



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 09:45 am GMT

PDB ID : 3TAL  
Title : Crystal structure of NurA with manganese  
Authors : Chae, J.; Kim, Y.C.; Cho, Y.  
Deposited on : 2011-08-04  
Resolution : 3.15 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

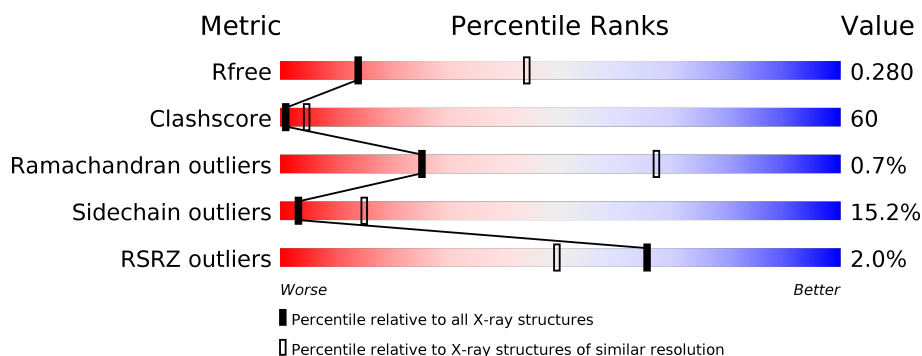
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 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))
$R_{free}$	100719	1259 (3.20-3.12)
Clashscore	112137	1397 (3.20-3.12)
Ramachandran outliers	110173	1368 (3.20-3.12)
Sidechain outliers	110143	1367 (3.20-3.12)
RSRZ outliers	101464	1264 (3.20-3.12)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	471	
1	B	471	

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	GOL	A	454	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6861 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 DNA double-strand break repair protein nurA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	Se	0	0	0
			3420	2188	587	638	7			
1	B	421	Total	C	N	O	Se	0	0	0
			3411	2186	584	634	7			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MSE	-	EXPRESSION TAG	UNP Q8U1N8
A	-18	GLY	-	EXPRESSION TAG	UNP Q8U1N8
A	-17	SER	-	EXPRESSION TAG	UNP Q8U1N8
A	-16	SER	-	EXPRESSION TAG	UNP Q8U1N8
A	-15	HIS	-	EXPRESSION TAG	UNP Q8U1N8
A	-14	HIS	-	EXPRESSION TAG	UNP Q8U1N8
A	-13	HIS	-	EXPRESSION TAG	UNP Q8U1N8
A	-12	HIS	-	EXPRESSION TAG	UNP Q8U1N8
A	-11	HIS	-	EXPRESSION TAG	UNP Q8U1N8
A	-10	HIS	-	EXPRESSION TAG	UNP Q8U1N8
A	-9	SER	-	EXPRESSION TAG	UNP Q8U1N8
A	-8	SER	-	EXPRESSION TAG	UNP Q8U1N8
A	-7	GLY	-	EXPRESSION TAG	UNP Q8U1N8
A	-6	LEU	-	EXPRESSION TAG	UNP Q8U1N8
A	-5	VAL	-	EXPRESSION TAG	UNP Q8U1N8
A	-4	PRO	-	EXPRESSION TAG	UNP Q8U1N8
A	-3	ARG	-	EXPRESSION TAG	UNP Q8U1N8
A	-2	GLY	-	EXPRESSION TAG	UNP Q8U1N8
A	-1	SER	-	EXPRESSION TAG	UNP Q8U1N8
A	0	HIS	-	EXPRESSION TAG	UNP Q8U1N8
B	-19	MSE	-	EXPRESSION TAG	UNP Q8U1N8
B	-18	GLY	-	EXPRESSION TAG	UNP Q8U1N8
B	-17	SER	-	EXPRESSION TAG	UNP Q8U1N8
B	-16	SER	-	EXPRESSION TAG	UNP Q8U1N8
B	-15	HIS	-	EXPRESSION TAG	UNP Q8U1N8

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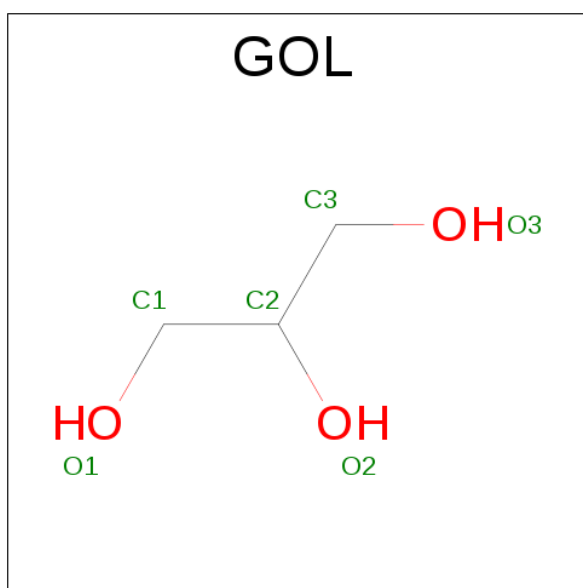
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	EXPRESSION TAG	UNP Q8U1N8
B	-13	HIS	-	EXPRESSION TAG	UNP Q8U1N8
B	-12	HIS	-	EXPRESSION TAG	UNP Q8U1N8
B	-11	HIS	-	EXPRESSION TAG	UNP Q8U1N8
B	-10	HIS	-	EXPRESSION TAG	UNP Q8U1N8
B	-9	SER	-	EXPRESSION TAG	UNP Q8U1N8
B	-8	SER	-	EXPRESSION TAG	UNP Q8U1N8
B	-7	GLY	-	EXPRESSION TAG	UNP Q8U1N8
B	-6	LEU	-	EXPRESSION TAG	UNP Q8U1N8
B	-5	VAL	-	EXPRESSION TAG	UNP Q8U1N8
B	-4	PRO	-	EXPRESSION TAG	UNP Q8U1N8
B	-3	ARG	-	EXPRESSION TAG	UNP Q8U1N8
B	-2	GLY	-	EXPRESSION TAG	UNP Q8U1N8
B	-1	SER	-	EXPRESSION TAG	UNP Q8U1N8
B	0	HIS	-	EXPRESSION TAG	UNP Q8U1N8

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Mn 2 2	0	0
2	A	2	Total Mn 2 2	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total	O	0	0
			13	13		
4	B	7	Total	O	0	0
			7	7		



PRO	LEU	GLU
I388	E389	K390
I391	L392	P393
I394	L396	H397
H398	K399	A400
GLY	GLY	TYR
L404	R405	P406
L407	Q408	L409
A410	H411	H412
G413	V414	K415
T416	S417	Y418
K419	E420	A421
H422	H423	T424
L425	E426	A427
L428	L429	L432
R433	N434	R435
D436	P437	A438
L439	K440	ILE
PHE	VAL	LYS
TYR	GLY	ARG
SER		
L325	I326	GLY
HIS	GLU	K330
E331	G332	Y333
L334	E335	I336
V340	V341	P342
P343	K344	V345
S346	F347	P348
D349	F350	L351
L352	S353	K354
F355	R356	N357
I358	E359	K360
L361	I362	D363
K364	G365	I366
H367	L368	A369
Y370	V371	R372
F373	E374	Q375
G376	D377	V378
I379	Y380	M381
L382	Q383	S384
T385		
L260	L261	I266
Y267	D268	A269
H271	L270	H272
T273	L274	S275
Y276	I277	E278
Y279	L280	Y281
S282	I283	D284
K285	L286	L287
E288	N291	L292
A293	Y294	I295
A296	R297	P298
Y299	Y300	T301
K302	T303	L304
A305	R306	THR
LEU	GLY	V310
E311	L312	V313
D314	L317	L318
D319	A320	V321
I322	R323	T324
K256	V257	E258
L259		
D193	N194	V195
E197	K198	L199
R200	K201	K202
Y203	I204	D205
T206	K207	V208
ILE	ALA	TYR
GLY	SER	GLY
K215	V216	K217
V218	K219	I220
K223	A224	L225
G226	S228	P229
R230	V231	I232
P233	L234	E235
V236	S240	R241
G242	K243	S244
V245	D246	E247
L248	L249	Q250
K256	V257	E258
L259		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.80Å 114.65Å 121.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.48 – 3.15 34.37 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.8 (29.48-3.15) 94.4 (34.37-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.218 , 0.285 0.214 , 0.280	Depositor DCC
$R_{free}$ test set	1583 reflections (10.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	97.2	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 89.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6861	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, MN

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	0.34	0/3470	0.60	0/4670
1	B	0.32	0/3459	0.62	1/4652 (0.0%)
All	All	0.33	0/6929	0.61	1/9322 (0.0%)

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	B	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	274	LEU	CA-CB-CG	5.97	129.03	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	228	SER	Peptide
1	B	417	SER	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	3420	0	3526	400	0
1	B	3411	0	3532	474	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	6	0	8	3	0
4	A	13	0	0	3	0
4	B	7	0	0	1	0
All	All	6861	0	7066	829	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 60.

