Full wwPDB X-ray Structure Validation Report (i)

Jan 30, 2024 – 09:59 PM EST

PDB ID	:	1K7L
Title	:	The 2.5 Angstrom resolution crystal structure of the human PPARalpha ligand binding domain bound with GW409544 and a co-activator peptide.
Authors	:	Xu, H.E.; Lambert, M.H.; Montana, V.G.; Moore, L.B.; Collins, J.L.; Oplinger, J.A.; Kliewer, S.A.; Gampe Jr., R.T.; McKee, D.D.; Moore, J.T.; Willson, T.M.
Deposited on	:	2001-10-19
Resolution	:	2.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

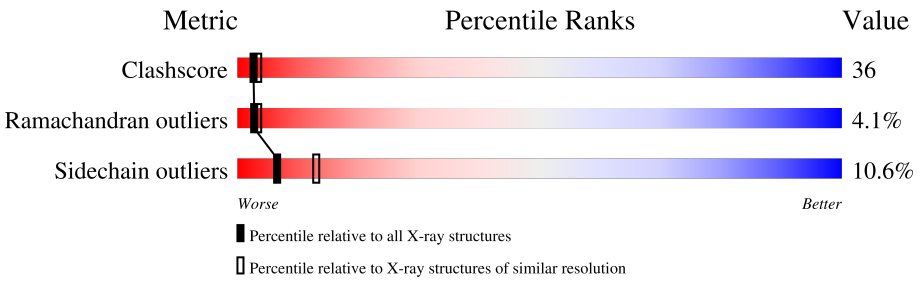
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	288	45% 39% 7% • 7%
1	C	288	55% 29% 8% • 7%
1	E	288	55% 30% 7% • 7%
1	G	288	46% 38% 9% 7%
2	B	21	24% 33% 5% 38%
2	D	21	24% 24% 14% 38%
2	F	21	19% 38% 5% 38%
2	H	21	14% 43% 5% 38%

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	544	A	469	X	-	-	-
3	544	C	470	X	-	-	-
3	544	E	501	X	-	-	-
3	544	G	601	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9308 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 Peroxisome proliferator activated receptor alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	267	2118	1359	355	386	18	0	0	0
1	C	267	2118	1359	355	386	18	0	0	0
1	E	267	2118	1359	355	386	18	0	0	0
1	G	267	2118	1359	355	386	18	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	MET	-	expression tag	UNP Q07869
A	182	LYS	-	expression tag	UNP Q07869
A	183	LYS	-	expression tag	UNP Q07869
A	184	GLY	-	expression tag	UNP Q07869
A	185	HIS	-	expression tag	UNP Q07869
A	186	HIS	-	expression tag	UNP Q07869
A	187	HIS	-	expression tag	UNP Q07869
A	188	HIS	-	expression tag	UNP Q07869
A	189	HIS	-	expression tag	UNP Q07869
A	190	HIS	-	expression tag	UNP Q07869
A	191	GLY	-	expression tag	UNP Q07869
C	181	MET	-	expression tag	UNP Q07869
C	182	LYS	-	expression tag	UNP Q07869
C	183	LYS	-	expression tag	UNP Q07869
C	184	GLY	-	expression tag	UNP Q07869
C	185	HIS	-	expression tag	UNP Q07869
C	186	HIS	-	expression tag	UNP Q07869
C	187	HIS	-	expression tag	UNP Q07869
C	188	HIS	-	expression tag	UNP Q07869
C	189	HIS	-	expression tag	UNP Q07869
C	190	HIS	-	expression tag	UNP Q07869

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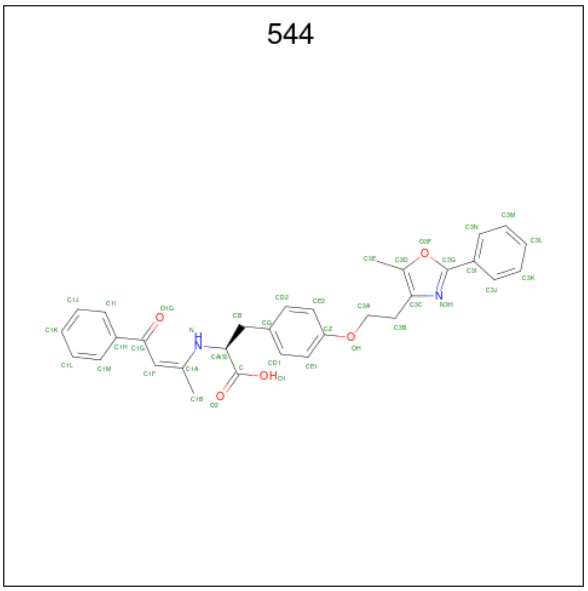
Chain	Residue	Modelled	Actual	Comment	Reference
C	191	GLY	-	expression tag	UNP Q07869
E	181	MET	-	expression tag	UNP Q07869
E	182	LYS	-	expression tag	UNP Q07869
E	183	LYS	-	expression tag	UNP Q07869
E	184	GLY	-	expression tag	UNP Q07869
E	185	HIS	-	expression tag	UNP Q07869
E	186	HIS	-	expression tag	UNP Q07869
E	187	HIS	-	expression tag	UNP Q07869
E	188	HIS	-	expression tag	UNP Q07869
E	189	HIS	-	expression tag	UNP Q07869
E	190	HIS	-	expression tag	UNP Q07869
E	191	GLY	-	expression tag	UNP Q07869
G	181	MET	-	expression tag	UNP Q07869
G	182	LYS	-	expression tag	UNP Q07869
G	183	LYS	-	expression tag	UNP Q07869
G	184	GLY	-	expression tag	UNP Q07869
G	185	HIS	-	expression tag	UNP Q07869
G	186	HIS	-	expression tag	UNP Q07869
G	187	HIS	-	expression tag	UNP Q07869
G	188	HIS	-	expression tag	UNP Q07869
G	189	HIS	-	expression tag	UNP Q07869
G	190	HIS	-	expression tag	UNP Q07869
G	191	GLY	-	expression tag	UNP Q07869

- Molecule 2 is a protein called steroid receptor coactivator.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	13	110	68	24	18	0	0	0
2	D	13	110	68	24	18	0	0	0
2	F	13	110	68	24	18	0	0	0
2	H	13	110	68	24	18	0	0	0

- Molecule 3 is 2-(1-METHYL-3-OXO-3-PHENYL-PROPYLAMINO)-3-{4-[2-(5-METHYL-2-PHENYL-OXAZOL-4-YL)-ETHOXY]-PHENYL}-PROPIONIC ACID (three-letter code: 544) (formula: $C_{31}H_{30}N_2O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	38	31	2	5	0	0
3	C	1	38	31	2	5	0	0
3	E	1	38	31	2	5	0	0
3	G	1	38	31	2	5	0	0

- Molecule 4 is YTTRIUM (III) ION (three-letter code: YT3) (formula: Y).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Y		
4	C	1	1	1	0	0
4	E	1	1	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	46	46	46	0	0
5	C	76	76	76	0	0
5	D	7	7	7	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	E	51	51	51	0	0
			Total	O		
5	F	1	1	1	0	0
			Total	O		
5	G	57	57	57	0	0
			Total	O		
5	H	4	4	4	0	0

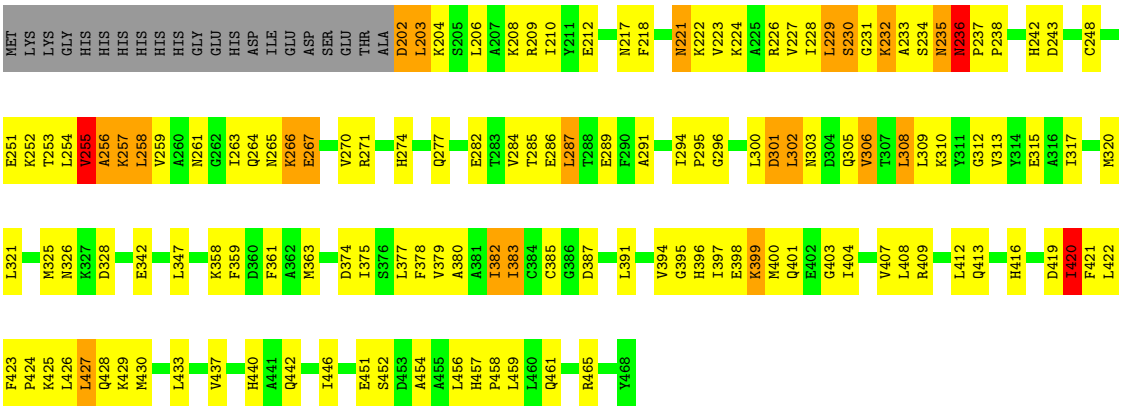
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

