLU:HB3	2.15	0.46
1:B:96:ASN:OD1	1:B:98:SER:OG	2.32	0.46
1:A:172:TRP:CZ3	1:A:411:LEU:HB3	2.51	0.46
1:A:169:ASN:HB3	1:A:173:TRP:HB3	1.96	0.46
1:A:99:VAL:HG21	1:A:210:GLU:HG3	1.98	0.46
1:C:383:ALA:HB3	1:C:437:VAL:HG13	1.98	0.46
1:D:283:ILE:HG23	1:D:345:THR:HG22	1.98	0.46
1:B:162:LEU:O	1:B:177:MET:CE	2.62	0.46
1:C:234:GLY:O	1:C:238:VAL:HG23	2.15	0.46
1:C:363:TYR:O	1:C:367:LEU:N	2.48	0.46
1:D:191:ALA:HA	1:D:206:LEU:HG	1.97	0.46
1:A:337:TRP:CD1	1:A:388:SER:O	2.68	0.46
1:C:406:SER:O	1:C:409:ARG:HB2	2.16	0.45
1:D:220:LEU:O	1:D:220:LEU:HD12	2.16	0.45
1:D:277:THR:HG21	1:D:284:THR:HB	1.98	0.45
1:D:389:HIS:O	1:D:390:GLU:HB2	2.17	0.45
1:A:203:MET:HE3	1:A:206:LEU:HD12	1.98	0.45
1:B:246:ALA:O	1:B:250:GLU:HG3	2.15	0.45
1:D:91:LEU:HB2	1:D:110:TYR:CE2	2.51	0.45
1:B:161:ILE:O	1:B:177:MET:HE3	2.16	0.45
1:C:337:TRP:CE3	1:C:386:CYS:HB2	2.51	0.45
1:A:213:ARG:HG2	1:A:252:LEU:HD11	1.99	0.45
1:D:106:PRO:O	1:D:149:SER:CB	2.64	0.45
1:B:348:ASN:C	1:B:348:ASN:HD22	2.15	0.45
1:C:347:ASP:O	1:C:348:ASN:HB3	2.17	0.45
1:D:110:TYR:HB2	1:D:179:PHE:HB3	1.99	0.45
1:D:89:LEU:HD21	1:D:177:MET:HB2	1.99	0.45
1:D:248:GLN:HA	1:D:251:LYS:HE3	1.99	0.45
1:D:446:ASN:OD1	1:D:447:PRO:HD2	2.17	0.45
1:A:114:SER:N	1:A:176:ASN:OD1	2.48	0.44
1:B:162:LEU:C	1:B:177:MET:HE1	2.37	0.44
1:B:285:CYS:HB3	1:B:290:ALA:HB2	2.00	0.44
1:C:240:LEU:HD23	1:C:303:PRO:HD2	1.98	0.44
1:C:288:THR:CG2	1:C:316:TRP:CZ3	2.93	0.44
1:C:394:ARG:HG3	1:C:396:HIS:NE2	2.32	0.44
1:D:291:ILE:HG22	1:D:316:TRP:CB	2.40	0.44
1:B:216:LEU:HD23	1:B:220:LEU:HB3	1.97	0.44
1:B:241:ASN:O	1:B:245:VAL:HG23	2.17	0.44
1:C:271:ASN:OD1	1:C:347:ASP:OD1	2.36	0.44
1:C:271:ASN:CG	1:C:347:ASP:OD1	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:GLY:HA3	1:C:392:ILE:O	2.17	0.44
1:A:407:LEU:HB3	1:A:408:PRO:HD3	2.00	0.44
1:C:409:ARG:O	1:C:412:HIS:N	2.51	0.44
1:D:213:ARG:HA	1:D:216:LEU:HD12	2.00	0.44
1:C:102:ASN:ND2	1:C:184:SER:O	2.48	0.44
1:A:191:ALA:HB2	1:A:301:VAL:HG21	1.99	0.44
1:A:262:LEU:HD22	1:A:411:LEU:HD21	1.98	0.44
1:B:401:GLN:CA	1:B:405:THR:O	2.63	0.44
1:A:295:ILE:HD11	1:A:319:PHE:CE1	2.53	0.44
1:B:98:SER:O	1:B:100:THR:HG23	2.17	0.44
1:B:378:VAL:HA	1:B:379:PRO:HD3	1.88	0.44
1:A:322:TYR:OH	1:A:323:LYS:HE3	2.17	0.44
1:D:188:TRP:HA	1:D:204:GLY:HA3	2.00	0.44
1:D:338:LEU:O	1:D:371:LEU:HD12	2.17	0.44
1:A:348:ASN:O	1:A:348:ASN:ND2	2.49	0.43
1:C:175:ALA:HB3	1:C:177:MET:HE1	1.98	0.43
1:D:187:VAL:O	1:D:188:TRP:HB2	2.18	0.43
1:B:216:LEU:HA	1:B:220:LEU:HB3	2.00	0.43
1:C:298:TRP:O	1:C:299:ASN:HB2	2.18	0.43
1:A:336:GLN:O	1:A:383:ALA:HA	2.19	0.43
1:D:449:CYS:SG	1:D:450:PRO:HD2	2.59	0.43
1:A:378:VAL:O	1:A:435:HIS:CD2	2.72	0.43
1:C:114:SER:HB3	1:C:117:SER:HB3	2.00	0.43
1:C:110:TYR:HE1	1:C:181:PRO:HG3	1.83	0.43
1:D:339:PHE:O	1:D:387:LEU:HA	2.18	0.43
1:A:162:LEU:CD1	1:A:393:ILE:CD1	2.97	0.43
1:C:238:VAL:O	1:C:242:VAL:HB	2.19	0.43
1:D:262:LEU:HD21	1:D:392:ILE:HD13	2.00	0.43
1:A:91:LEU:HD12	1:A:92:HIS:N	2.34	0.43
1:B:92:HIS:CD2	1:B:218:ARG:NH2	2.87	0.43
1:D:89:LEU:HB3	1:D:110:TYR:HB3	2.01	0.42