All (829) 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:172:HIS:ND1	1:B:191:LEU:HD11	1.57	1.20
1:A:54:ARG:HB3	1:A:101:MSE:HE3	1.29	1.14
1:B:98:ARG:HH22	1:B:137:PRO:HB3	0.99	1.10
1:A:244:SER:HA	1:B:244:SER:HA	1.24	1.09
1:A:240:SER:HB3	1:A:243:LYS:HD2	1.31	1.08
1:A:310:VAL:HG12	1:A:311:GLU:H	1.18	1.04
1:A:87:LYS:HZ3	1:B:19:GLU:HG3	1.21	1.02
1:A:231:VAL:HB	1:B:231:VAL:HG11	1.41	1.02
1:B:405:ARG:HG3	1:B:406:PRO:HD3	1.43	0.99
1:A:135:ARG:HH22	1:A:140:PRO:HD3	1.26	0.99
1:A:21:GLU:HB3	1:A:24:ARG:HD3	1.43	0.99
1:A:169:LEU:HD23	1:A:191:LEU:HD12	1.43	0.99
1:A:87:LYS:NZ	1:B:19:GLU:HG3	1.78	0.99
1:A:95:GLN:HE22	1:A:138:VAL:HA	1.24	0.98
1:A:419:LYS:HG3	1:A:420:GLU:H	1.29	0.98
1:A:300:TYR:HE1	1:A:304:LEU:H	1.06	0.97
1:B:98:ARG:NH2	1:B:137:PRO:HB3	1.79	0.95
1:A:217:LYS:HG3	1:A:258:GLU:OE2	1.67	0.95
1:B:217:LYS:HG2	1:B:260:TYR:HE1	1.29	0.95
1:B:217:LYS:HG2	1:B:260:TYR:CE1	2.02	0.95
1:A:374:GLU:HB3	1:A:377:ASP:HB2	1.48	0.94
1:A:44:LYS:HA	1:A:397:HIS:ND1	1.85	0.92
1:A:320:ALA:HA	1:B:436:ASP:OD2	1.69	0.91
1:B:28:GLN:C	1:B:30:ARG:H	1.64	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:SER:HB2	1:B:7:GLN:HE22	1.35	0.91
1:B:111:LEU:HD23	1:B:180:LEU:HD12	1.53	0.91
1:B:361:LEU:HD11	1:B:366:ILE:HG22	1.53	0.90
1:B:192:THR:HG21	1:B:275:SER:HA	1.51	0.90
1:A:321:VAL:HG13	1:A:325:LEU:HD21	1.51	0.90
1:B:284:ASP:OD1	1:B:357:ASN:HB2	1.72	0.89
1:B:98:ARG:HH22	1:B:137:PRO:CB	1.85	0.89
1:A:310:VAL:HG12	1:A:311:GLU:N	1.85	0.89
1:B:172:HIS:CG	1:B:191:LEU:HD11	2.08	0.89
1:B:232:ILE:HG12	1:B:236:VAL:HG11	1.55	0.88
1:B:96:ILE:HD11	1:B:272:MSE:HE1	1.53	0.88
1:A:374:GLU:HB2	1:A:402:GLY:HA2	1.53	0.87
1:A:99:MSE:O	1:A:103:THR:HG22	1.74	0.87
1:B:110:TYR:HD2	1:B:111:LEU:HD12	1.39	0.87
1:B:172:HIS:CE1	1:B:191:LEU:HD11	2.12	0.85
1:A:340:VAL:HG12	1:A:341:VAL:H	1.41	0.85
1:B:114:ARG:HH12	1:B:170:ARG:NH1	1.75	0.85
1:A:304:LEU:HA	1:A:307:THR:HB	1.59	0.84
1:A:300:TYR:OH	1:A:304:LEU:HB2	1.78	0.84
1:B:370:TYR:HB3	1:B:379:ILE:HD11	1.60	0.84
1:B:129:LEU:HG	1:B:294:TYR:CE2	2.12	0.83
1:A:340:VAL:CG1	1:A:341:VAL:H	1.90	0.83
1:B:357:ASN:HA	1:B:360:LYS:HE3	1.58	0.83
1:A:425:LEU:HD23	1:A:428:LEU:HD21	1.60	0.83
1:B:43:GLU:O	1:B:397:HIS:HB2	1.79	0.83
1:B:174:ARG:HG3	1:B:175:LYS:N	1.94	0.82
1:B:192:THR:HG22	1:B:274:LEU:HD13	1.60	0.82
1:A:300:TYR:CZ	1:A:303:THR:HB	2.14	0.82
1:A:299:PHE:CE1	1:A:304:LEU:HD22	2.15	0.82
1:A:208:VAL:HB	1:A:216:VAL:CG1	2.10	0.82
1:B:322:ILE:HA	1:B:325:LEU:HD23	1.60	0.81
1:A:21:GLU:HB3	1:A:24:ARG:NH1	1.96	0.81
1:B:426:GLU:CD	1:B:427:ALA:H	1.83	0.81
1:A:107:MSE:HE1	1:A:189:PRO:HB2	1.62	0.81
1:A:340:VAL:HG12	1:A:341:VAL:N	1.96	0.81
1:B:5:SER:HB2	1:B:7:GLN:NE2	1.95	0.81
1:A:21:GLU:HB3	1:A:24:ARG:HH11	1.45	0.80
1:A:374:GLU:HB2	1:A:402:GLY:CA	2.11	0.80
1:B:219:LYS:HB3	1:B:256:LYS:HD3	1.64	0.80
1:B:32:ILE:HD13	1:B:325:LEU:HD22	1.62	0.80
1:A:300:TYR:CE1	1:A:304:LEU:N	2.49	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:ILE:HD12	1:B:33:ILE:N	1.95	0.79
1:B:331:GLU:HB3	1:B:373:PHE:O	1.82	0.79
1:A:208:VAL:HB	1:A:216:VAL:HG11	1.63	0.79
1:A:176:VAL:HG22	1:A:186:TYR:HE2	1.48	0.79
1:A:321:VAL:HG13	1:A:325:LEU:CD2	2.13	0.78
1:B:107:MSE:O	1:B:111:LEU:HD13	1.82	0.78
1:B:137:PRO:HG2	1:B:279:TYR:CZ	2.17	0.78
1:B:399:LYS:HD2	1:B:400:ALA:N	1.99	0.78
1:B:29:ILE:O	1:B:30:ARG:HG2	1.82	0.78
1:A:430:ASN:OD1	1:A:431:ALA:N	2.15	0.77
1:B:205:ASP:HA	1:B:208:VAL:HG23	1.66	0.77
1:B:146:LEU:HD12	1:B:273:THR:HG22	1.65	0.77
1:B:230:ARG:HG3	1:B:231:VAL:H	1.49	0.77
1:A:21:GLU:CB	1:A:24:ARG:HD3	2.14	0.77
1:B:191:LEU:N	1:B:191:LEU:HD12	2.00	0.77
1:B:342:PRO:HD2	1:B:362:ILE:HA	1.67	0.76
1:A:428:LEU:N	1:A:435:ARG:HH22	1.83	0.76
1:A:144:ARG:HH12	1:B:229:PRO:HG2	1.48	0.76
1:B:32:ILE:HD13	1:B:325:LEU:CD2	2.16	0.76
1:B:420:GLU:HA	1:B:423:HIS:CD2	2.21	0.76
1:A:133:LEU:HD11	1:A:347:PHE:CZ	2.20	0.76
1:B:47:ILE:HD12	1:B:122:ALA:HB3	1.66	0.76
1:B:228:SER:O	1:B:230:ARG:HG2	1.85	0.76
1:B:179:HIS:HA	1:B:182:LYS:HG2	1.66	0.75
1:A:378:VAL:HG13	1:B:440:LYS:HE3	1.66	0.75
1:A:304:LEU:CD2	1:A:312:ILE:HD12	2.16	0.75
1:A:24:ARG:HG2	1:A:25:GLU:N	2.02	0.75
1:A:307:THR:HG23	1:A:309:GLY:H	1.51	0.75
1:A:245:VAL:HG22	1:B:243:LYS:O	1.87	0.75
1:B:370:TYR:HD1	1:B:379:ILE:HD11	1.52	0.75
1:B:123:ILE:HG22	1:B:292:LEU:HD13	1.68	0.74
1:B:362:ILE:HG13	1:B:363:ASP:N	2.00	0.74
1:A:428:LEU:H	1:A:428:LEU:HD12	1.51	0.74
1:B:301:THR:HG21	1:B:314:ASP:HB2	1.69	0.74
1:B:426:GLU:N	1:B:426:GLU:OE1	2.20	0.74
1:B:373:PHE:CE2	1:B:399:LYS:HE3	2.23	0.74
1:A:20:LEU:O	1:A:23:VAL:HB	1.88	0.73
1:A:37:LYS:HG2	1:A:38:PRO:HD2	1.69	0.73
1:B:114:ARG:HH12	1:B:170:ARG:HH12	1.36	0.73
1:A:44:LYS:HG3	1:A:397:HIS:HE1	1.53	0.73
1:B:433:ARG:HG3	1:B:434:ASN:H	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:LYS:CE	1:A:306:ARG:NH2	2.52	0.73
1:B:244:SER:N	1:B:247:GLU:OE2	2.22	0.73
1:B:325:LEU:HG	1:B:326:ILE:H	1.54	0.73
1:B:89:ASN:OD1	1:B:92:THR:HB	1.88	0.73
1:B:207:LYS:HD2	1:B:207:LYS:N	2.03	0.73
1:A:135:ARG:NH2	1:A:140:PRO:HD3	2.03	0.73
1:B:21:GLU:HA	1:B:24:ARG:HG3	1.71	0.73
1:B:348:PRO:HG2	1:B:351:LEU:HD13	1.70	0.72
1:B:433:ARG:HG3	1:B:434:ASN:N	2.04	0.72
1:A:176:VAL:HG22	1:A:186:TYR:CE2	2.25	0.72
1:A:395:ILE:HD12	1:A:404:LEU:HD13	1.72	0.72
1:B:325:LEU:HG	1:B:326:ILE:N	2.04	0.72
1:B:48:TYR:CD1	1:B:112:ALA:HB1	2.25	0.72
1:A:248:LEU:HD12	1:A:248:LEU:O	1.90	0.72
1:A:129:LEU:HD23	1:A:366:ILE:HG12	1.71	0.71
1:B:240:SER:HB3	1:B:243:LYS:HD2	1.72	0.71
1:A:29:ILE:O	1:A:32:ILE:HG22	1.89	0.71
1:B:243:LYS:HB3	1:B:247:GLU:OE2	1.90	0.71
1:B:373:PHE:CZ	1:B:399:LYS:HE3	2.26	0.71
1:A:95:GLN:OE1	1:A:137:PRO:O	2.08	0.71
1:A:113:TYR:CG	1:A:289:VAL:HG22	2.25	0.71
1:B:191:LEU:CD1	1:B:191:LEU:N	2.53	0.71
1:A:126:ASP:O	1:A:126:ASP:OD1	2.08	0.70
1:A:28:GLN:OE1	1:A:28:GLN:HA	1.91	0.70
1:B:172:HIS:HB2	1:B:191:LEU:HD21	1.72	0.70
1:B:172:HIS:O	1:B:176:VAL:HG13	1.91	0.70
1:A:231:VAL:HB	1:B:231:VAL:CG1	2.19	0.70
1:B:216:VAL:O	1:B:260:TYR:HA	1.91	0.70
1:B:124:LEU:HD13	1:B:395:ILE:HD11	1.74	0.70
1:B:370:TYR:HB3	1:B:379:ILE:CD1	2.20	0.70
1:A:134:VAL:O	1:A:345:TRP:HH2	1.74	0.70
1:A:300:TYR:CZ	1:A:304:LEU:HB2	2.27	0.70
1:B:101:MSE:HA	1:B:101:MSE:HE3	1.74	0.70
1:B:370:TYR:CD1	1:B:379:ILE:HD11	2.27	0.70
1:A:21:GLU:HB3	1:A:24:ARG:CD	2.21	0.69
1:A:136:PRO:HB2	1:A:138:VAL:HG13	1.73	0.69
1:A:230:ARG:HG3	1:B:234:ILE:CG1	2.22	0.69
1:A:64:ILE:HD11	1:A:425:LEU:HD22	1.74	0.69
1:A:428:LEU:CD1	1:A:429:ILE:H	2.06	0.69
1:B:204:ILE:HD11	1:B:270:LEU:HD12	1.75	0.69
1:A:285:LYS:O	1:A:288:GLU:HB2	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:TYR:HE1	1:A:304:LEU:N	1.85	0.69
1:A:21:GLU:CB	1:A:24:ARG:HH11	2.06	0.69
1:A:217:LYS:CG	1:A:258:GLU:OE2	2.40	0.69
1:A:378:VAL:HG13	1:B:440:LYS:CE	2.22	0.69
1:A:302:LYS:HE3	1:A:306:ARG:NH2	2.08	0.69
1:B:416:ILE:HG22	1:B:416:ILE:O	1.92	0.69
1:A:230:ARG:HG3	1:B:234:ILE:HG12	1.75	0.69
1:A:134:VAL:O	1:A:345:TRP:CH2	2.46	0.68
1:B:163:ASN:O	1:B:167:GLU:HG3	1.94	0.68
1:A:315:THR:HG22	1:A:370:TYR:CD1	2.29	0.68
1:A:313:VAL:HG12	1:A:318:LEU:HB2	1.75	0.68
1:A:364:LYS:HE3	4:A:461:HOH:O	1.94	0.68
1:B:182:LYS:HG3	1:B:183:ASN:H	1.59	0.68
1:B:30:ARG:O	1:B:33:ILE:HG22	1.94	0.68
1:B:368:LEU:HB3	1:B:381:MSE:HE1	1.74	0.68
1:B:21:GLU:HG3	1:B:24:ARG:HD2	1.74	0.68
1:B:104:LEU:HA	1:B:107:MSE:HE2	1.75	0.68