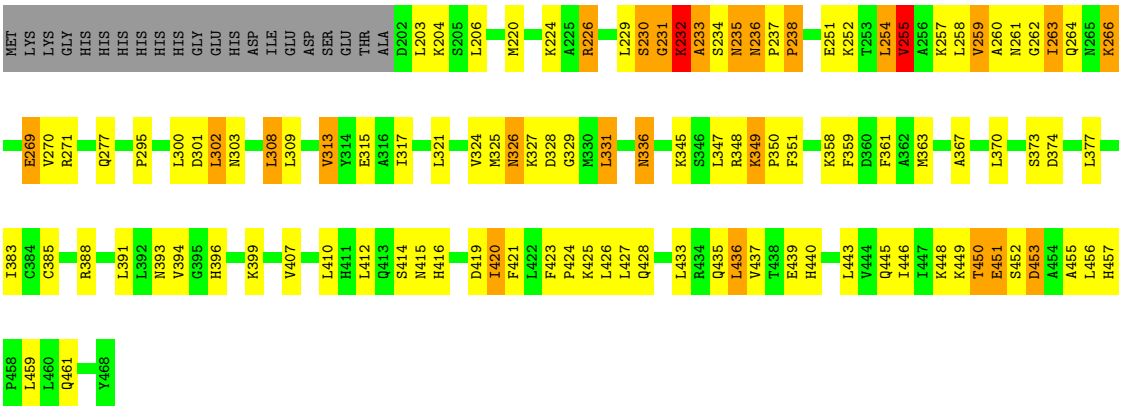
• Molecule 1: Peroxisome proliferator activated receptor alpha

Chain A: 45% 39% 7% • 7%



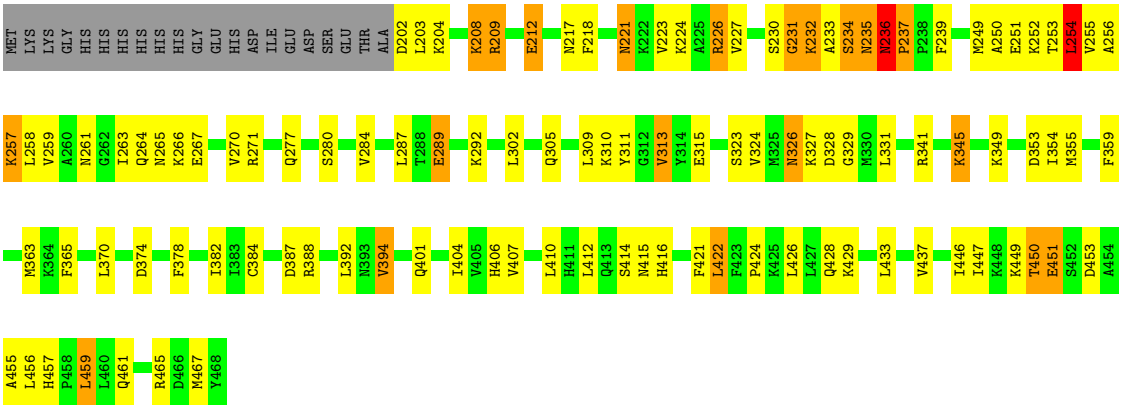
• Molecule 1: Peroxisome proliferator activated receptor alpha

Chain C: 55% 29% 8% • 7%



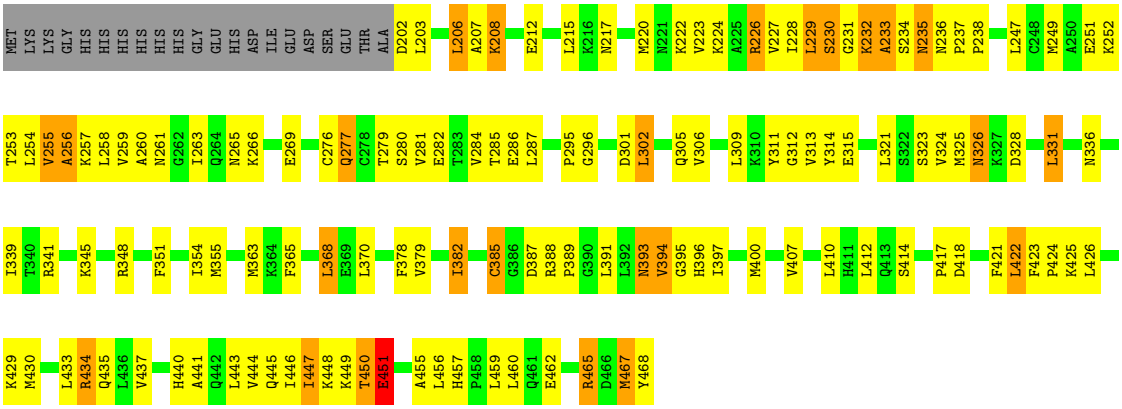
• Molecule 1: Peroxisome proliferator activated receptor alpha

Chain E: 55% 30% 7% • 7%



• Molecule 1: Peroxisome proliferator activated receptor alpha

Chain G:

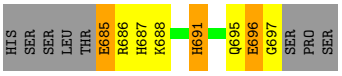


• Molecule 2: steroid receptor coactivator

Chain B:

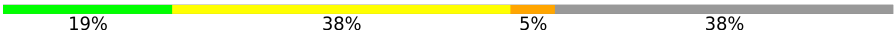
• Molecule 2: steroid receptor coactivator

Chain D:



• Molecule 2: steroid receptor coactivator

Chain F:



• Molecule 2: steroid receptor coactivator

Chain H: 14% 43% 5% 38%

HIS SER SER LEU THR E685 R686 H687 K688 I689 L690 H691 R692 L693 L694 Q695 E696 G697 SER PRO SER

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	95.56Å 121.60Å 121.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.50	Depositor
% Data completeness (in resolution range)	98.3 (19.99-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	CNX 2000.1	Depositor
R, R_{free}	0.247 , 0.284	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9308	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 544, YT3

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	0.40	0/2156	0.63	3/2906 (0.1%)
1	C	0.44	0/2156	0.68	1/2906 (0.0%)
1	E	0.42	0/2156	0.65	0/2906
1	G	0.42	0/2156	0.65	1/2906 (0.0%)
2	B	0.30	0/111	0.48	0/147
2	D	0.37	0/111	0.67	0/147
2	F	0.40	0/111	0.53	0/147
2	H	0.30	0/111	0.41	0/147
All	All	0.42	0/9068	0.65	5/12212 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	256	ALA	N-CA-C	-5.90	95.07	111.00
1	G	256	ALA	N-CA-C	-5.74	95.50	111.00
1	A	266	LYS	N-CA-C	-5.57	95.96	111.00
1	C	266	LYS	N-CA-C	-5.17	97.04	111.00
1	A	258	LEU	CA-CB-CG	5.13	127.09	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2118	0	2161	179	0
1	C	2118	0	2161	179	0
1	E	2118	0	2161	122	0
1	G	2118	0	2161	167	0
2	B	110	0	108	14	0
2	D	110	0	108	11	0
2	F	110	0	108	12	0
2	H	110	0	108	16	0
3	A	38	0	28	1	0
3	C	38	0	28	2	0
3	E	38	0	29	0	0
3	G	38	0	29	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
5	A	46	0	0	0	0
5	C	76	0	0	10	0
5	D	7	0	0	1	0
5	E	51	0	0	2	0
5	F	1	0	0	0	0
5	G	57	0	0	3	0
5	H	4	0	0	1	0
All	All	9308	0	9190	660	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 36.