1:A:172:TRP:CH2	1:A:411:LEU:HB3	2.54	0.42
1:C:435:HIS:O	1:C:436:LEU:HD13	2.19	0.42
1:D:391:ILE:CG2	1:D:392:ILE:N	2.82	0.42
1:C:330:CYS:HA	1:C:331:PRO:HD2	1.86	0.42
1:D:246:ALA:O	1:D:250:GLU:HG2	2.19	0.42
1:B:302:VAL:HG11	1:B:318:CYS:HB2	2.00	0.42
1:D:337:TRP:HB3	1:D:386:CYS:O	2.20	0.42
1:A:132:ASN:OD1	1:A:135:ASN:HB2	2.19	0.42
1:A:325:TYR:N	1:A:326:PRO:CD	2.80	0.42
1:D:252:LEU:O	1:D:254:TYR:CD2	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:ILE:CD1	1:A:407:LEU:HD21	2.50	0.42
1:B:433:PRO:C	1:B:436:LEU:HD21	2.35	0.42
1:D:247:GLU:HG2	1:D:251:LYS:HE2	2.02	0.42
1:B:162:LEU:CD2	1:B:177:MET:HB3	2.50	0.42
1:B:314:GLU:HA	1:B:314:GLU:OE1	2.19	0.42
1:D:258:GLN:OE1	1:D:260:ARG:NH2	2.44	0.42
1:A:110:TYR:HB2	1:A:179:PHE:HB3	2.01	0.41
1:A:311:GLN:O	1:A:314:GLU:HB2	2.20	0.41
1:C:129:TYR:O	1:C:282:THR:HG21	2.20	0.41
1:C:322:TYR:OH	1:C:323:LYS:HE3	2.19	0.41
1:C:363:TYR:HB3	1:C:364:ILE:HD13	2.02	0.41
1:C:378:VAL:HA	1:C:379:PRO:HD2	1.78	0.41
1:C:394:ARG:HG2	1:C:396:HIS:NE2	2.34	0.41
1:B:304:GLU:HG3	1:B:307:ARG:HH21	1.83	0.41
1:B:380:ALA:HA	1:B:434:VAL:CG1	2.44	0.41
1:C:367:LEU:C	1:C:367:LEU:CD2	2.89	0.41
1:D:102:ASN:ND2	1:D:184:SER:O	2.46	0.41
1:C:283:ILE:HG23	1:C:345:THR:CG2	2.50	0.41
1:C:363:TYR:O	1:C:366:ASN:HB3	2.20	0.41
1:A:180:ILE:HG22	1:A:188:TRP:HH2	1.85	0.41
1:A:152:TRP:HA	1:A:153:PRO:HD3	1.88	0.41
1:B:442:TRP:O	1:B:445:CYS:HB3	2.21	0.41
1:C:172:TRP:CH2	1:C:411:LEU:HB3	2.56	0.41
1:A:288:THR:O	1:A:292:ARG:HG3	2.20	0.41
1:A:401:GLN:HA	1:A:405:THR:O	2.21	0.41
1:A:99:VAL:HA	1:A:203:MET:CE	2.51	0.41
1:A:302:VAL:HG23	1:A:307:ARG:HG3	2.02	0.41
1:B:108:GLY:O	1:B:181:PRO:HD2	2.21	0.41
1:B:274:TYR:CD1	1:B:363:TYR:HD2	2.39	0.41
1:C:186:ASP:O	1:C:187:VAL:HB	2.21	0.41
1:D:434:VAL:O	1:D:434:VAL:HG12	2.19	0.41
1:C:89:LEU:HB3	1:C:110:TYR:HB3	2.03	0.41
1:C:338:LEU:O	1:C:371:LEU:HD12	2.21	0.41
1:D:178:VAL:HG21	1:D:215:LEU:HD11	2.03	0.41
1:D:325:TYR:N	1:D:326:PRO:HD2	2.36	0.41
1:A:184:SER:O	1:A:185:SER:HB2	2.21	0.41
1:B:111:LEU:HD21	1:B:113:GLU:HG3	2.03	0.41
1:B:405:THR:CG2	1:B:436:LEU:CD1	2.99	0.41
1:B:405:THR:HG21	1:B:436:LEU:CD1	2.51	0.41
1:C:281:ASP:N	1:C:284:THR:OG1	2.51	0.41
1:C:278:ASP:OD1	1:C:279:CYS:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:LEU:CD1	1:C:393:ILE:HD11	2.45	0.40
1:C:121:LEU:HD12	1:C:177:MET:HE1	1.99	0.40
1:C:339:PHE:CD2	1:C:443:PRO:CG	2.91	0.40
1:D:210:GLU:HA	1:D:213:ARG:HG2	2.03	0.40
1:D:302:VAL:O	1:D:307:ARG:NH2	2.54	0.40
1:A:130:CYS:HB2	1:A:139:ARG:HD2	2.03	0.40
1:D:210:GLU:CD	1:D:213:ARG:HE	2.02	0.40
1:A:165:GLN:O	1:A:168:GLU:N	2.52	0.40
1:C:159:THR:HG23	1:C:393:ILE:O	2.22	0.40
1:D:127:GLY:O	1:D:139:ARG:NH2	2.54	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	337/471 (72%)	324 (96%)	11 (3%)	2 (1%)	25	56
1	B	327/471 (69%)	312 (95%)	14 (4%)	1 (0%)	41	72
1	C	329/471 (70%)	308 (94%)	19 (6%)	2 (1%)	25	56
1	D	361/471 (77%)	340 (94%)	19 (5%)	2 (1%)	25	56
2	E	8/10 (80%)	8 (100%)	0	0	100	100
All	All	1362/1894 (72%)	1292 (95%)	63 (5%)	7 (0%)	29	61