1:B:28:GLN:C	1:B:30:ARG:N	2.39	0.68
1:A:363:ASP:OD1	1:A:363:ASP:C	2.32	0.67
1:A:302:LYS:HE3	1:A:306:ARG:CZ	2.24	0.67
1:B:325:LEU:HG	1:B:326:ILE:HG22	1.76	0.67
1:A:299:PHE:CZ	1:A:304:LEU:HD22	2.29	0.67
1:A:304:LEU:HD23	1:A:312:ILE:HD12	1.77	0.67
1:B:269:ALA:O	1:B:273:THR:HG23	1.94	0.67
1:B:106:ASN:HB2	1:B:282:SER:HB2	1.76	0.67
1:B:334:LEU:HD12	1:B:335:GLU:O	1.95	0.67
1:B:439:LEU:HD12	1:B:440:LYS:N	2.09	0.67
1:B:127:GLY:O	1:B:296:ALA:HB2	1.95	0.66
1:A:419:LYS:HG3	1:A:420:GLU:N	2.07	0.66
1:A:302:LYS:HG2	1:A:306:ARG:CZ	2.25	0.66
1:A:24:ARG:HG2	1:A:25:GLU:H	1.60	0.66
1:B:294:TYR:HB2	1:B:383:GLN:HB2	1.77	0.66
1:A:355:PHE:HB3	1:A:358:ILE:HD12	1.78	0.66
1:A:302:LYS:HE2	1:A:306:ARG:NH2	2.11	0.66
1:A:307:THR:O	1:A:308:LEU:HB2	1.95	0.66
1:A:32:ILE:O	1:A:35:SER:HB3	1.96	0.66
1:A:29:ILE:HA	1:A:32:ILE:HG22	1.77	0.65
1:A:304:LEU:O	1:A:307:THR:HG22	1.96	0.65
1:B:336:ILE:HD11	1:B:370:TYR:HE2	1.61	0.65
1:A:64:ILE:CD1	1:A:425:LEU:HD22	2.27	0.65
1:A:48:TYR:CD1	1:A:116:LEU:HD13	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:GLU:O	1:B:312:ILE:HG23	1.97	0.65
1:B:161:LEU:HA	1:B:203:TYR:CZ	2.32	0.65
1:B:283:ILE:HG22	1:B:287:LEU:HD11	1.78	0.65
1:A:26:ASN:HB2	1:A:30:ARG:CG	2.26	0.65
1:A:300:TYR:CE1	1:A:304:LEU:HB2	2.32	0.65
1:B:248:LEU:HD12	1:B:248:LEU:O	1.97	0.65
1:A:310:VAL:CG1	1:A:311:GLU:N	2.58	0.65
1:A:209:ILE:O	1:A:216:VAL:HG13	1.97	0.64
1:B:172:HIS:ND1	1:B:191:LEU:CD1	2.48	0.64
1:B:231:VAL:HG12	1:B:232:ILE:N	2.13	0.64
1:B:56:VAL:HG22	1:B:65:TYR:HB3	1.78	0.64
1:A:29:ILE:HD11	1:A:33:ILE:HG12	1.80	0.64
1:B:172:HIS:CE1	1:B:191:LEU:CD1	2.81	0.64
1:A:24:ARG:CG	1:A:25:GLU:N	2.61	0.64
1:A:87:LYS:NZ	1:B:19:GLU:CG	2.58	0.64
1:B:174:ARG:HG3	1:B:175:LYS:H	1.63	0.64
1:B:420:GLU:HA	1:B:423:HIS:NE2	2.13	0.63
1:B:411:HIS:O	1:B:414:VAL:HG12	1.99	0.63
1:B:336:ILE:HD11	1:B:370:TYR:CE2	2.34	0.63
1:A:21:GLU:CD	1:A:24:ARG:HD3	2.19	0.63
1:A:100:GLN:HA	1:A:103:THR:HG23	1.81	0.63
1:B:375:GLN:HG3	1:B:376:GLY:N	2.13	0.63
1:A:176:VAL:HG13	1:A:186:TYR:HD2	1.62	0.63
1:B:142:ASP:OD1	1:B:143:ILE:N	2.31	0.63
1:B:347:PHE:CB	1:B:352:LEU:HD11	2.28	0.63
1:B:123:ILE:HG22	1:B:292:LEU:CD1	2.29	0.62
1:A:65:TYR:CZ	1:A:84:ASN:HB3	2.34	0.62
1:B:215:LYS:HA	1:B:261:LEU:O	1.99	0.62
1:A:151:ALA:HB1	1:A:233:PRO:HD3	1.80	0.62
1:B:182:LYS:HG3	1:B:183:ASN:N	2.14	0.62
1:A:115:LYS:HZ3	1:A:181:GLU:HA	1.64	0.62
1:A:28:GLN:O	1:A:31:ASN:OD1	2.18	0.62
1:B:138:VAL:O	1:B:139:TYR:HB2	1.99	0.62
1:A:95:GLN:HE22	1:A:138:VAL:CA	2.08	0.62
1:A:304:LEU:HD21	1:A:312:ILE:HD12	1.82	0.62
1:B:357:ASN:CA	1:B:360:LYS:HE3	2.30	0.62
1:A:16:LEU:HD21	1:B:62:THR:HG21	1.82	0.62
1:B:89:ASN:CG	1:B:92:THR:HB	2.20	0.62
1:B:391:ILE:O	1:B:394:LEU:HB2	2.00	0.61
1:B:92:THR:HG22	1:B:96:ILE:HD13	1.82	0.61
1:A:428:LEU:HD13	1:A:429:ILE:H	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:GLU:HA	1:B:180:LEU:HB2	1.82	0.61
1:B:179:HIS:HA	1:B:182:LYS:CG	2.28	0.61
1:A:202:LYS:HE2	1:A:203:TYR:CE1	2.36	0.61
1:B:341:VAL:HG23	1:B:342:PRO:O	2.00	0.61
1:B:398:HIS:O	1:B:405:ARG:HG2	2.00	0.61
1:A:43:GLU:HG2	1:A:120:LYS:NZ	2.14	0.61
1:A:430:ASN:HB3	1:A:435:ARG:CZ	2.29	0.61
1:B:405:ARG:HG3	1:B:406:PRO:CD	2.25	0.61
1:A:171:ASP:HA	1:A:174:ARG:HD3	1.82	0.61
1:B:439:LEU:HD12	1:B:440:LYS:HG3	1.82	0.61
1:B:95:GLN:HB3	1:B:138:VAL:HG23	1.81	0.61
1:B:232:ILE:CG1	1:B:236:VAL:HG11	2.30	0.61
1:B:11:ARG:O	1:B:15:ILE:HG13	2.01	0.61
1:B:378:VAL:HG12	1:B:379:ILE:H	1.66	0.61
1:A:240:SER:HB3	1:A:243:LYS:CD	2.21	0.60
1:A:200:ARG:HD3	1:A:267:TYR:CE1	2.36	0.60
1:A:245:VAL:HG21	1:B:241:ARG:HA	1.82	0.60
1:A:346:SER:O	1:A:347:PHE:CD1	2.55	0.60
1:B:355:PHE:O	1:B:359:GLU:HB2	2.01	0.60
1:A:306:ARG:O	1:A:308:LEU:HD12	2.01	0.60
1:B:26:ASN:O	1:B:28:GLN:HG2	2.01	0.60
1:B:435:ARG:O	1:B:438:ALA:HB3	2.01	0.60
1:A:323:ARG:HG2	1:A:329:GLU:HB2	1.83	0.60
1:B:375:GLN:HG3	1:B:376:GLY:H	1.67	0.60
1:A:104:LEU:HD11	1:A:189:PRO:HG2	1.82	0.60
1:A:419:LYS:CG	1:A:420:GLU:H	2.11	0.60
1:B:373:PHE:CD2	1:B:374:GLU:N	2.70	0.60
1:A:130:THR:HG23	1:A:383:GLN:OE1	2.01	0.60
1:B:439:LEU:CD1	1:B:440:LYS:HG3	2.32	0.60
1:A:427:ALA:C	1:A:435:ARG:HH22	2.04	0.60
1:B:172:HIS:CD2	1:B:176:VAL:HG12	2.36	0.60
1:B:173:TYR:O	1:B:176:VAL:HG22	2.02	0.60
1:A:92:THR:HA	1:A:95:GLN:HB3	1.84	0.60
1:A:17:LEU:HD21	1:B:432:LEU:CD2	2.32	0.59
1:B:407:LEU:HD23	1:B:408:GLN:N	2.17	0.59
1:B:31:ASN:O	1:B:35:SER:N	2.36	0.59
1:A:29:ILE:CD1	1:A:33:ILE:HG12	2.32	0.59
1:A:422:ARG:O	1:A:425:LEU:N	2.35	0.59
1:A:302:LYS:HE3	1:A:306:ARG:NH1	2.17	0.59
1:A:425:LEU:O	1:A:428:LEU:HD11	2.02	0.59
1:B:110:TYR:CD2	1:B:111:LEU:HD12	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:GLU:O	1:B:29:ILE:HG13	2.02	0.59
1:A:142:ASP:OD1	1:A:142:ASP:C	2.40	0.59
1:B:191:LEU:CD1	1:B:191:LEU:H	2.16	0.59
1:A:243:LYS:HB2	1:A:247:GLU:OE1	2.02	0.59
1:A:432:LEU:HD22	1:B:13:THR:HG21	1.84	0.59
1:B:149:MSE:HE3	1:B:270:LEU:N	2.18	0.59
1:A:234:ILE:HB	1:B:229:PRO:O	2.02	0.58
1:A:422:ARG:HG3	1:A:423:HIS:N	2.18	0.58
1:B:271:HIS:HA	1:B:274:LEU:HD11	1.85	0.58
1:A:113:TYR:CD2	1:A:289:VAL:HG22	2.37	0.58
1:A:130:THR:OG1	1:A:299:PHE:CZ	2.57	0.58
1:B:392:LEU:C	1:B:392:LEU:HD23	2.24	0.58
1:A:378:VAL:HG13	1:B:440:LYS:NZ	2.18	0.58
1:B:405:ARG:CG	1:B:406:PRO:HD3	2.23	0.58
1:A:366:ILE:HG22	1:A:368:LEU:HD22	1.85	0.58
1:B:19:GLU:O	1:B:23:VAL:HG23	2.03	0.58
1:B:436:ASP:HB2	1:B:437:PRO:HD3	1.85	0.58
1:B:388:ILE:CG2	1:B:389:GLU:N	2.65	0.58
1:B:138:VAL:CG1	1:B:142:ASP:HB3	2.34	0.58
1:B:235:GLU:HA	1:B:235:GLU:OE1	2.04	0.58
1:A:428:LEU:H	1:A:428:LEU:CD1	2.12	0.57
1:A:320:ALA:HB1	1:B:434:ASN:ND2	2.19	0.57
1:A:104:LEU:HD11	1:A:189:PRO:CG	2.34	0.57
1:A:202:LYS:HE2	1:A:203:TYR:CZ	2.40	0.57
1:A:176:VAL:HG13	1:A:186:TYR:CD2	2.39	0.57
1:A:172:HIS:O	1:A:176:VAL:HG23	2.03	0.57
1:A:21:GLU:CB	1:A:24:ARG:NH1	2.64	0.57
1:B:172:HIS:CD2	1:B:176:VAL:CG1	2.87	0.57
1:B:192:THR:HG21	1:B:275:SER:CA	2.31	0.57
1:A:141:GLU:HA	1:A:144:ARG:HE	1.68	0.57
1:A:99:MSE:O	1:A:103:THR:CG2	2.51	0.57
1:A:169:LEU:CD2	1:A:191:LEU:HD12	2.26	0.57
1:A:428:LEU:N	1:A:428:LEU:HD12	2.19	0.57
1:B:110:TYR:CD1	1:B:285:LYS:HB3	2.39	0.57
1:B:82:TYR:CD2	1:B:190:ILE:HD12	2.40	0.57
1:B:225:LEU:CD1	1:B:227:TYR:HB2	2.35	0.57
1:A:79:ARG:HB3	1:A:185:ASN:HB2	1.86	0.57
1:A:140:PRO:O	1:A:144:ARG:HD3	2.05	0.57
1:B:304:LEU:HB3	1:B:312:ILE:CD1	2.35	0.57
1:A:141:GLU:O	1:A:144:ARG:HG2	2.05	0.57
1:A:232:ILE:O	1:B:231:VAL:HG13	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:VAL:HG12	1:B:249:LEU:HD12	1.86	0.56
1:A:124:LEU:HD21	1:A:295:ILE:HG12	1.87	0.56
1:B:312:ILE:N	1:B:312:ILE:HD12	2.20	0.56
1:A:181:GLU:OE1	1:A:181:GLU:HA	2.05	0.56
1:A:104:LEU:HD12	1:A:107:MSE:CE	2.35	0.56
1:A:232:ILE:HD13	1:B:234:ILE:HD13	1.88	0.56
1:A:374:GLU:HB3	1:A:377:ASP:CB	2.31	0.56
1:B:180:LEU:O	1:B:184:GLY:HA2	2.04	0.56
1:B:208:VAL:O	1:B:208:VAL:HG12	2.05	0.56
1:B:351:LEU:O	1:B:354:LYS:HB2	2.06	0.56
1:B:423:HIS:O	1:B:426:GLU:CD	2.44	0.56
1:A:292:LEU:HD12	1:A:293:ALA:N	2.21	0.56
1:A:373:PHE:HB2	1:A:402:GLY:O	2.06	0.56
1:B:202:LYS:HE2	1:B:203:TYR:CE2	2.41	0.56
1:B:258:GLU:OE1	1:B:260:TYR:OH	2.22	0.56
1:B:304:LEU:HB3	1:B:312:ILE:HD11	1.86	0.56
1:B:80:LEU:CD1	1:B:107:MSE:HE3	2.34	0.56
1:B:426:GLU:CG	1:B:427:ALA:N	2.68	0.56
1:B:436:ASP:O	1:B:439:LEU:HG	2.05	0.56