All (660) 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:E:253:THR:HG23	1:E:254:LEU:H	1.09	1.09
1:A:252:LYS:HG3	1:A:259:VAL:HG21	1.39	1.04
1:E:251:GLU:HA	1:E:255:VAL:HB	1.41	1.02
1:C:420:ILE:HG13	1:C:421:PHE:H	1.23	1.00
1:E:202:ASP:O	1:E:204:LYS:N	1.93	1.00
1:E:208:LYS:O	1:E:212:GLU:HG2	1.61	0.99
1:C:252:LYS:HA	1:C:259:VAL:HG11	1.43	0.98
1:C:420:ILE:HB	1:G:336:ASN:HB3	1.44	0.98
1:A:258:LEU:HD22	1:A:263:ILE:HG21	1.43	0.97
1:A:302:LEU:HA	1:A:305:GLN:HE21	1.27	0.97
2:F:685:GLU:HG3	2:F:686:ARG:H	1.27	0.97
1:A:263:ILE:HG23	1:A:266:LYS:HD2	1.47	0.96
1:C:255:VAL:HG13	1:C:257:LYS:HB3	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:VAL:HG21	1:A:258:LEU:HB2	1.51	0.93
1:C:232:LYS:HZ2	1:C:235:ASN:HA	1.33	0.92
1:G:263:ILE:HG23	1:G:266:LYS:HD2	1.52	0.91
1:A:379:VAL:O	1:A:383:ILE:HG22	1.70	0.91
1:E:457:HIS:HD2	1:E:459:LEU:H	1.10	0.91
1:A:255:VAL:HB	1:A:257:LYS:H	1.38	0.89
1:E:253:THR:HG23	1:E:254:LEU:N	1.88	0.88
1:G:354:ILE:HG12	1:G:443:LEU:HD21	1.54	0.88
2:D:685:GLU:HG3	2:D:686:ARG:H	1.40	0.87
1:G:284:VAL:HG22	1:G:313:VAL:HG21	1.56	0.86
1:G:418:ASP:HB2	5:G:602:HOH:O	1.76	0.86
1:C:255:VAL:CG1	1:C:258:LEU:H	1.89	0.86
1:A:255:VAL:HG11	1:A:258:LEU:HG	1.57	0.85
1:C:255:VAL:CG1	1:C:257:LYS:H	1.89	0.85
1:A:255:VAL:HB	1:A:258:LEU:H	1.43	0.84
1:E:253:THR:CG2	1:E:254:LEU:H	1.91	0.84
1:E:326:ASN:C	1:E:326:ASN:HD22	1.80	0.84
1:C:254:LEU:O	1:C:255:VAL:HB	1.78	0.83
1:A:224:LYS:O	1:A:227:VAL:HG12	1.78	0.83
1:A:277:GLN:OE1	1:A:457:HIS:N	2.08	0.83
1:A:302:LEU:HD12	1:A:303:ASN:N	1.92	0.83
1:A:255:VAL:HG12	1:A:257:LYS:HB3	1.61	0.83
1:G:447:ILE:HD12	1:G:451:GLU:HB3	1.58	0.83
1:C:457:HIS:HD2	1:C:459:LEU:H	1.27	0.83
1:A:385:CYS:HA	1:A:401:GLN:NE2	1.92	0.83
1:G:326:ASN:HD22	1:G:326:ASN:C	1.83	0.82
1:C:235:ASN:CG	1:C:237:PRO:HD3	2.00	0.82
1:C:420:ILE:HG13	1:C:421:PHE:N	1.96	0.81
1:C:420:ILE:HD12	1:G:336:ASN:O	1.79	0.81
1:C:420:ILE:HD11	1:C:425:LYS:CE	2.09	0.81
1:C:302:LEU:HD12	1:C:303:ASN:N	1.96	0.81
1:C:421:PHE:HB3	1:C:424:PRO:CG	2.10	0.81
1:E:354:ILE:HG22	1:E:355:MET:HE2	1.61	0.81
1:G:277:GLN:NE2	1:G:456:LEU:HA	1.95	0.81
1:A:208:LYS:O	1:A:212:GLU:HG3	1.81	0.80
1:C:232:LYS:NZ	1:C:235:ASN:HD22	1.77	0.80
1:C:226:ARG:HG2	1:C:226:ARG:HH11	1.45	0.80
1:A:420:ILE:CG2	1:A:421:PHE:N	2.43	0.80
1:C:446:ILE:O	1:C:450:THR:HB	1.82	0.79
1:G:257:LYS:HA	1:G:261:ASN:ND2	1.97	0.79
1:A:403:GLY:O	1:A:407:VAL:HG23	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:222:LYS:HE3	1:G:370:LEU:O	1.82	0.79
1:A:232:LYS:HE3	1:A:237:PRO:HD3	1.62	0.79
1:C:421:PHE:HB3	1:C:424:PRO:HG3	1.63	0.79
1:C:252:LYS:HG2	1:C:259:VAL:HG21	1.64	0.79
1:A:420:ILE:CG2	1:A:421:PHE:H	1.96	0.78
1:A:412:LEU:HD11	1:A:426:LEU:HD12	1.65	0.78
1:E:263:ILE:HG23	1:E:266:LYS:HD2	1.65	0.78
1:G:263:ILE:HG12	1:G:266:LYS:NZ	1.97	0.78
1:C:255:VAL:HG12	1:C:257:LYS:H	1.46	0.78
1:C:232:LYS:NZ	1:C:235:ASN:HA	1.97	0.78
1:C:235:ASN:CG	1:C:236:ASN:H	1.86	0.78
1:E:457:HIS:CD2	1:E:459:LEU:H	1.99	0.78
1:G:448:LYS:HE2	1:G:449:LYS:HE3	1.66	0.78
1:G:354:ILE:HG22	1:G:355:MET:HE2	1.63	0.78
1:A:263:ILE:HA	1:A:266:LYS:HG3	1.66	0.78
1:G:351:PHE:CZ	1:G:447:ILE:HD13	2.19	0.77
1:G:281:VAL:O	1:G:285:THR:HG23	1.84	0.77
1:G:231:GLY:O	1:G:233:ALA:N	2.15	0.77
1:C:420:ILE:HD11	1:C:425:LYS:NZ	1.99	0.77
1:A:217:ASN:HD21	1:A:289:GLU:HB3	1.50	0.77
1:C:255:VAL:HG12	1:C:258:LEU:H	1.50	0.77
1:A:420:ILE:HG23	1:A:421:PHE:N	2.00	0.76
1:C:232:LYS:HE2	5:C:503:HOH:O	1.85	0.76
1:E:263:ILE:HA	1:E:266:LYS:HG3	1.67	0.76
1:E:221:ASN:C	1:E:221:ASN:HD22	1.89	0.76
1:A:255:VAL:C	1:A:257:LYS:N	2.38	0.75
1:C:255:VAL:HG11	1:C:258:LEU:HG	1.66	0.75
1:C:235:ASN:ND2	1:C:237:PRO:HD3	2.02	0.75
1:G:263:ILE:HA	1:G:266:LYS:HE3	1.69	0.75
1:G:277:GLN:HG2	1:G:460:LEU:CD1	2.16	0.75
1:C:255:VAL:CG1	1:C:258:LEU:N	2.50	0.74
1:A:229:LEU:O	1:A:230:SER:HB2	1.86	0.74
1:E:354:ILE:HD11	1:E:447:ILE:HD11	1.68	0.73
1:A:251:GLU:O	1:A:255:VAL:HG23	1.87	0.73
1:A:420:ILE:HG22	1:A:421:PHE:H	1.51	0.73
1:C:420:ILE:HB	1:G:336:ASN:CB	2.18	0.73
1:A:309:LEU:O	1:A:313:VAL:HB	1.89	0.73
1:C:419:ASP:OD1	1:C:420:ILE:HG12	1.89	0.72
1:E:446:ILE:O	1:E:450:THR:HG23	1.89	0.72
1:E:257:LYS:HA	1:E:257:LYS:HE2	1.71	0.72
1:G:235:ASN:ND2	1:G:237:PRO:HD3	2.05	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ILE:HG12	1:A:266:LYS:NZ	2.04	0.72
1:A:315:GLU:HB2	1:A:382:ILE:HD13	1.71	0.72
1:C:420:ILE:HG22	1:G:336:ASN:CG	2.09	0.72
1:E:235:ASN:OD1	1:E:236:ASN:N	2.23	0.72
2:F:685:GLU:CG	2:F:686:ARG:H	2.03	0.72
1:E:449:LYS:HG3	1:E:450:THR:N	2.05	0.71
1:G:444:VAL:HA	1:G:447:ILE:CG2	2.20	0.71
1:C:326:ASN:C	1:C:326:ASN:HD22	1.92	0.71
2:H:695:GLN:HE21	2:H:695:GLN:HA	1.56	0.71
1:C:232:LYS:HZ1	1:C:235:ASN:HD22	1.36	0.71
1:G:305:GLN:HE21	2:H:694:LEU:HD13	1.55	0.71
1:C:301:ASP:OD2	1:C:303:ASN:HB2	1.90	0.71
1:E:384:CYS:O	1:E:401:GLN:HB2	1.90	0.71
1:A:302:LEU:HD13	2:B:691:HIS:HE1	1.54	0.71
1:A:312:GLY:O	1:A:382:ILE:HD11	1.89	0.71
1:G:354:ILE:HG12	1:G:443:LEU:CD2	2.21	0.71
1:G:277:GLN:HE22	1:G:457:HIS:N	1.89	0.71
1:A:377:LEU:HD22	1:A:404:ILE:HD11	1.73	0.70
1:C:326:ASN:ND2	1:C:328:ASP:H	1.90	0.69
1:C:324:VAL:HB	1:C:331:LEU:HB2	1.74	0.69
1:E:202:ASP:C	1:E:204:LYS:H	1.95	0.69
1:A:302:LEU:O	1:A:306:VAL:HG13	1.92	0.69
1:C:420:ILE:HG22	1:G:336:ASN:ND2	2.07	0.69
1:E:252:LYS:HA	1:E:259:VAL:HG11	1.75	0.69
1:G:277:GLN:NE2	1:G:457:HIS:N	2.40	0.69
2:B:695:GLN:HE21	2:B:695:GLN:HA	1.57	0.69
2:D:685:GLU:HG3	2:D:686:ARG:N	2.07	0.69
1:G:277:GLN:HG2	1:G:460:LEU:HD12	1.74	0.69
1:G:315:GLU:HB2	1:G:382:ILE:HD13	1.74	0.69
1:A:306:VAL:HG12	2:B:694:LEU:CD1	2.23	0.68
1:C:255:VAL:HG13	1:C:257:LYS:CB	2.23	0.68
1:C:254:LEU:O	1:C:255:VAL:CB	2.42	0.68
1:G:277:GLN:NE2	1:G:457:HIS:H	1.92	0.68
1:G:326:ASN:ND2	1:G:328:ASP:H	1.92	0.68
1:A:421:PHE:O	1:A:425:LYS:HG3	1.94	0.68
1:G:446:ILE:O	1:G:450:THR:HB	1.93	0.68
1:A:258:LEU:HD22	1:A:263:ILE:CG2	2.22	0.68