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	390	GLU
1	A	390	GLU
1	A	187	VAL
1	C	187	VAL

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Mol	Chain	Res	Type
1	D	187	VAL
1	B	187	VAL
1	C	391	ILE

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	293/405 (72%)	288 (98%)	5 (2%)	60	87
1	B	278/405 (69%)	270 (97%)	8 (3%)	42	76
1	C	285/405 (70%)	279 (98%)	6 (2%)	53	84
1	D	303/405 (75%)	294 (97%)	9 (3%)	41	75
All	All	1159/1620 (72%)	1131 (98%)	28 (2%)	49	81

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	TRP
1	A	177	MET
1	A	183	CYS
1	A	348	ASN
1	A	448	SER
1	B	139	ARG
1	B	285	CYS
1	B	308	ARG
1	B	314	GLU
1	B	348	ASN
1	B	367	LEU
1	B	381	SER
1	B	417	SER
1	C	183	CYS
1	C	185	SER
1	C	189	SER
1	C	285	CYS
1	C	372	ARG

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Mol	Chain	Res	Type
1	C	432	CYS
1	D	121	LEU
1	D	183	CYS
1	D	282	THR
1	D	301	VAL
1	D	326	PRO
1	D	365	GLN
1	D	411	LEU
1	D	432	CYS
1	D	444	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	366	ASN
1	B	273	GLN
1	C	271	ASN
1	C	273	GLN
1	C	373	HIS
1	D	365	GLN
1	D	469	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\#\|Z\| > 2$
3	NAG	B	1452	1	14,14,15	0.97	1 (7%)	17,19,21	1.95	6 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1452	1	1/1/5/7	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1452	NAG	C1-C2	2.63	1.56	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1452	NAG	O5-C1-C2	-4.36	104.40	111.29
3	B	1452	NAG	C1-C2-N2	3.14	115.85	110.49
3	B	1452	NAG	O5-C5-C4	-2.80	104.01	110.83
3	B	1452	NAG	C2-N2-C7	2.73	126.78	122.90
3	B	1452	NAG	C3-C4-C5	-2.60	105.60	110.24
3	B	1452	NAG	O6-C6-C5	-2.01	104.38	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	1452	NAG	C1

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1452	NAG	O5-C5-C6-O6
3	B	1452	NAG	C4-C5-C6-O6
3	B	1452	NAG	C1-C2-N2-C7
3	B	1452	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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, 95^{th} 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	345/471 (73%)	-0.10	1 (0%)	94	93	28, 43, 68, 84	0
1	B	335/471 (71%)	-0.15	3 (0%)	84	80	25, 42, 88, 108	0
1	C	337/471 (71%)	-0.09	3 (0%)	84	80	25, 45, 92, 130	0
1	D	369/471 (78%)	-0.16	1 (0%)	94	93	26, 44, 67, 84	0
2	E	10/10 (100%)	-0.38	0	100	100	50, 62, 69, 71	0
All	All	1396/1894 (73%)	-0.13	8 (0%)	89	86	25, 44, 79, 130	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	442	TRP	4.3
1	D	353	GLY	4.2
1	B	387	LEU	3.3
1	B	279	CYS	2.4
1	A	439	SER	2.3
1	C	440	CYS	2.2
1	C	116	GLY	2.1
1	B	341	GLU	2.1

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, 95^{th} 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	NAG	B	1452	14/15	0.84	0.17	60,62,66,67	0
4	CL	B	1453	1/1	0.87	0.11	72,72,72,72	0

6.5 Other polymers

There are no such residues in this entry.