1:B:139:TYR:C	1:B:141:GLU:H	2.09	0.56
1:A:138:VAL:HG23	1:A:139:TYR:N	2.21	0.56
1:A:401:GLY:C	1:A:403:TYR:H	2.08	0.56
1:A:326:ILE:HG23	1:A:328:HIS:HB2	1.88	0.56
1:B:205:ASP:HA	1:B:208:VAL:CG2	2.35	0.55
1:A:27:GLU:O	1:A:27:GLU:HG2	2.06	0.55
1:A:427:ALA:C	1:A:435:ARG:HH12	2.09	0.55
1:B:200:ARG:HB3	1:B:270:LEU:HD13	1.88	0.55
1:B:400:ALA:H	1:B:404:LEU:HA	1.69	0.55
1:A:291:ASN:HB3	1:A:391:ILE:HD12	1.88	0.55
1:B:207:LYS:O	1:B:208:VAL:C	2.44	0.55
1:A:26:ASN:ND2	1:A:30:ARG:HD2	2.22	0.55
1:B:139:TYR:O	1:B:141:GLU:N	2.40	0.55
1:B:319:ASP:HB2	1:B:379:ILE:CG2	2.37	0.55
1:A:316:ALA:HA	1:B:440:LYS:CD	2.36	0.55
1:B:347:PHE:HB3	1:B:352:LEU:HD11	1.89	0.55
1:B:426:GLU:CD	1:B:427:ALA:N	2.59	0.55
1:A:26:ASN:HB3	1:A:30:ARG:HG2	1.89	0.55
1:B:293:ALA:HB3	1:B:395:ILE:HD11	1.88	0.55
1:A:368:LEU:N	1:A:368:LEU:HD23	2.22	0.55
1:A:57:SER:O	1:A:64:ILE:HG22	2.06	0.55
1:B:429:ILE:HD12	1:B:438:ALA:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:LEU:O	1:B:164:GLU:HB3	2.06	0.54
1:B:381:MSE:HE3	1:B:383:GLN:HE21	1.72	0.54
1:A:126:ASP:O	3:A:454:GOL:H31	2.07	0.54
1:B:347:PHE:HB2	1:B:352:LEU:HD11	1.88	0.54
1:A:135:ARG:HG2	1:B:90:TYR:CE2	2.42	0.54
1:A:27:GLU:C	1:A:29:ILE:H	2.10	0.54
1:A:374:GLU:HG3	1:A:375:GLN:OE1	2.07	0.54
1:A:430:ASN:CG	1:A:431:ALA:N	2.60	0.54
1:B:191:LEU:O	1:B:192:THR:C	2.46	0.54
1:B:201:LYS:HA	1:B:205:ASP:OD2	2.07	0.54
1:B:389:GLU:O	1:B:393:PRO:HD2	2.07	0.54
1:B:21:GLU:O	1:B:24:ARG:HB2	2.06	0.54
1:B:343:PRO:HG2	1:B:346:SER:HB3	1.89	0.54
1:A:102:GLU:HG3	3:A:454:GOL:H2	1.88	0.54
1:A:133:LEU:HB3	1:A:342:PRO:HB3	1.89	0.54
1:B:137:PRO:HG2	1:B:279:TYR:CE2	2.41	0.54
1:B:206:THR:HB	1:B:207:LYS:NZ	2.23	0.54
1:A:133:LEU:CD1	1:A:347:PHE:CZ	2.91	0.54
1:A:325:LEU:HG	1:A:326:ILE:H	1.73	0.54
1:A:397:HIS:HD2	1:A:397:HIS:O	1.90	0.54
1:A:44:LYS:HG3	1:A:397:HIS:CE1	2.38	0.54
1:B:172:HIS:NE2	1:B:176:VAL:HG12	2.22	0.54
1:B:21:GLU:HA	1:B:24:ARG:CG	2.36	0.54
1:B:301:THR:O	1:B:304:LEU:HB2	2.07	0.54
1:A:166:LEU:CD1	1:A:354:LYS:HD2	2.38	0.54
1:A:244:SER:N	1:A:247:GLU:OE1	2.41	0.54
1:B:218:VAL:HG12	1:B:220:ILE:HG12	1.90	0.54
1:A:197:GLU:O	1:A:201:LYS:HG3	2.08	0.54
1:A:302:LYS:CE	1:A:306:ARG:HH22	2.21	0.54
1:B:10:GLU:OE2	1:B:14:LYS:HE2	2.08	0.54
1:B:322:ILE:HG13	1:B:323:ARG:N	2.22	0.54
1:A:326:ILE:HG23	1:A:328:HIS:H	1.72	0.53
1:A:200:ARG:HG3	1:A:201:LYS:N	2.23	0.53
1:A:230:ARG:HG3	1:B:234:ILE:HG13	1.89	0.53
1:A:70:LEU:HD11	1:A:72:VAL:HG12	1.91	0.53
1:B:172:HIS:CB	1:B:191:LEU:HD21	2.38	0.53
1:A:378:VAL:CG1	1:B:440:LYS:HE3	2.36	0.53
1:A:130:THR:OG1	1:A:299:PHE:HZ	1.92	0.53
1:A:197:GLU:CG	1:A:201:LYS:HE3	2.39	0.53
1:A:119:GLU:HG2	1:A:120:LYS:HG3	1.90	0.53
1:A:392:LEU:N	1:A:393:PRO:HD2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ARG:CG	1:A:201:LYS:N	2.71	0.53
1:A:313:VAL:CG1	1:A:313:VAL:O	2.57	0.53
1:B:350:PHE:CD1	1:B:351:LEU:HD12	2.44	0.53
1:B:95:GLN:HA	1:B:98:ARG:HG2	1.91	0.53
1:A:133:LEU:HD11	1:A:347:PHE:HZ	1.71	0.53
1:A:136:PRO:HB2	1:A:138:VAL:CG1	2.39	0.53
1:A:124:LEU:CD1	1:A:395:ILE:HD11	2.39	0.53
1:B:166:LEU:HD12	1:B:169:LEU:HD12	1.89	0.53
1:B:418:TYR:CD2	1:B:419:LYS:HG2	2.44	0.53
1:B:171:ASP:HA	1:B:174:ARG:NH1	2.24	0.53
1:B:29:ILE:C	1:B:30:ARG:HG2	2.29	0.53
1:B:362:ILE:HG13	1:B:363:ASP:H	1.72	0.53
1:A:132:SER:O	1:A:136:PRO:HB3	2.09	0.53
1:B:220:ILE:O	1:B:256:LYS:HA	2.09	0.53
1:B:381:MSE:CE	1:B:383:GLN:HE21	2.22	0.53
1:B:175:LYS:NZ	1:B:186:TYR:OH	2.42	0.52
1:B:247:GLU:O	1:B:250:GLN:HB3	2.08	0.52
1:B:305:ALA:N	1:B:312:ILE:HD11	2.24	0.52
1:A:343:PRO:HG3	1:A:345:TRP:CZ2	2.44	0.52
1:B:104:LEU:HD22	1:B:107:MSE:HE1	1.92	0.52
1:B:169:LEU:HD13	1:B:281:TYR:CG	2.44	0.52
1:B:357:ASN:HA	1:B:360:LYS:CE	2.36	0.52
1:A:200:ARG:HD3	1:A:267:TYR:CZ	2.44	0.52
1:A:26:ASN:CB	1:A:30:ARG:HG2	2.39	0.52
1:A:44:LYS:HA	1:A:397:HIS:CE1	2.43	0.52
1:B:175:LYS:O	1:B:179:HIS:ND1	2.43	0.52
1:A:432:LEU:CD2	1:B:13:THR:HG21	2.39	0.52
1:B:80:LEU:HD13	1:B:107:MSE:HE3	1.92	0.52
1:A:23:VAL:O	1:A:25:GLU:O	2.27	0.52
1:B:304:LEU:C	1:B:312:ILE:HD11	2.30	0.52
1:A:279:TYR:CE2	1:A:283:ILE:HD11	2.44	0.52
1:A:429:ILE:HD13	1:A:434:ASN:O	2.10	0.52
1:B:106:ASN:HB2	1:B:282:SER:CB	2.39	0.52
1:B:114:ARG:NH1	1:B:170:ARG:HH12	2.04	0.52
1:B:400:ALA:HB2	1:B:405:ARG:HB3	1.92	0.52
1:A:197:GLU:O	1:A:200:ARG:HG2	2.10	0.52
1:A:300:TYR:CE1	1:A:303:THR:HB	2.45	0.52
1:A:72:VAL:HG21	1:A:409:LEU:HB3	1.91	0.52
1:B:79:ARG:O	1:B:185:ASN:HB2	2.10	0.52
1:A:26:ASN:CB	1:A:30:ARG:CG	2.88	0.52
1:B:392:LEU:HB3	1:B:393:PRO:HD3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:HIS:O	1:B:426:GLU:OE1	2.27	0.52
1:A:81:SER:O	1:A:189:PRO:CD	2.58	0.52
1:B:283:ILE:HG22	1:B:287:LEU:CD1	2.39	0.52
1:A:27:GLU:H	1:A:27:GLU:CD	2.13	0.51
1:A:428:LEU:O	1:A:430:ASN:OD1	2.27	0.51
1:A:281:TYR:HA	1:A:355:PHE:CE1	2.45	0.51
1:A:352:LEU:HD21	1:A:362:ILE:CD1	2.40	0.51
1:B:138:VAL:HG12	1:B:142:ASP:OD2	2.11	0.51
1:B:26:ASN:C	1:B:28:GLN:N	2.62	0.51
1:B:378:VAL:HG12	1:B:379:ILE:N	2.26	0.51
1:A:29:ILE:HD11	1:A:33:ILE:CG1	2.39	0.51
1:B:205:ASP:C	1:B:207:LYS:N	2.62	0.51
1:A:29:ILE:HA	1:A:32:ILE:CG2	2.41	0.51
1:B:176:VAL:CG2	1:B:177:GLU:N	2.74	0.51
1:A:87:LYS:HZ1	1:B:19:GLU:CD	2.14	0.51
1:B:31:ASN:HD22	1:B:35:SER:HB2	1.76	0.51
1:B:89:ASN:OD1	1:B:92:THR:N	2.44	0.51
1:A:321:VAL:CG1	1:A:325:LEU:HD21	2.33	0.51
1:A:300:TYR:CE1	1:A:304:LEU:CB	2.93	0.51
1:B:271:HIS:O	1:B:275:SER:HB2	2.10	0.51
1:B:335:GLU:C	1:B:336:ILE:HD12	2.31	0.51
1:B:26:ASN:C	1:B:28:GLN:H	2.12	0.51
1:B:195:VAL:CG1	1:B:199:LEU:HD22	2.41	0.50
1:B:225:LEU:HD13	1:B:227:TYR:HB2	1.94	0.50
1:A:144:ARG:NH1	1:B:229:PRO:HG2	2.22	0.50
1:B:219:LYS:O	1:B:220:ILE:HG12	2.11	0.50
1:B:271:HIS:HA	1:B:274:LEU:CD1	2.41	0.50
1:B:137:PRO:HG2	1:B:279:TYR:OH	2.11	0.50
1:A:135:ARG:HG2	1:B:90:TYR:CD2	2.46	0.50
1:B:231:VAL:CG1	1:B:232:ILE:N	2.75	0.50
1:B:285:LYS:O	1:B:288:GLU:HB2	2.12	0.50
1:B:72:VAL:HG21	1:B:409:LEU:CB	2.42	0.50
1:A:104:LEU:HD12	1:A:107:MSE:HE1	1.92	0.50
1:B:114:ARG:NH1	1:B:170:ARG:NH1	2.54	0.50
1:A:94:ASP:OD2	1:A:98:ARG:HD2	2.12	0.50
1:B:256:LYS:O	1:B:257:VAL:HG13	2.12	0.50
1:B:357:ASN:O	1:B:360:LYS:HG2	2.11	0.50
1:A:54:ARG:CB	1:A:101:MSE:HE3	2.20	0.50
1:B:359:GLU:O	1:B:362:ILE:HG12	2.12	0.50
1:B:191:LEU:O	1:B:193:ASP:N	2.45	0.50
1:B:352:LEU:HD12	1:B:352:LEU:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:GLN:HA	1:A:103:THR:CG2	2.42	0.50
1:A:308:LEU:C	1:A:310:VAL:H	2.14	0.50
1:B:106:ASN:HA	1:B:286:LEU:HD22	1.92	0.50
1:B:82:TYR:OH	1:B:193:ASP:OD2	2.28	0.49
1:B:284:ASP:OD1	1:B:357:ASN:CB	2.51	0.49
1:B:47:ILE:HB	1:B:398:HIS:CD2	2.47	0.49
1:B:404:LEU:N	1:B:404:LEU:HD12	2.27	0.49
1:A:302:LYS:HG2	1:A:306:ARG:NH1	2.27	0.49
1:A:390:LYS:HB3	1:A:390:LYS:HZ3	1.78	0.49
1:B:204:ILE:HG22	1:B:208:VAL:CG2	2.42	0.49
1:B:228:SER:O	1:B:229:PRO:C	2.48	0.49
1:B:259:LEU:HB3	1:B:261:LEU:HD21	1.94	0.49
1:B:418:TYR:CE2	1:B:419:LYS:HG2	2.47	0.49
1:A:10:GLU:O	1:A:11:ARG:C	2.49	0.49
1:A:333:TYR:HB2	1:A:371:VAL:HG22	1.94	0.49
1:A:392:LEU:O	1:A:396:LEU:HG	2.12	0.49
1:B:102:GLU:HB3	1:B:279:TYR:HE1	1.77	0.49
1:B:175:LYS:O	1:B:178:GLU:HB2	2.12	0.49
1:B:182:LYS:CG	1:B:183:ASN:H	2.24	0.49
1:B:360:LYS:O	1:B:364:LYS:HB3	2.12	0.49
1:A:285:LYS:HE2	1:A:285:LYS:HA	1.94	0.49
1:B:305:ALA:HA	1:B:310:VAL:O	2.12	0.49
1:A:43:GLU:HG2	1:A:120:LYS:HZ2	1.76	0.49