1:A:385:CYS:HA	1:A:401:GLN:HE22	1.57	0.67
1:G:440:HIS:O	1:G:444:VAL:HG12	1.94	0.67
1:C:308:LEU:HD13	1:C:391:LEU:HD21	1.76	0.67
1:G:208:LYS:O	1:G:212:GLU:HG3	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:207:ALA:HB2	1:G:407:VAL:HG11	1.76	0.67
1:G:423:PHE:HB3	1:G:424:PRO:HD3	1.77	0.67
1:G:450:THR:HG22	5:G:620:HOH:O	1.95	0.67
1:A:302:LEU:HA	1:A:305:GLN:NE2	2.05	0.66
1:C:428:GLN:HG3	5:C:472:HOH:O	1.94	0.66
1:E:277:GLN:OE1	1:E:456:LEU:HA	1.95	0.66
1:A:203:LEU:HG	1:A:407:VAL:HG22	1.78	0.66
1:A:433:LEU:O	1:A:437:VAL:HG23	1.95	0.66
1:A:358:LYS:NZ	1:A:440:HIS:HD2	1.94	0.66
1:C:451:GLU:OE1	1:C:453:ASP:HB2	1.94	0.66
1:C:350:PRO:HB2	1:C:443:LEU:HD11	1.77	0.66
1:C:226:ARG:HG2	1:C:226:ARG:NH1	2.06	0.65
1:C:255:VAL:HG13	1:C:257:LYS:N	2.11	0.65
1:E:263:ILE:HG12	1:E:266:LYS:NZ	2.11	0.65
1:E:263:ILE:HG12	1:E:266:LYS:CE	2.26	0.65
1:G:462:GLU:O	1:G:465:ARG:HB3	1.97	0.65
1:G:263:ILE:HG12	1:G:266:LYS:HZ2	1.60	0.65
1:C:220:MET:CE	1:C:224:LYS:HB2	2.26	0.65
1:A:202:ASP:HA	1:E:449:LYS:HD3	1.78	0.64
1:E:235:ASN:OD1	1:E:237:PRO:HD3	1.96	0.64
1:C:257:LYS:HG2	1:C:263:ILE:HD12	1.79	0.64
1:C:252:LYS:HA	1:C:259:VAL:CG1	2.22	0.64
1:C:327:LYS:HB3	1:C:363:MET:HE2	1.79	0.64
2:F:691:HIS:O	2:F:695:GLN:HG2	1.97	0.64
1:G:441:ALA:HA	1:G:444:VAL:CG1	2.28	0.64
1:A:209:ARG:NH1	1:A:295:PRO:HD3	2.13	0.64
1:A:258:LEU:HA	1:A:263:ILE:HB	1.79	0.64
1:G:282:GLU:O	1:G:286:GLU:HG3	1.97	0.63
1:A:203:LEU:O	1:A:206:LEU:HB3	1.97	0.63
1:A:277:GLN:OE1	1:A:456:LEU:HD12	1.98	0.63
1:A:255:VAL:HB	1:A:258:LEU:N	2.12	0.63
1:C:255:VAL:HG11	1:C:258:LEU:N	2.14	0.63
1:G:254:LEU:O	1:G:255:VAL:HG13	1.98	0.63
1:A:251:GLU:O	1:A:255:VAL:CG2	2.47	0.63
1:A:263:ILE:HG12	1:A:266:LYS:CE	2.29	0.63
1:G:326:ASN:HA	1:G:363:MET:HE1	1.80	0.63
1:G:388:ARG:NH1	1:G:434:ARG:NH1	2.46	0.63
1:A:302:LEU:HD13	2:B:691:HIS:CE1	2.32	0.62
1:A:284:VAL:HG22	1:A:313:VAL:HG21	1.79	0.62
1:G:421:PHE:O	1:G:424:PRO:HD2	1.98	0.62
1:A:306:VAL:HG12	2:B:694:LEU:HD12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:VAL:HB	1:A:257:LYS:N	2.10	0.62
1:C:424:PRO:HD3	1:G:253:THR:OG1	1.99	0.62
1:A:206:LEU:O	1:A:209:ARG:HB3	2.00	0.62
1:A:412:LEU:HD11	1:A:426:LEU:CD1	2.30	0.62
1:G:235:ASN:OD1	1:G:237:PRO:HD2	1.99	0.62
1:G:315:GLU:HB2	1:G:382:ILE:CD1	2.30	0.62
1:A:255:VAL:CB	1:A:258:LEU:H	2.11	0.62
1:C:257:LYS:HA	1:C:261:ASN:CG	2.18	0.62
1:C:449:LYS:O	1:C:449:LYS:HG2	1.98	0.62
1:G:388:ARG:NH1	1:G:434:ARG:HH11	1.97	0.62
1:A:217:ASN:ND2	1:A:289:GLU:HB3	2.13	0.62
1:G:207:ALA:HB2	1:G:407:VAL:CG1	2.29	0.62
1:G:379:VAL:HA	1:G:382:ILE:HG23	1.82	0.62
1:G:220:MET:CE	1:G:224:LYS:HB2	2.30	0.62
1:E:263:ILE:HG21	5:E:545:HOH:O	1.99	0.61
2:F:685:GLU:HG3	2:F:686:ARG:N	2.06	0.61
1:G:229:LEU:O	1:G:230:SER:HB2	2.00	0.61
1:A:358:LYS:HZ1	1:A:440:HIS:CD2	2.17	0.61
1:G:284:VAL:HG22	1:G:313:VAL:CG2	2.28	0.61
1:A:255:VAL:C	1:A:257:LYS:H	2.01	0.61
1:C:416:HIS:HD2	5:C:500:HOH:O	1.81	0.61
1:A:251:GLU:OE2	1:A:271:ARG:HD2	2.01	0.61
1:A:255:VAL:CG1	1:A:257:LYS:HB3	2.29	0.61
1:G:220:MET:HE2	1:G:224:LYS:HB2	1.83	0.61
1:G:444:VAL:HA	1:G:447:ILE:HG23	1.82	0.61
1:G:277:GLN:HE21	1:G:456:LEU:HA	1.66	0.61
1:G:443:LEU:O	1:G:447:ILE:HG22	2.01	0.60
1:G:258:LEU:HD22	1:G:263:ILE:HG21	1.83	0.60
1:E:412:LEU:HD22	1:E:422:LEU:HD13	1.83	0.60
1:C:336:ASN:N	1:C:336:ASN:HD22	2.00	0.60
1:E:236:ASN:N	1:E:237:PRO:HD3	2.16	0.60
1:E:326:ASN:C	1:E:326:ASN:ND2	2.52	0.60
1:E:392:LEU:O	1:E:394:VAL:HG12	1.99	0.60
1:A:378:PHE:O	1:A:382:ILE:HG23	2.02	0.60
1:A:202:ASP:OD1	1:A:202:ASP:N	2.34	0.60
1:A:308:LEU:CD1	1:A:391:LEU:HD21	2.31	0.60
1:G:257:LYS:HD2	1:G:261:ASN:HD22	1.66	0.60
1:E:226:ARG:NH1	1:E:323:SER:O	2.35	0.60
1:C:427:LEU:HD11	1:G:252:LYS:HE3	1.84	0.59
1:A:302:LEU:CA	1:A:305:GLN:HE21	2.10	0.59
1:G:365:PHE:O	1:G:368:LEU:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ASN:ND2	1:A:289:GLU:CB	2.65	0.59
1:G:280:SER:O	1:G:284:VAL:HG23	2.02	0.59
1:E:370:LEU:HD11	1:E:426:LEU:HD21	1.83	0.59
1:E:421:PHE:O	1:E:424:PRO:HG2	2.02	0.59
1:A:217:ASN:HD21	1:A:289:GLU:CB	2.15	0.59
1:A:421:PHE:O	1:A:424:PRO:HG2	2.03	0.59
1:E:258:LEU:O	1:E:264:GLN:HA	2.03	0.59
1:G:348:ARG:O	1:G:351:PHE:HB2	2.03	0.58
1:E:378:PHE:CE2	1:E:382:ILE:HD11	2.38	0.58
2:F:695:GLN:HE21	2:F:695:GLN:HA	1.67	0.58
1:G:255:VAL:HB	1:G:257:LYS:H	1.68	0.58
1:E:404:ILE:O	1:E:407:VAL:HG22	2.02	0.58
1:E:221:ASN:ND2	1:E:224:LYS:H	2.01	0.58
1:G:302:LEU:HD12	2:H:691:HIS:ND1	2.18	0.58
2:D:685:GLU:O	2:D:687:HIS:N	2.34	0.58
1:C:420:ILE:HD11	1:C:425:LYS:HE3	1.82	0.58
1:G:234:SER:O	1:G:235:ASN:HB2	2.04	0.58
1:E:223:VAL:O	1:E:227:VAL:HG23	2.03	0.58
1:G:396:HIS:O	1:G:400:MET:HG3	2.04	0.58
2:H:695:GLN:HA	2:H:695:GLN:NE2	2.18	0.58
1:G:394:VAL:HG23	1:G:394:VAL:O	2.03	0.58
1:G:467:MET:HG2	1:G:468:TYR:CD1	2.39	0.57
1:C:232:LYS:HZ2	1:C:235:ASN:CA	2.12	0.57
1:C:236:ASN:N	1:C:237:PRO:CD	2.68	0.57
1:A:374:ASP:OD2	1:A:416:HIS:HE1	1.87	0.57
1:C:374:ASP:OD2	1:C:416:HIS:HE1	1.87	0.57
1:G:315:GLU:CB	1:G:382:ILE:HD13	2.34	0.57
1:C:309:LEU:O	1:C:313:VAL:HB	2.04	0.57
1:G:226:ARG:NH1	1:G:323:SER:O	2.36	0.57
1:G:235:ASN:CG	1:G:237:PRO:HD3	2.25	0.57
1:G:326:ASN:C	1:G:326:ASN:ND2	2.55	0.57
1:A:361:PHE:CZ	1:A:433:LEU:HD21	2.38	0.57
1:C:236:ASN:H	1:C:237:PRO:HD3	1.69	0.57
1:A:461:GLN:O	1:A:465:ARG:HB2	2.05	0.57
1:C:269:GLU:OE1	1:C:348:ARG:HG2	2.03	0.57
1:E:257:LYS:HZ1	1:E:261:ASN:ND2	2.02	0.57
1:A:235:ASN:CG	1:A:236:ASN:N	2.58	0.57
1:G:450:THR:HG22	1:G:450:THR:O	2.05	0.57
1:C:277:GLN:OE1	1:C:456:LEU:HA	2.05	0.57
1:E:235:ASN:OD1	1:E:237:PRO:CD	2.52	0.57
1:C:277:GLN:NE2	1:C:455:ALA:O	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:309:LEU:CD1	2:F:694:LEU:HD21	2.35	0.56
1:A:203:LEU:H	1:A:203:LEU:HD22	1.71	0.56
2:B:685:GLU:HG3	2:B:686:ARG:H	1.70	0.56
1:A:235:ASN:O	1:A:236:ASN:CB	2.53	0.56
1:E:263:ILE:O	1:E:271:ARG:HD3	2.06	0.56
1:G:378:PHE:CE1	1:G:430:MET:HG3	2.40	0.56
1:G:388:ARG:HH12	1:G:434:ARG:HH11	1.53	0.56