1:B:172:HIS:HD2	1:B:175:LYS:HE3	1.78	0.49
1:A:136:PRO:HG2	1:A:138:VAL:CG2	2.43	0.49
1:A:299:PHE:CE2	1:A:300:TYR:CE2	3.00	0.49
1:A:419:LYS:O	1:A:422:ARG:HG2	2.13	0.49
1:B:110:TYR:HE2	1:B:114:ARG:CZ	2.25	0.49
1:B:13:THR:O	1:B:17:LEU:HG	2.13	0.49
1:B:369:ALA:CB	1:B:388:ILE:HG12	2.42	0.49
1:B:368:LEU:HD13	1:B:381:MSE:HE1	1.93	0.49
1:A:316:ALA:HB3	1:B:60:SER:OG	2.12	0.49
1:B:65:TYR:CZ	1:B:84:ASN:HB3	2.48	0.49
1:A:209:ILE:HG22	1:A:210:ALA:N	2.28	0.49
1:A:23:VAL:HG12	1:A:321:VAL:HG21	1.95	0.49
1:A:322:ILE:HG23	1:A:326:ILE:CG2	2.42	0.49
1:A:428:LEU:HD12	1:A:429:ILE:H	1.78	0.49
1:A:430:ASN:HB3	1:A:435:ARG:NE	2.28	0.49
1:B:267:TYR:C	1:B:267:TYR:CD2	2.85	0.48
1:B:31:ASN:ND2	1:B:35:SER:HB2	2.28	0.48
1:B:325:LEU:CG	1:B:326:ILE:N	2.74	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:THR:HG21	1:B:278:GLU:HG2	1.94	0.48
1:B:124:LEU:HD13	1:B:395:ILE:CD1	2.43	0.48
1:B:134:VAL:CG2	1:B:135:ARG:N	2.76	0.48
1:B:26:ASN:O	1:B:28:GLN:N	2.46	0.48
1:B:434:ASN:OD1	1:B:434:ASN:C	2.52	0.48
1:A:305:ALA:HA	1:A:312:ILE:H	1.78	0.48
1:B:114:ARG:HH22	1:B:170:ARG:HH12	1.59	0.48
1:A:329:GLU:HG2	1:A:329:GLU:O	2.13	0.48
1:A:370:TYR:HB3	1:A:379:ILE:HG21	1.95	0.48
1:B:141:GLU:O	1:B:144:ARG:HB3	2.13	0.48
1:A:27:GLU:O	1:A:29:ILE:N	2.46	0.48
1:A:343:PRO:HG2	1:A:346:SER:HB3	1.95	0.48
1:B:199:LEU:HD12	1:B:203:TYR:CD2	2.49	0.48
1:B:219:LYS:HA	1:B:257:VAL:O	2.13	0.48
1:A:324:THR:HG22	1:A:325:LEU:N	2.28	0.48
1:A:358:ILE:O	1:A:362:ILE:HG13	2.14	0.48
1:A:397:HIS:CD2	1:A:397:HIS:O	2.67	0.48
1:B:145:SER:HB3	1:B:269:ALA:HA	1.96	0.48
1:B:37:LYS:HD2	1:B:333:TYR:CZ	2.49	0.48
1:A:82:TYR:OH	1:A:193:ASP:OD1	2.29	0.48
1:A:241:ARG:HD2	1:B:246:ASP:OD1	2.13	0.48
1:A:29:ILE:CA	1:A:32:ILE:HG22	2.44	0.48
1:B:197:GLU:O	1:B:201:LYS:HG2	2.14	0.48
1:B:381:MSE:HE3	1:B:383:GLN:HG2	1.95	0.48
1:A:47:ILE:HG13	1:A:122:ALA:HB3	1.96	0.48
1:B:223:LYS:N	4:B:457:HOH:O	2.46	0.48
1:A:374:GLU:HB2	1:A:402:GLY:HA3	1.92	0.48
1:A:245:VAL:CG2	1:B:241:ARG:HA	2.44	0.48
1:B:348:PRO:O	1:B:352:LEU:HD13	2.14	0.48
1:B:354:LYS:N	1:B:354:LYS:HD2	2.28	0.48
1:A:138:VAL:HG23	1:A:139:TYR:H	1.79	0.47
1:A:328:HIS:CE1	1:A:330:LYS:HE3	2.49	0.47
1:A:87:LYS:HZ1	1:B:19:GLU:HG3	1.71	0.47
1:B:415:LYS:O	1:B:416:ILE:C	2.51	0.47
1:A:8:SER:HA	1:A:11:ARG:HD3	1.97	0.47
1:A:204:ILE:HD13	1:A:270:LEU:HD22	1.96	0.47
1:B:204:ILE:O	1:B:207:LYS:HB2	2.14	0.47
1:B:248:LEU:C	1:B:248:LEU:HD12	2.34	0.47
1:B:381:MSE:HE3	1:B:383:GLN:CG	2.44	0.47
1:B:72:VAL:HG21	1:B:409:LEU:HB3	1.97	0.47
1:A:378:VAL:HG13	1:B:440:LYS:HZ2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:PHE:CD2	1:B:399:LYS:HE3	2.49	0.47
1:B:164:GLU:OE2	1:B:203:TYR:OH	2.21	0.47
1:B:179:HIS:HA	1:B:182:LYS:HD3	1.96	0.47
1:B:232:ILE:HD11	1:B:236:VAL:HG21	1.96	0.47
1:B:243:LYS:CB	1:B:247:GLU:OE2	2.62	0.47
1:B:45:SER:OG	1:B:398:HIS:CD2	2.68	0.47
1:B:90:TYR:CD1	1:B:91:GLY:N	2.78	0.47
1:A:292:LEU:HB3	1:A:385:THR:CG2	2.45	0.47
1:A:80:LEU:HD13	1:A:108:LEU:HD13	1.96	0.47
1:A:124:LEU:HD21	1:A:295:ILE:CG1	2.44	0.47
1:B:149:MSE:CE	1:B:266:ILE:O	2.63	0.47
1:A:320:ALA:CA	1:B:434:ASN:HD21	2.28	0.47
1:A:133:LEU:HD13	1:A:133:LEU:N	2.29	0.47
1:A:29:ILE:O	1:A:30:ARG:C	2.53	0.47
1:A:31:ASN:OD1	1:A:32:ILE:N	2.46	0.47
1:B:135:ARG:HG2	1:B:136:PRO:HD2	1.96	0.47
1:B:247:GLU:HG2	1:B:248:LEU:N	2.29	0.47
1:B:400:ALA:HB2	1:B:405:ARG:N	2.30	0.47
1:A:21:GLU:HA	1:A:24:ARG:HB3	1.97	0.47
1:A:386:THR:HG21	1:A:390:LYS:NZ	2.30	0.47
1:B:64:ILE:HG21	1:B:422:ARG:NH2	2.30	0.47
1:A:33:ILE:O	1:A:36:TRP:CB	2.64	0.47
1:A:63:VAL:O	1:A:85:ALA:HA	2.15	0.47
1:B:128:THR:HG23	1:B:296:ALA:CB	2.45	0.47
1:A:23:VAL:O	1:A:24:ARG:C	2.52	0.46
1:B:273:THR:O	1:B:277:ILE:HG13	2.14	0.46
1:B:345:TRP:CE3	1:B:346:SER:HA	2.50	0.46
1:B:98:ARG:O	1:B:101:MSE:HB3	2.15	0.46
1:A:222:ARG:NH1	1:A:255:GLU:OE2	2.49	0.46
1:A:386:THR:HB	4:A:465:HOH:O	2.15	0.46
1:A:43:GLU:O	1:A:397:HIS:HB2	2.16	0.46
1:A:67:LEU:HD22	1:A:101:MSE:CE	2.46	0.46
1:A:141:GLU:O	1:A:144:ARG:CG	2.63	0.46
1:A:221:PRO:O	1:A:230:ARG:NH2	2.48	0.46
1:A:92:THR:O	1:A:96:ILE:HG12	2.15	0.46
1:A:249:LEU:O	1:A:252:LEU:HB2	2.16	0.46
1:A:323:ARG:NH2	1:A:376:GLY:O	2.48	0.46
1:A:57:SER:HB3	1:A:64:ILE:HG23	1.96	0.46
1:B:130:THR:O	1:B:134:VAL:HG13	2.16	0.46
1:B:195:VAL:HG12	1:B:199:LEU:HD22	1.98	0.46
1:B:343:PRO:HG2	1:B:346:SER:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:GLU:O	1:B:393:PRO:CD	2.63	0.46
1:A:136:PRO:O	1:A:138:VAL:N	2.49	0.46
1:A:49:ALA:HA	1:A:124:LEU:O	2.15	0.46
1:A:281:TYR:HA	1:A:355:PHE:HE1	1.80	0.46
1:B:114:ARG:NH2	1:B:170:ARG:HH22	2.14	0.46
1:B:191:LEU:C	1:B:193:ASP:N	2.65	0.46
1:A:130:THR:HG1	1:A:299:PHE:HZ	1.53	0.46
1:A:133:LEU:CD1	1:A:133:LEU:N	2.79	0.46
1:A:234:ILE:HA	1:A:234:ILE:HD12	1.65	0.46
1:A:89:ASN:CG	1:A:92:THR:HG23	2.37	0.46
1:B:164:GLU:CD	1:B:202:LYS:HZ1	2.19	0.46
1:B:405:ARG:HA	1:B:408:GLN:NE2	2.31	0.46
1:B:333:TYR:HE1	1:B:335:GLU:HB2	1.81	0.46
1:B:98:ARG:NH2	1:B:137:PRO:CB	2.59	0.46
1:B:187:ASP:C	1:B:189:PRO:HD3	2.36	0.45
1:B:47:ILE:HB	1:B:398:HIS:NE2	2.31	0.45
1:A:21:GLU:HB3	1:A:24:ARG:CZ	2.47	0.45
1:B:230:ARG:HG3	1:B:231:VAL:N	2.26	0.45
1:B:48:TYR:HA	1:B:73:GLY:HA3	1.98	0.45
1:A:126:ASP:C	1:A:126:ASP:OD1	2.55	0.45
1:A:217:LYS:HD2	1:A:260:TYR:HE1	1.81	0.45
1:A:300:TYR:HE1	1:A:304:LEU:CB	2.29	0.45
1:A:37:LYS:CG	1:A:38:PRO:HD2	2.42	0.45
1:B:172:HIS:CD2	1:B:175:LYS:HE3	2.51	0.45
1:A:115:LYS:HZ3	1:A:181:GLU:CA	2.30	0.45
1:A:9:ILE:O	1:A:13:THR:OG1	2.34	0.45
1:A:27:GLU:OE2	1:A:29:ILE:HG22	2.16	0.45
1:A:302:LYS:HE3	1:A:306:ARG:HH22	1.80	0.45
1:A:431:ALA:O	1:A:432:LEU:HD12	2.17	0.45
1:B:313:VAL:CG1	1:B:317:LEU:HB3	2.46	0.45
1:B:364:LYS:HG2	1:B:365:GLY:O	2.16	0.45
1:B:422:ARG:C	1:B:422:ARG:CD	2.85	0.45
1:A:320:ALA:HA	1:B:434:ASN:HD21	1.80	0.45
1:B:136:PRO:HB3	1:B:142:ASP:OD2	2.17	0.45
1:B:196:VAL:HG12	1:B:274:LEU:HD21	1.99	0.45
1:B:407:LEU:HD23	1:B:408:GLN:HG3	1.97	0.45
1:B:82:TYR:CE2	1:B:193:ASP:OD2	2.70	0.45
1:A:346:SER:O	1:A:347:PHE:HD1	1.98	0.45
1:B:172:HIS:O	1:B:175:LYS:HG2	2.17	0.45
1:B:192:THR:O	1:B:196:VAL:HG13	2.17	0.45
1:B:218:VAL:HB	1:B:259:LEU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:GLN:NE2	1:B:30:ARG:HB3	2.32	0.45
1:B:350:PHE:HD2	1:B:350:PHE:H	1.60	0.45
1:A:67:LEU:HA	1:A:101:MSE:HE1	1.98	0.45
1:A:307:THR:HG23	1:A:309:GLY:N	2.26	0.45
1:A:104:LEU:HA	1:A:107:MSE:HE3	1.99	0.45
1:A:222:ARG:HD3	1:A:255:GLU:OE2	2.17	0.45
1:A:67:LEU:HD22	1:A:101:MSE:HE2	1.98	0.45
1:A:87:LYS:HZ1	1:B:19:GLU:CG	2.26	0.45
1:B:172:HIS:NE2	1:B:176:VAL:CG1	2.80	0.45
1:A:139:TYR:O	1:A:140:PRO:C	2.55	0.44
1:A:48:TYR:CD1	1:A:112:ALA:HB1	2.52	0.44
1:B:217:LYS:HG2	1:B:260:TYR:CD1	2.48	0.44
1:A:21:GLU:CG	1:A:24:ARG:HD3	2.47	0.44
1:B:240:SER:O	1:B:243:LYS:HB2	2.18	0.44
1:B:295:ILE:HD11	1:B:382:LEU:HD13	2.00	0.44
1:B:130:THR:HG23	1:B:383:GLN:NE2	2.33	0.44
1:B:388:ILE:HG22	1:B:389:GLU:N	2.31	0.44
1:B:408:GLN:O	1:B:412:HIS:HB2	2.17	0.44
1:A:102:GLU:HG3	3:A:454:GOL:C2	2.47	0.44
1:A:146:LEU:HD22	1:A:273:THR:HG23	2.00	0.44
1:A:230:ARG:O	1:B:233:PRO:HA	2.16	0.44
1:A:430:ASN:C	1:A:432:LEU:N	2.71	0.44
1:B:138:VAL:HG11	1:B:272:MSE:SE	2.67	0.44
1:A:299:PHE:C	1:A:299:PHE:CD2	2.91	0.44
1:A:300:TYR:CD1	1:A:300:TYR:C	2.91	0.44
1:B:205:ASP:C	1:B:207:LYS:H	2.20	0.44
1:B:407:LEU:HD23	1:B:408:GLN:CA	2.48	0.44
1:A:356:ARG:O	1:A:360:LYS:HG3	2.17	0.44
1:A:422:ARG:CG	1:A:423:HIS:N	2.81	0.44
1:A:428:LEU:CD1	1:A:429:ILE:N	2.79	0.44
1:B:103:THR:OG1	1:B:279:TYR:HA	2.18	0.44
1:B:134:VAL:HG23	1:B:135:ARG:N	2.32	0.44
1:B:420:GLU:HG3	1:B:423:HIS:NE2	2.32	0.44
1:A:320:ALA:HB1	1:B:434:ASN:HD21	1.83	0.44
1:B:89:ASN:OD1	1:B:92:THR:CB	2.61	0.44
1:A:299:PHE:HD2	1:A:299:PHE:C	2.21	0.44
1:A:299:PHE:HE2	1:A:300:TYR:CE2	2.35	0.44
1:B:179:HIS:HA	1:B:182:LYS:CD	2.48	0.44
1:B:206:THR:C	1:B:207:LYS:HD2	2.38	0.44
1:B:318:LEU:HD23	1:B:370:TYR:CD1	2.53	0.44
1:A:320:ALA:CB	1:B:434:ASN:HD21	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:LEU:O	1:A:395:ILE:HG22	2.17	0.44
1:A:51:ASP:C	1:A:414:VAL:HG21	2.38	0.44
1:B:319:ASP:O	1:B:322:ILE:HG12	2.17	0.44
1:A:263:LYS:HE3	1:A:263:LYS:HB2	1.74	0.43
1:A:27:GLU:C	1:A:29:ILE:N	2.71	0.43
1:B:180:LEU:HA	1:B:180:LEU:HD23	1.51	0.43
1:B:191:LEU:O	1:B:194:ASN:N	2.51	0.43
1:B:333:TYR:CE1	1:B:388:ILE:HG21	2.53	0.43
1:B:373:PHE:CE1	1:B:399:LYS:HE3	2.53	0.43
1:B:188:SER:N	1:B:189:PRO:HD3	2.33	0.43
1:B:89:ASN:ND2	1:B:92:THR:HB	2.33	0.43
1:A:153:ILE:HD11	1:A:158:PHE:HA	2.00	0.43
1:A:313:VAL:HG12	1:A:313:VAL:O	2.18	0.43
1:A:313:VAL:CG1	1:A:318:LEU:HB2	2.46	0.43
1:B:199:LEU:HD12	1:B:203:TYR:CE2	2.53	0.43
1:A:8:SER:OG	1:B:83:ALA:HB3	2.18	0.43
1:A:26:ASN:HD22	1:A:30:ARG:NE	2.16	0.43
1:A:386:THR:CG2	1:A:390:LYS:HB2	2.48	0.43
1:B:223:LYS:HA	1:B:223:LYS:HD3	1.63	0.43
1:B:28:GLN:HG3	1:B:29:ILE:N	2.32	0.43
1:A:27:GLU:OE2	1:A:29:ILE:CG2	2.66	0.43
1:B:116:LEU:HA	1:B:116:LEU:HD12	1.88	0.43
1:B:276:TYR:O	1:B:279:TYR:HB3	2.18	0.43
1:B:136:PRO:CB	1:B:142:ASP:OD2	2.67	0.43
1:B:130:THR:HG23	1:B:383:GLN:HE22	1.83	0.43
1:A:316:ALA:HB2	1:B:440:LYS:HD3	2.01	0.43
1:B:101:MSE:CE	1:B:101:MSE:HA	2.47	0.43
1:B:116:LEU:HB3	1:B:121:ARG:HD3	2.00	0.43
1:B:138:VAL:HG22	1:B:138:VAL:O	2.18	0.43
1:B:191:LEU:HD13	1:B:191:LEU:H	1.82	0.43
1:A:232:ILE:C	1:B:231:VAL:HG13	2.39	0.43
1:A:21:GLU:OE1	1:A:24:ARG:NH1	2.50	0.43
1:A:386:THR:CG2	1:A:387:ASN:N	2.82	0.43
1:A:243:LYS:HE2	1:A:243:LYS:HB3	1.81	0.43
1:A:33:ILE:HA	1:A:33:ILE:HD13	1.77	0.43
1:A:80:LEU:HD23	1:A:107:MSE:HE3	2.01	0.43
1:B:14:LYS:O	1:B:18:ASP:OD2	2.36	0.43
1:B:280:LEU:HD23	1:B:283:ILE:HD12	2.01	0.43
1:B:304:LEU:HD13	1:B:304:LEU:HA	1.87	0.43
1:B:39:LEU:HG	1:B:332:GLY:HA2	2.01	0.43
1:B:343:PRO:CG	1:B:346:SER:HB3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:ASP:OD2	1:B:355:PHE:HA	2.19	0.43
1:B:360:LYS:O	1:B:363:ASP:HB2	2.19	0.43
1:B:370:TYR:CB	1:B:379:ILE:HD11	2.40	0.43
1:A:79:ARG:HB3	1:A:185:ASN:CB	2.48	0.42
1:A:247:GLU:O	1:A:251:GLU:HG3	2.19	0.42
1:A:425:LEU:O	1:A:428:LEU:HD21	2.19	0.42
1:B:260:TYR:C	1:B:261:LEU:HD23	2.39	0.42
1:A:170:ARG:O	1:A:174:ARG:HG3	2.18	0.42
1:A:369:ALA:HB2	1:A:388:ILE:HG13	1.99	0.42
1:A:130:THR:HG23	1:A:383:GLN:HE22	1.83	0.42
1:B:106:ASN:HB3	1:B:282:SER:O	2.19	0.42
1:A:26:ASN:HD22	1:A:30:ARG:HD2	1.83	0.42
1:A:319:ASP:OD1	1:A:319:ASP:C	2.58	0.42
1:A:89:ASN:CB	1:A:92:THR:HG23	2.49	0.42
1:B:206:THR:HB	1:B:207:LYS:HZ3	1.83	0.42
1:B:96:ILE:HD11	1:B:272:MSE:CE	2.37	0.42
1:A:279:TYR:CZ	1:A:283:ILE:HD11	2.54	0.42
1:A:60:SER:OG	1:A:61:GLY:N	2.52	0.42
1:A:64:ILE:O	1:A:64:ILE:HG23	2.20	0.42
1:B:202:LYS:O	1:B:207:LYS:NZ	2.53	0.42
1:B:373:PHE:CE2	1:B:399:LYS:CE	2.98	0.42
1:B:368:LEU:HD22	1:B:383:GLN:HG2	2.02	0.42
1:B:95:GLN:CB	1:B:138:VAL:HG23	2.47	0.42
1:B:179:HIS:CA	1:B:182:LYS:HG2	2.44	0.42
1:B:218:VAL:N	1:B:259:LEU:O	2.52	0.42
1:B:284:ASP:OD2	1:B:355:PHE:HB3	2.20	0.42
1:A:136:PRO:HG2	1:A:138:VAL:HG21	2.01	0.42
1:A:125:MSE:HE1	1:A:286:LEU:HD11	2.01	0.42
1:A:316:ALA:HA	1:B:440:LYS:HD2	2.01	0.42
1:B:256:LYS:O	1:B:257:VAL:CG1	2.68	0.42
1:B:318:LEU:O	1:B:321:VAL:HB	2.20	0.42
1:B:287:LEU:CD1	1:B:358:ILE:HD13	2.50	0.42
1:A:342:PRO:HG2	1:A:362:ILE:HG12	2.01	0.42
1:A:89:ASN:N	1:A:93:SER:HB3	2.34	0.42
1:B:65:TYR:CE1	1:B:100:GLN:OE1	2.73	0.42
1:B:171:ASP:HA	1:B:174:ARG:HH11	1.83	0.42
1:A:167:GLU:HG3	1:A:168:LYS:N	2.35	0.42
1:A:29:ILE:O	1:A:29:ILE:HD12	2.19	0.42
1:A:374:GLU:OE1	1:A:374:GLU:HA	2.19	0.42
1:A:386:THR:HG21	1:A:390:LYS:HZ3	1.84	0.42
1:B:369:ALA:HB2	1:B:388:ILE:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:LEU:HD12	1:B:440:LYS:H	1.84	0.42
1:B:350:PHE:CD2	1:B:350:PHE:N	2.76	0.42
1:B:405:ARG:O	1:B:406:PRO:C	2.56	0.42
1:A:236:VAL:HG12	1:A:248:LEU:HD11	2.02	0.41
1:B:129:LEU:HA	1:B:129:LEU:HD23	1.70	0.41
1:B:27:GLU:O	1:B:28:GLN:C	2.56	0.41
1:B:433:ARG:CG	1:B:434:ASN:N	2.79	0.41
1:A:236:VAL:CG1	1:A:248:LEU:HD11	2.50	0.41
1:A:367:HIS:CE1	4:A:461:HOH:O	2.72	0.41
1:B:334:LEU:HD12	1:B:334:LEU:C	2.41	0.41
1:B:84:ASN:ND2	1:B:193:ASP:OD2	2.54	0.41
1:B:364:LYS:HG2	1:B:365:GLY:N	2.35	0.41
1:B:64:ILE:HG13	1:B:422:ARG:HH22	1.86	0.41
1:B:56:VAL:HG13	1:B:63:VAL:HG13	2.02	0.41
1:A:57:SER:HB3	1:A:64:ILE:CG2	2.51	0.41
1:A:89:ASN:HB3	1:A:92:THR:HG23	2.02	0.41
1:B:293:ALA:CB	1:B:395:ILE:HD11	2.50	0.41
1:A:173:TYR:CE1	1:A:285:LYS:HG3	2.56	0.41
1:A:250:GLN:O	1:A:254:GLU:HB2	2.20	0.41
1:B:196:VAL:HG23	1:B:197:GLU:N	2.35	0.41
1:B:295:ILE:CD1	1:B:382:LEU:HD13	2.51	0.41
1:B:32:ILE:HD13	1:B:325:LEU:HD21	1.97	0.41
1:B:362:ILE:CG1	1:B:363:ASP:N	2.79	0.41
1:B:434:ASN:OD1	1:B:436:ASP:CG	2.59	0.41
1:A:129:LEU:HD13	1:A:294:TYR:CE2	2.55	0.41
1:A:138:VAL:CG2	1:A:139:TYR:N	2.83	0.41
1:A:198:LYS:HB2	1:A:198:LYS:HE3	1.86	0.41
1:B:396:LEU:HA	1:B:396:LEU:HD23	1.76	0.41
1:A:27:GLU:N	1:A:27:GLU:CD	2.74	0.41
1:A:340:VAL:CG1	1:A:341:VAL:N	2.54	0.41
1:A:395:ILE:HA	1:A:395:ILE:HD13	1.68	0.41
1:B:135:ARG:CG	1:B:136:PRO:HD2	2.51	0.41
1:B:95:GLN:HB3	1:B:138:VAL:HA	2.03	0.41
1:B:153:ILE:O	1:B:157:ASP:HB2	2.19	0.41
1:B:166:LEU:HA	1:B:166:LEU:HD12	1.83	0.41
1:B:371:VAL:O	1:B:379:ILE:HA	2.21	0.41
1:A:352:LEU:HA	1:A:352:LEU:HD12	1.82	0.41
1:B:139:TYR:C	1:B:141:GLU:N	2.73	0.41
1:B:176:VAL:HG12	1:B:186:TYR:HE2	1.86	0.41
1:B:336:ILE:HD13	1:B:368:LEU:O	2.21	0.41
1:B:70:LEU:HD12	1:B:78:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ASN:OD1	1:B:92:THR:CA	2.69	0.41
1:A:95:GLN:NE2	1:A:138:VAL:O	2.53	0.41
1:A:59:LEU:HD13	1:A:64:ILE:HG22	2.02	0.41
1:A:6:LYS:O	1:A:9:ILE:HG22	2.21	0.41
1:B:149:MSE:HG3	1:B:273:THR:HG21	2.02	0.41
1:B:190:ILE:HG23	1:B:192:THR:OG1	2.21	0.41
1:B:304:LEU:O	1:B:310:VAL:HG13	2.21	0.41
1:A:43:GLU:HG2	1:A:120:LYS:HZ3	1.85	0.41
1:B:47:ILE:HG21	1:B:406:PRO:HG2	2.03	0.41
1:A:104:LEU:HA	1:A:107:MSE:CE	2.51	0.41
1:B:245:VAL:HG12	1:B:249:LEU:CD1	2.48	0.41
1:B:436:ASP:O	1:B:437:PRO:C	2.58	0.41
1:B:166:LEU:O	1:B:169:LEU:HB2	2.21	0.40
1:A:434:ASN:OD1	1:A:434:ASN:O	2.40	0.40
1:B:169:LEU:O	1:B:172:HIS:HB3	2.21	0.40
1:A:11:ARG:H	1:A:11:ARG:CD	2.34	0.40
1:A:79:ARG:O	1:A:185:ASN:HA	2.22	0.40
1:B:164:GLU:OE2	1:B:202:LYS:CE	2.70	0.40
1:B:356:ARG:HA	1:B:359:GLU:HB3	2.04	0.40
1:B:373:PHE:CE2	1:B:374:GLU:CD	2.95	0.40
1:A:171:ASP:O	1:A:174:ARG:HB2	2.21	0.40
1:A:26:ASN:HD22	1:A:30:ARG:CD	2.34	0.40
1:B:419:LYS:O	1:B:422:ARG:HB3	2.21	0.40
1:A:130:THR:HG23	1:A:383:GLN:NE2	2.36	0.40
1:A:67:LEU:HD13	1:A:101:MSE:HA	2.03	0.40
1:B:404:LEU:O	1:B:407:LEU:HB3	2.22	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	418/471 (89%)	370 (88%)	46 (11%)	2 (0%)	32	73
1	B	411/471 (87%)	345 (84%)	62 (15%)	4 (1%)	18	60
All	All	829/942 (88%)	715 (86%)	108 (13%)	6 (1%)	25	67