1:A:235:ASN:OD1	1:A:236:ASN:N	2.38	0.56
1:C:257:LYS:HA	1:C:261:ASN:OD1	2.05	0.56
1:C:420:ILE:CG1	1:C:421:PHE:N	2.62	0.56
1:A:203:LEU:HD23	1:A:204:LYS:N	2.20	0.56
1:C:229:LEU:HD21	1:C:331:LEU:HD13	1.86	0.56
1:A:308:LEU:HD13	1:A:391:LEU:HD21	1.88	0.56
1:C:367:ALA:HB1	1:G:235:ASN:ND2	2.20	0.56
1:E:231:GLY:O	1:E:233:ALA:N	2.29	0.56
1:C:457:HIS:CD2	1:C:459:LEU:H	2.15	0.56
1:C:435:GLN:O	1:C:439:GLU:HG3	2.05	0.55
2:D:696:GLU:HB3	5:D:58:HOH:O	2.06	0.55
1:E:218:PHE:HZ	1:E:287:LEU:HD23	1.71	0.55
1:E:421:PHE:HB3	1:E:424:PRO:HG2	1.89	0.55
1:C:255:VAL:CG1	1:C:257:LYS:N	2.62	0.55
1:E:292:LYS:HE2	2:F:694:LEU:O	2.06	0.55
1:A:282:GLU:O	1:A:286:GLU:HG3	2.06	0.55
1:C:262:GLY:C	1:C:264:GLN:H	2.07	0.55
1:A:284:VAL:HG22	1:A:313:VAL:CG2	2.36	0.55
1:A:427:LEU:HD12	1:A:430:MET:HE1	1.89	0.55
1:A:229:LEU:O	1:A:230:SER:CB	2.54	0.55
1:C:236:ASN:N	1:C:237:PRO:HD3	2.22	0.55
1:C:263:ILE:HG23	1:C:266:LYS:HD2	1.87	0.55
2:H:687:HIS:HD2	2:H:690:LEU:HD12	1.71	0.55
1:A:394:VAL:HG13	1:A:395:GLY:N	2.22	0.55
1:G:287:LEU:HD13	1:G:313:VAL:HG23	1.88	0.55
1:C:427:LEU:CD1	1:G:252:LYS:HE3	2.37	0.55
1:E:255:VAL:C	1:E:257:LYS:H	2.10	0.55
1:G:235:ASN:ND2	1:G:237:PRO:CD	2.69	0.55
1:C:232:LYS:HZ3	1:C:235:ASN:HD22	1.54	0.54
1:G:311:TYR:CE2	1:G:389:PRO:HD2	2.43	0.54
1:E:251:GLU:OE1	1:E:271:ARG:NH1	2.41	0.54
1:E:374:ASP:OD2	1:E:416:HIS:HE1	1.90	0.54
1:A:209:ARG:HG2	1:A:209:ARG:HH11	1.72	0.54
1:G:321:LEU:O	1:G:325:MET:HG3	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:PHE:O	1:A:363:MET:HG2	2.07	0.54
1:C:238:PRO:HA	1:C:336:ASN:O	2.08	0.54
1:G:228:ILE:C	1:G:230:SER:H	2.10	0.54
2:H:685:GLU:HG3	2:H:686:ARG:H	1.71	0.54
1:E:263:ILE:HG12	1:E:266:LYS:HE3	1.89	0.54
1:C:252:LYS:CG	1:C:259:VAL:HG21	2.37	0.54
1:G:412:LEU:HD11	1:G:426:LEU:HD12	1.89	0.54
1:A:255:VAL:O	1:A:256:ALA:HB3	2.08	0.53
1:C:220:MET:HE3	1:C:224:LYS:HB2	1.90	0.53
2:B:687:HIS:HD2	2:B:690:LEU:HD12	1.73	0.53
1:A:222:LYS:HD2	1:A:375:ILE:HD11	1.90	0.53
1:C:204:LYS:NZ	1:C:410:LEU:HD12	2.23	0.53
1:C:358:LYS:NZ	1:C:440:HIS:HD2	2.06	0.53
1:A:263:ILE:HA	1:A:266:LYS:CG	2.37	0.53
1:G:235:ASN:CG	1:G:237:PRO:CD	2.77	0.53
1:A:301:ASP:OD1	1:A:303:ASN:HB2	2.09	0.53
2:F:688:LYS:O	2:F:692:ARG:HG3	2.08	0.53
1:A:440:HIS:HE1	3:A:469:544:O1	1.92	0.53
1:E:255:VAL:C	1:E:257:LYS:N	2.62	0.53
1:E:412:LEU:HD11	1:E:426:LEU:HD12	1.90	0.53
1:G:302:LEU:HD12	2:H:691:HIS:CE1	2.44	0.53
1:C:302:LEU:HD13	2:D:691:HIS:CE1	2.44	0.53
1:A:302:LEU:HD12	1:A:303:ASN:H	1.70	0.52
1:A:358:LYS:NZ	1:A:440:HIS:CD2	2.73	0.52
1:C:373:SER:O	1:C:377:LEU:HD13	2.08	0.52
1:E:451:GLU:OE1	1:E:453:ASP:HB2	2.09	0.52
2:H:685:GLU:HG3	2:H:686:ARG:N	2.24	0.52
1:A:270:VAL:HG22	1:A:454:ALA:HB2	1.92	0.52
1:A:374:ASP:OD2	1:A:416:HIS:CE1	2.62	0.52
1:C:252:LYS:HA	1:C:259:VAL:HG21	1.91	0.52
1:A:380:ALA:HA	1:A:383:ILE:CG2	2.39	0.52
1:E:236:ASN:CG	1:E:236:ASN:O	2.47	0.52
1:E:457:HIS:HD2	1:E:459:LEU:N	1.94	0.52
1:A:210:ILE:CD1	1:A:404:ILE:HD13	2.39	0.52
1:E:217:ASN:ND2	1:E:289:GLU:HB3	2.24	0.52
1:G:277:GLN:HG2	1:G:460:LEU:HD11	1.89	0.52
1:A:210:ILE:HD12	1:A:404:ILE:HD13	1.92	0.52
1:A:310:LYS:HD2	2:B:687:HIS:NE2	2.25	0.52
1:A:457:HIS:ND1	1:A:458:PRO:HD2	2.25	0.52
2:B:685:GLU:CG	2:B:686:ARG:H	2.23	0.52
1:C:255:VAL:HG13	1:C:257:LYS:CA	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:255:VAL:HG12	1:E:258:LEU:HG	1.92	0.52
1:A:235:ASN:O	1:A:236:ASN:HB2	2.10	0.51
1:G:412:LEU:HD22	1:G:422:LEU:HD13	1.93	0.51
1:E:257:LYS:NZ	1:E:261:ASN:ND2	2.58	0.51
1:C:302:LEU:HD12	1:C:302:LEU:C	2.30	0.51
1:A:326:ASN:OD1	1:A:328:ASP:N	2.41	0.51
1:A:409:ARG:O	1:A:413:GLN:HG3	2.09	0.51
1:C:421:PHE:O	1:C:425:LYS:HG3	2.10	0.51
1:G:255:VAL:HB	1:G:257:LYS:HB3	1.92	0.51
1:A:263:ILE:O	1:A:271:ARG:HD3	2.09	0.51
1:C:450:THR:HG22	1:C:450:THR:O	2.11	0.51
1:A:254:LEU:O	1:A:255:VAL:HG13	2.11	0.51
1:C:232:LYS:NZ	1:C:235:ASN:CA	2.72	0.51
1:G:441:ALA:O	1:G:444:VAL:HG13	2.11	0.51
1:A:251:GLU:OE1	1:A:271:ARG:NH1	2.43	0.51
1:E:227:VAL:O	1:E:230:SER:C	2.49	0.51
1:C:235:ASN:OD1	1:C:237:PRO:HD3	2.11	0.51
1:C:448:LYS:NZ	1:C:461:GLN:HE22	2.08	0.51
1:E:255:VAL:O	1:E:257:LYS:N	2.43	0.51
1:E:433:LEU:O	1:E:437:VAL:HG23	2.11	0.51
1:G:277:GLN:NE2	1:G:456:LEU:CA	2.69	0.51
1:C:423:PHE:HE2	1:G:252:LYS:HD2	1.76	0.50
1:G:354:ILE:CG1	1:G:443:LEU:HD21	2.34	0.50
1:C:270:VAL:HG21	1:C:453:ASP:HB3	1.93	0.50
1:C:367:ALA:HB1	1:G:235:ASN:CG	2.32	0.50
1:A:266:LYS:O	1:A:267:GLU:C	2.48	0.50
1:C:255:VAL:HG11	1:C:258:LEU:CG	2.40	0.50
1:C:315:GLU:HG3	1:C:437:VAL:HG21	1.93	0.50
1:C:420:ILE:CG2	1:G:336:ASN:CG	2.79	0.50
1:C:421:PHE:CB	1:C:424:PRO:CG	2.87	0.50
1:E:236:ASN:N	1:E:237:PRO:CD	2.74	0.50
1:A:203:LEU:H	1:A:203:LEU:CD2	2.25	0.50
1:A:394:VAL:HG13	1:A:395:GLY:H	1.75	0.50
1:G:263:ILE:HG12	1:G:266:LYS:CE	2.42	0.50
1:C:232:LYS:HE3	1:C:232:LYS:C	2.32	0.50
1:C:261:ASN:O	1:C:263:ILE:HG13	2.12	0.50
1:C:308:LEU:HG	1:C:383:ILE:O	2.11	0.50
1:G:277:GLN:HE22	1:G:456:LEU:C	2.15	0.50
1:C:263:ILE:HG23	1:C:266:LYS:CE	2.42	0.50
2:D:695:GLN:HE21	2:D:695:GLN:HA	1.77	0.50
1:G:341:ARG:O	1:G:345:LYS:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:GLU:OE1	1:C:271:ARG:NH2	2.40	0.49
1:E:255:VAL:HG11	1:E:258:LEU:HD12	1.94	0.49
1:G:228:ILE:O	1:G:230:SER:N	2.45	0.49
1:A:375:ILE:O	1:A:379:VAL:HG23	2.12	0.49
1:E:359:PHE:O	1:E:363:MET:HG2	2.11	0.49
1:G:385:CYS:C	1:G:387:ASP:H	2.15	0.49
1:C:420:ILE:HG21	1:G:336:ASN:HA	1.94	0.49
1:G:263:ILE:HA	1:G:266:LYS:HG3	1.94	0.49
1:E:309:LEU:O	1:E:313:VAL:HB	2.13	0.49
2:F:685:GLU:CG	2:F:686:ARG:N	2.71	0.49
1:E:341:ARG:O	1:E:345:LYS:HG2	2.12	0.49
1:G:441:ALA:HA	1:G:444:VAL:HG12	1.93	0.49
1:A:263:ILE:HG12	1:A:266:LYS:HZ1	1.76	0.49
1:C:421:PHE:CB	1:C:424:PRO:HG2	2.43	0.49
1:E:235:ASN:C	1:E:237:PRO:HD3	2.33	0.49
1:E:234:SER:O	1:E:235:ASN:C	2.51	0.49
1:C:235:ASN:CG	1:C:236:ASN:N	2.60	0.49
1:C:257:LYS:O	1:C:261:ASN:HB2	2.13	0.49
1:G:287:LEU:CD1	1:G:313:VAL:HG23	2.43	0.49