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	29	ILE
1	A	310	VAL
1	B	27	GLU
1	B	312	ILE
1	B	230	ARG
1	A	375	GLN

### 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	378/410 (92%)	325 (86%)	53 (14%)	4	18
1	B	380/410 (93%)	318 (84%)	62 (16%)	3	12
All	All	758/820 (92%)	643 (85%)	115 (15%)	3	15

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	13	THR
1	A	27	GLU
1	A	29	ILE
1	A	48	TYR
1	A	50	VAL
1	A	56	VAL
1	A	58	ARG
1	A	72	VAL
1	A	90	TYR

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Mol	Chain	Res	Type
1	A	92	THR
1	A	95	GLN
1	A	102	GLU
1	A	103	THR
1	A	126	ASP
1	A	128	THR
1	A	133	LEU
1	A	142	ASP
1	A	144	ARG
1	A	155	GLU
1	A	160	ASN
1	A	188	SER
1	A	191	LEU
1	A	234	ILE
1	A	246	ASP
1	A	249	LEU
1	A	258	GLU
1	A	266	ILE
1	A	280	LEU
1	A	282	SER
1	A	292	LEU
1	A	299	PHE
1	A	300	TYR
1	A	303	THR
1	A	318	LEU
1	A	321	VAL
1	A	324	THR
1	A	325	LEU
1	A	328	HIS
1	A	349	ASP
1	A	352	LEU
1	A	353	SER
1	A	363	ASP
1	A	368	LEU
1	A	381	MSE
1	A	385	THR
1	A	386	THR
1	A	395	ILE
1	A	414	VAL
1	A	423	HIS
1	A	424	THR
1	A	425	LEU