1:A:277:GLN:CD	1:A:456:LEU:HD12	2.33	0.48
1:E:251:GLU:CA	1:E:255:VAL:HB	2.28	0.48
1:E:326:ASN:ND2	1:E:328:ASP:H	2.11	0.48
1:E:354:ILE:HG22	1:E:355:MET:CE	2.39	0.48
1:A:222:LYS:HD2	1:A:375:ILE:CD1	2.43	0.48
1:C:359:PHE:O	1:C:363:MET:HG2	2.13	0.48
1:A:202:ASP:HA	1:E:449:LYS:CE	2.44	0.48
1:A:377:LEU:HD22	1:A:404:ILE:CD1	2.40	0.48
1:C:226:ARG:HH11	1:C:226:ARG:CG	2.18	0.48
1:E:349:LYS:HG2	1:E:353:ASP:OD2	2.12	0.48
1:G:235:ASN:CG	1:G:236:ASN:N	2.66	0.48
1:G:393:ASN:OD1	1:G:396:HIS:CE1	2.66	0.48
1:C:420:ILE:HA	1:G:336:ASN:OD1	2.13	0.48
1:C:421:PHE:CE2	1:G:254:LEU:HD13	2.49	0.48
1:G:257:LYS:HE3	1:G:263:ILE:CD1	2.43	0.48
1:C:252:LYS:CA	1:C:259:VAL:HG11	2.29	0.48
1:C:327:LYS:N	1:C:363:MET:HE1	2.29	0.48
1:G:257:LYS:CD	1:G:261:ASN:HD22	2.27	0.48
1:C:327:LYS:HB3	1:C:363:MET:CE	2.43	0.48
1:G:351:PHE:HZ	1:G:447:ILE:HD13	1.74	0.48
1:C:231:GLY:O	1:C:233:ALA:N	2.47	0.48
1:C:313:VAL:O	1:C:317:ILE:HG13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:324:VAL:HB	1:G:331:LEU:HB2	1.95	0.48
1:A:274:HIS:O	1:A:277:GLN:HB3	2.14	0.48
1:A:427:LEU:HD12	1:A:430:MET:CE	2.43	0.48
1:E:252:LYS:HA	1:E:259:VAL:HG21	1.96	0.48
1:E:252:LYS:HA	1:E:259:VAL:CG1	2.44	0.47
1:G:391:LEU:HD22	1:G:397:ILE:CD1	2.44	0.47
1:A:221:ASN:HD22	1:A:223:VAL:N	2.12	0.47
1:A:242:HIS:CE1	1:A:243:ASP:OD2	2.67	0.47
1:G:276:CYS:O	1:G:279:THR:HB	2.14	0.47
1:A:221:ASN:ND2	1:A:223:VAL:HB	2.28	0.47
1:A:228:ILE:C	1:A:230:SER:H	2.17	0.47
1:C:374:ASP:OD2	1:C:416:HIS:CE1	2.68	0.47
1:E:235:ASN:CG	1:E:237:PRO:HD3	2.35	0.47
1:A:287:LEU:HD11	1:A:320:MET:CE	2.44	0.47
1:G:235:ASN:CG	1:G:236:ASN:H	2.17	0.47
1:A:306:VAL:HG12	2:B:694:LEU:HD11	1.96	0.47
2:D:685:GLU:CG	2:D:686:ARG:N	2.77	0.47
1:G:227:VAL:O	1:G:231:GLY:N	2.48	0.47
1:C:421:PHE:O	1:C:424:PRO:HG2	2.15	0.47
1:A:326:ASN:OD1	1:A:326:ASN:C	2.53	0.47
1:A:382:ILE:HG13	1:A:383:ILE:N	2.29	0.47
1:C:236:ASN:H	1:C:237:PRO:CD	2.27	0.47
1:C:277:GLN:OE1	1:C:457:HIS:N	2.41	0.47
1:C:326:ASN:ND2	1:C:329:GLY:H	2.12	0.47
1:G:391:LEU:HB3	1:G:394:VAL:HG12	1.97	0.47
1:A:261:ASN:C	1:A:263:ILE:H	2.18	0.47
1:C:349:LYS:HE2	5:C:521:HOH:O	2.15	0.47
1:E:394:VAL:CG2	1:E:394:VAL:O	2.62	0.47
1:G:414:SER:O	1:G:417:PRO:HD3	2.15	0.47
1:A:231:GLY:O	1:A:232:LYS:C	2.53	0.47
1:G:311:TYR:CB	1:G:388:ARG:HD2	2.45	0.47
1:C:361:PHE:CZ	1:C:433:LEU:HD21	2.50	0.47
1:E:326:ASN:ND2	1:E:329:GLY:H	2.13	0.47
1:C:224:LYS:HD3	5:C:523:HOH:O	2.14	0.46
1:G:277:GLN:CG	1:G:460:LEU:HD12	2.44	0.46
2:H:689:ILE:O	2:H:693:LEU:HG	2.14	0.46
1:A:224:LYS:O	1:A:228:ILE:HG13	2.15	0.46
2:D:686:ARG:NH1	2:D:688:LYS:CB	2.78	0.46
2:F:695:GLN:HA	2:F:695:GLN:NE2	2.31	0.46
1:G:444:VAL:O	1:G:444:VAL:CG2	2.64	0.46
1:A:248:CYS:HA	1:A:251:GLU:OE1	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:LEU:HB3	1:A:325:MET:CE	2.46	0.46
1:A:383:ILE:HD12	1:A:383:ILE:O	2.16	0.46
1:E:280:SER:O	1:E:284:VAL:HG23	2.15	0.46
1:E:449:LYS:HG3	1:E:450:THR:H	1.80	0.46
1:A:231:GLY:O	1:A:233:ALA:N	2.49	0.46
1:A:252:LYS:HA	1:A:259:VAL:HB	1.98	0.46
1:E:253:THR:CG2	1:E:254:LEU:N	2.60	0.46
1:C:436:LEU:HD22	5:C:510:HOH:O	2.16	0.46
1:G:236:ASN:N	1:G:237:PRO:CD	2.79	0.46
1:G:259:VAL:O	1:G:259:VAL:HG13	2.16	0.46
1:A:258:LEU:O	1:A:264:GLN:HA	2.15	0.46
1:C:232:LYS:NZ	1:C:235:ASN:ND2	2.54	0.46
1:E:221:ASN:C	1:E:221:ASN:ND2	2.62	0.46
1:E:277:GLN:HE21	1:E:277:GLN:HB3	1.43	0.46
1:E:310:LYS:HZ3	2:F:687:HIS:CE1	2.33	0.46
1:A:296:GLY:O	1:A:400:MET:HE1	2.15	0.46
1:C:388:ARG:O	1:C:391:LEU:HG	2.15	0.46
2:D:695:GLN:HA	2:D:695:GLN:NE2	2.31	0.45
1:E:354:ILE:HD11	1:E:447:ILE:CD1	2.42	0.45
1:G:203:LEU:O	1:G:206:LEU:HB3	2.17	0.45
1:A:412:LEU:HD22	1:A:422:LEU:HD23	1.98	0.45
1:G:259:VAL:O	1:G:259:VAL:CG1	2.64	0.45
1:C:229:LEU:HG	1:C:331:LEU:HD21	1.98	0.45
1:E:292:LYS:CE	2:F:694:LEU:HA	2.46	0.45
1:G:305:GLN:NE2	2:H:694:LEU:HD13	2.28	0.45
1:A:223:VAL:HG12	1:A:224:LYS:N	2.32	0.45
1:A:419:ASP:O	1:A:419:ASP:OD1	2.35	0.45
1:C:326:ASN:C	1:C:326:ASN:ND2	2.62	0.45
1:A:254:LEU:HD12	1:A:254:LEU:HA	1.76	0.45
1:E:327:LYS:HB3	1:E:363:MET:HE2	1.99	0.45
1:G:249:MET:O	1:G:252:LYS:HB3	2.17	0.45
2:B:695:GLN:HA	2:B:695:GLN:NE2	2.28	0.45
1:C:231:GLY:O	1:C:232:LYS:C	2.55	0.45
1:C:326:ASN:ND2	1:C:328:ASP:N	2.62	0.45
1:C:461:GLN:OE1	1:C:461:GLN:O	2.34	0.45
1:E:224:LYS:HE2	5:H:44:HOH:O	2.16	0.45
1:G:326:ASN:C	1:G:363:MET:HE3	2.37	0.45
1:G:459:LEU:HD13	2:H:689:ILE:CG2	2.47	0.45
1:A:263:ILE:HG12	1:A:266:LYS:HE3	1.97	0.45
1:A:302:LEU:CD1	2:B:691:HIS:HE1	2.24	0.45
1:C:230:SER:OG	1:C:231:GLY:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:GLU:H	1:C:269:GLU:HG2	1.31	0.45
1:G:296:GLY:C	1:G:400:MET:HE1	2.37	0.45
1:E:251:GLU:HA	1:E:255:VAL:CB	2.30	0.45
1:E:365:PHE:HD2	1:E:429:LYS:HD3	1.81	0.44
1:G:312:GLY:O	1:G:382:ILE:HD11	2.18	0.44
1:C:300:LEU:HD23	1:C:396:HIS:CD2	2.51	0.44
1:G:277:GLN:HE22	1:G:456:LEU:HA	1.76	0.44
1:G:393:ASN:C	1:G:395:GLY:H	2.20	0.44
1:A:202:ASP:HA	1:E:449:LYS:CD	2.44	0.44
1:A:255:VAL:CB	1:A:257:LYS:HB3	2.48	0.44
1:E:449:LYS:HG3	1:E:450:THR:CG2	2.47	0.44
1:A:380:ALA:O	1:A:383:ILE:HG23	2.17	0.44
1:A:461:GLN:HA	1:A:461:GLN:NE2	2.32	0.44
1:C:435:GLN:NE2	5:C:546:HOH:O	2.49	0.44
2:D:696:GLU:CD	2:D:697:GLY:H	2.20	0.44
1:E:239:PHE:HE2	1:E:250:ALA:HB2	1.81	0.44
1:G:314:TYR:OH	1:G:460:LEU:HD22	2.17	0.44
1:G:391:LEU:CB	1:G:394:VAL:HG12	2.47	0.44
1:A:300:LEU:HG	1:A:400:MET:HE1	1.99	0.44
1:C:226:ARG:HD3	1:C:226:ARG:HA	1.79	0.44
1:C:270:VAL:CG2	1:C:451:GLU:OE2	2.64	0.44
1:E:284:VAL:HG22	1:E:313:VAL:HG21	1.99	0.44
1:G:258:LEU:CD2	1:G:263:ILE:HG21	2.48	0.44
1:E:311:TYR:CB	1:E:388:ARG:HD2	2.48	0.44
1:E:221:ASN:HD21	1:E:224:LYS:H	1.66	0.44
1:G:277:GLN:HE22	1:G:456:LEU:CA	2.31	0.44
1:A:391:LEU:HD22	1:A:397:ILE:CD1	2.48	0.44
1:A:412:LEU:HD22	1:A:422:LEU:CD2	2.48	0.44
1:G:315:GLU:OE1	1:G:382:ILE:HD13	2.18	0.44
1:G:433:LEU:O	1:G:437:VAL:HG23	2.18	0.44
1:A:202:ASP:CA	1:E:449:LYS:HD3	2.46	0.44
1:E:239:PHE:CE2	1:E:250:ALA:HB2	2.52	0.44
1:C:348:ARG:HH22	1:C:451:GLU:HG2	1.83	0.43
1:E:404:ILE:HA	1:E:407:VAL:HG22	2.00	0.43
1:G:339:ILE:HG23	1:G:339:ILE:O	2.18	0.43
1:A:228:ILE:O	1:A:230:SER:N	2.49	0.43
1:G:309:LEU:CD1	2:H:694:LEU:HD21	2.48	0.43
1:A:232:LYS:O	1:A:233:ALA:HB3	2.18	0.43
2:B:695:GLN:HE21	2:B:695:GLN:CA	2.23	0.43
1:C:255:VAL:C	1:C:257:LYS:N	2.72	0.43
1:C:420:ILE:HD11	1:C:425:LYS:HZ1	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:313:VAL:HG12	5:G:621:HOH:O	2.18	0.43
1:A:203:LEU:CD2	1:A:203:LEU:N	2.80	0.43
1:C:259:VAL:HG22	1:C:259:VAL:O	2.18	0.43
1:C:358:LYS:NZ	1:C:440:HIS:CD2	2.85	0.43
1:E:315:GLU:HG3	1:E:437:VAL:HG21	2.00	0.43
1:A:221:ASN:HD22	1:A:223:VAL:H	1.67	0.43
1:A:301:ASP:OD1	1:A:303:ASN:N	2.51	0.43
1:C:358:LYS:HZ1	1:C:440:HIS:CD2	2.37	0.43
1:A:287:LEU:HD11	1:A:320:MET:HE2	2.00	0.43
1:A:313:VAL:O	1:A:317:ILE:HG13	2.18	0.43
1:C:204:LYS:HE2	1:C:204:LYS:HB2	1.87	0.43
1:A:265:ASN:CG	1:A:265:ASN:O	2.55	0.43
1:E:404:ILE:O	1:E:407:VAL:CG2	2.65	0.43
1:G:305:GLN:O	1:G:306:VAL:C	2.57	0.43
1:A:461:GLN:HA	1:A:461:GLN:HE21	1.83	0.43
1:E:227:VAL:O	1:E:231:GLY:N	2.52	0.43
1:A:287:LEU:HD12	1:A:287:LEU:HA	1.81	0.43
1:A:425:LYS:O	1:A:429:LYS:HG3	2.18	0.43
2:B:685:GLU:HG3	2:B:686:ARG:N	2.31	0.43
1:A:218:PHE:HZ	1:A:287:LEU:HD12	1.84	0.42
1:C:263:ILE:HG23	1:C:266:LYS:CD	2.48	0.42
1:C:203:LEU:O	1:C:407:VAL:HG21	2.19	0.42
1:C:325:MET:HE2	1:C:359:PHE:HA	2.02	0.42
1:A:255:VAL:HG11	1:A:258:LEU:CG	2.40	0.42
1:C:370:LEU:HD11	1:C:426:LEU:HD21	2.01	0.42
1:C:420:ILE:CB	1:G:336:ASN:CB	2.93	0.42
1:A:398:GLU:O	1:A:401:GLN:HB3	2.19	0.42
1:C:348:ARG:O	1:C:351:PHE:HB2	2.18	0.42
1:E:252:LYS:HE3	1:E:252:LYS:HB2	1.80	0.42
1:E:311:TYR:HB2	1:E:388:ARG:HD2	2.01	0.42
1:C:347:LEU:CD1	3:C:470:544:H1K1	2.49	0.42
1:E:208:LYS:HD3	1:E:208:LYS:HA	1.71	0.42
1:A:217:ASN:ND2	1:A:289:GLU:HB2	2.34	0.42
1:A:419:ASP:O	1:A:421:PHE:N	2.53	0.42
1:C:235:ASN:OD1	1:C:237:PRO:CD	2.68	0.42
1:C:321:LEU:O	1:C:325:MET:HG3	2.19	0.42
1:C:415:ASN:HB2	5:C:517:HOH:O	2.20	0.42
1:E:221:ASN:HD21	1:E:224:LYS:HG3	1.84	0.42
1:E:252:LYS:HA	1:E:259:VAL:CB	2.50	0.42
1:G:368:LEU:HB3	1:G:370:LEU:HD13	2.01	0.42
1:G:378:PHE:O	1:G:382:ILE:CG2	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:447:ILE:HD12	1:G:447:ILE:O	2.19	0.42
2:H:685:GLU:HB2	2:H:687:HIS:CE1	2.55	0.42
1:C:203:LEU:O	1:C:206:LEU:HB3	2.19	0.42
1:E:266:LYS:O	1:E:267:GLU:C	2.56	0.42
1:E:302:LEU:HD22	1:E:305:GLN:NE2	2.34	0.42
1:G:247:LEU:O	1:G:251:GLU:HG3	2.20	0.42
1:G:263:ILE:HA	1:G:266:LYS:CE	2.44	0.42
1:A:306:VAL:O	1:A:306:VAL:HG23	2.18	0.42
1:A:382:ILE:HD12	1:A:382:ILE:C	2.40	0.42
1:C:234:SER:O	1:C:235:ASN:HB3	2.19	0.42
1:C:261:ASN:O	1:C:263:ILE:N	2.47	0.42
1:C:262:GLY:C	1:C:264:GLN:N	2.73	0.42
1:C:414:SER:HB2	1:E:457:HIS:CE1	2.55	0.42
1:C:266:LYS:O	1:C:271:ARG:HD3	2.20	0.41
1:E:209:ARG:O	1:E:212:GLU:HG3	2.20	0.41
2:H:695:GLN:HE21	2:H:695:GLN:CA	2.23	0.41
1:E:267:GLU:HG3	1:E:270:VAL:HG23	2.02	0.41
1:G:217:ASN:O	1:G:286:GLU:HB3	2.20	0.41
1:A:252:LYS:HA	1:A:259:VAL:CB	2.51	0.41
1:C:421:PHE:HB3	1:C:424:PRO:HG2	1.95	0.41
1:E:204:LYS:NZ	1:E:410:LEU:HB3	2.36	0.41
1:G:231:GLY:C	1:G:233:ALA:H	2.19	0.41
1:G:237:PRO:HA	1:G:238:PRO:HD2	1.91	0.41
1:G:448:LYS:O	1:G:449:LYS:HG3	2.20	0.41
2:H:695:GLN:NE2	2:H:695:GLN:CA	2.81	0.41
1:C:327:LYS:CB	1:C:363:MET:HE2	2.48	0.41
1:E:277:GLN:OE1	1:E:455:ALA:O	2.38	0.41
1:E:324:VAL:HB	1:E:331:LEU:HB2	2.02	0.41
1:G:388:ARG:HA	1:G:389:PRO:HD3	1.77	0.41
1:G:425:LYS:O	1:G:429:LYS:HG2	2.20	0.41
1:A:291:ALA:O	1:A:294:ILE:HB	2.19	0.41
1:A:203:LEU:HD23	1:A:203:LEU:C	2.41	0.41
1:C:302:LEU:C	1:C:302:LEU:CD1	2.89	0.41
2:D:691:HIS:O	2:D:695:GLN:HG2	2.21	0.41
1:E:249:MET:O	1:E:252:LYS:HB3	2.21	0.41
1:G:311:TYR:CD2	1:G:389:PRO:HD2	2.55	0.41
1:A:282:GLU:O	1:A:285:THR:HB	2.20	0.41
1:C:204:LYS:HZ3	1:C:410:LEU:HD12	1.85	0.41
1:C:345:LYS:HE2	5:C:492:HOH:O	2.20	0.41
1:G:435:GLN:HA	1:G:435:GLN:OE1	2.20	0.41
1:A:226:ARG:HD3	1:A:226:ARG:HA	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:VAL:C	1:A:264:GLN:HB3	2.41	0.41
1:A:395:GLY:O	1:A:399:LYS:HD2	2.20	0.41
1:C:385:CYS:O	1:C:388:ARG:HG2	2.21	0.41
1:G:255:VAL:HG21	1:G:258:LEU:HG	2.02	0.41
1:A:237:PRO:HA	1:A:238:PRO:HD3	1.85	0.41
1:C:252:LYS:HA	1:C:259:VAL:CB	2.51	0.41
1:C:260:ALA:HA	1:C:264:GLN:OE1	2.21	0.41
1:C:350:PRO:HB3	5:C:512:HOH:O	2.21	0.41
1:C:449:LYS:HE2	1:C:449:LYS:HB3	1.72	0.41
1:C:450:THR:O	1:C:450:THR:CG2	2.68	0.41
1:E:465:ARG:HD2	5:E:532:HOH:O	2.20	0.41
1:G:326:ASN:CA	1:G:363:MET:HE1	2.48	0.41
1:C:440:HIS:HE1	3:C:470:544:O1	2.04	0.40
1:G:228:ILE:C	1:G:230:SER:N	2.74	0.40
1:G:459:LEU:HA	2:H:689:ILE:HD12	2.02	0.40
1:A:361:PHE:CD1	1:A:361:PHE:C	2.94	0.40
1:C:308:LEU:HA	1:C:308:LEU:HD12	1.80	0.40
1:C:349:LYS:HB3	1:C:350:PRO:HA	2.03	0.40
1:E:263:ILE:O	1:E:263:ILE:HG22	2.20	0.40
1:E:406:HIS:NE2	1:E:410:LEU:HD11	2.36	0.40
1:A:423:PHE:N	1:A:424:PRO:HD2	2.36	0.40
1:G:256:ALA:O	1:G:260:ALA:HB3	2.21	0.40
1:A:391:LEU:HD23	1:A:391:LEU:HA	1.87	0.40
1:C:220:MET:CE	1:C:224:LYS:CB	2.99	0.40
1:C:226:ARG:O	1:C:230:SER:HB3	2.21	0.40
1:E:261:ASN:C	1:E:263:ILE:H	2.25	0.40
1:G:229:LEU:HD21	1:G:331:LEU:HD13	2.02	0.40
1:G:378:PHE:HE1	1:G:430:MET:HG3	1.86	0.40
1:G:445:GLN:HE22	1:G:448:LYS:HZ2	1.69	0.40
1:A:254:LEU:C	1:A:255:VAL:HG22	2.41	0.40
1:A:408:LEU:HD23	1:A:412:LEU:HG	2.03	0.40
1:E:327:LYS:N	1:E:363:MET:HE1	2.36	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	265/288 (92%)	233 (88%)	23 (9%)	9 (3%)	3	5
1	C	265/288 (92%)	233 (88%)	18 (7%)	14 (5%)	2	2
1	E	265/288 (92%)	240 (91%)	16 (6%)	9 (3%)	3	5
1	G	265/288 (92%)	236 (89%)	18 (7%)	11 (4%)	3	3
2	B	11/21 (52%)	8 (73%)	3 (27%)	0	100	100
2	D	11/21 (52%)	8 (73%)	3 (27%)	0	100	100
2	F	11/21 (52%)	9 (82%)	2 (18%)	0	100	100
2	H	11/21 (52%)	9 (82%)	0	2 (18%)	0	0
All	All	1104/1236 (89%)	976 (88%)	83 (8%)	45 (4%)	3	3