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Mol	Chain	Res	Type
1	A	428	LEU
1	B	20	LEU
1	B	30	ARG
1	B	31	ASN
1	B	48	TYR
1	B	82	TYR
1	B	101	MSE
1	B	102	GLU
1	B	104	LEU
1	B	114	ARG
1	B	117	GLU
1	B	123	ILE
1	B	126	ASP
1	B	129	LEU
1	B	139	TYR
1	B	150	ARG
1	B	153	ILE
1	B	161	LEU
1	B	162	LEU
1	B	166	LEU
1	B	180	LEU
1	B	181	GLU
1	B	185	ASN
1	B	186	TYR
1	B	191	LEU
1	B	192	THR
1	B	199	LEU
1	B	216	VAL
1	B	225	LEU
1	B	236	VAL
1	B	247	GLU
1	B	248	LEU
1	B	249	LEU
1	B	274	LEU
1	B	275	SER
1	B	291	ASN
1	B	298	SER
1	B	301	THR
1	B	302	LYS
1	B	312	ILE
1	B	317	LEU
1	B	325	LEU

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Mol	Chain	Res	Type
1	B	326	ILE
1	B	333	TYR
1	B	334	LEU
1	B	340	VAL
1	B	341	VAL
1	B	350	PHE
1	B	366	ILE
1	B	371	VAL
1	B	374	GLU
1	B	377	ASP
1	B	379	ILE
1	B	385	THR
1	B	407	LEU
1	B	414	VAL
1	B	415	LYS
1	B	418	TYR
1	B	422	ARG
1	B	424	THR
1	B	426	GLU
1	B	428	LEU
1	B	432	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	26	ASN
1	A	95	GLN
1	A	271	HIS
1	A	397	HIS
1	B	28	GLN
1	B	172	HIS
1	B	185	ASN
1	B	398	HIS
1	B	408	GLN
1	B	411	HIS

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are 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	GOL	A	454	-	5,5,5	0.33	0	5,5,5	0.34	0

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	GOL	A	454	-	-	0/4/4/4	0/0/0/0

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.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	454	GOL	3	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	417/471 (88%)	-0.18	9 (2%)	62 46	52, 103, 201, 270	0
1	B	414/471 (87%)	-0.13	8 (1%)	67 51	72, 130, 200, 374	0
All	All	831/942 (88%)	-0.15	17 (2%)	65 49	52, 118, 201, 374	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	34	ASN	6.4
1	A	301	THR	5.9
1	B	35	SER	4.8
1	A	338	HIS	3.0
1	B	318	LEU	2.9
1	A	402	GLY	2.9
1	A	30	ARG	2.7
1	B	325	LEU	2.7
1	B	322	ILE	2.7
1	A	26	ASN	2.5
1	B	300	TYR	2.5
1	A	344	LYS	2.2
1	A	66	PHE	2.2
1	B	370	TYR	2.2
1	B	437	PRO	2.2
1	A	403	TYR	2.0
1	A	326	ILE	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 [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	A	454	6/6	0.80	0.86	13.80	95,114,126,129	0
2	MN	A	453	1/1	0.90	0.10	-	131,131,131,131	0
2	MN	B	453	1/1	0.29	0.26	-	235,235,235,235	0
2	MN	B	452	1/1	0.94	0.20	-	103,103,103,103	0
2	MN	A	452	1/1	0.99	0.28	-	93,93,93,93	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.