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	SER
1	A	232	LYS
1	A	236	ASN
1	A	420	ILE
1	C	232	LYS
1	C	233	ALA
1	C	255	VAL
1	C	420	ILE
1	E	203	LEU
1	E	232	LYS
1	E	235	ASN
1	G	230	SER
1	G	232	LYS
1	G	235	ASN
1	G	450	THR
1	G	467	MET
1	A	229	LEU
1	A	255	VAL
1	C	231	GLY
1	C	450	THR
1	G	229	LEU
1	G	394	VAL
1	A	451	GLU

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Mol	Chain	Res	Type
1	A	452	SER
1	C	235	ASN
1	C	259	VAL
1	E	256	ALA
1	G	455	ALA
1	E	254	LEU
1	G	233	ALA
1	G	451	GLU
1	C	236	ASN
1	C	263	ILE
1	C	452	SER
1	E	237	PRO
2	H	686	ARG
2	H	696	GLU
1	C	238	PRO
1	E	467	MET
1	A	446	ILE
1	E	231	GLY
1	C	295	PRO
1	E	236	ASN
1	G	295	PRO
1	C	394	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	234/252 (93%)	207 (88%)	27 (12%)	5 11
1	C	234/252 (93%)	214 (92%)	20 (8%)	10 21
1	E	234/252 (93%)	209 (89%)	25 (11%)	6 13
1	G	234/252 (93%)	209 (89%)	25 (11%)	6 13
2	B	11/20 (55%)	9 (82%)	2 (18%)	1 3
2	D	11/20 (55%)	8 (73%)	3 (27%)	0 0
2	F	11/20 (55%)	9 (82%)	2 (18%)	1 3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	H	11/20 (55%)	11 (100%)	0	100 100
All	All	980/1088 (90%)	876 (89%)	104 (11%)	6 13

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	202	ASP
1	A	203	LEU
1	A	221	ASN
1	A	234	SER
1	A	235	ASN
1	A	236	ASN
1	A	253	THR
1	A	255	VAL
1	A	257	LYS
1	A	267	GLU
1	A	287	LEU
1	A	301	ASP
1	A	302	LEU
1	A	306	VAL
1	A	308	LEU
1	A	342	GLU
1	A	347	LEU
1	A	382	ILE
1	A	383	ILE
1	A	387	ASP
1	A	396	HIS
1	A	399	LYS
1	A	420	ILE
1	A	427	LEU
1	A	428	GLN
1	A	442	GLN
1	A	459	LEU
2	B	695	GLN
2	B	696	GLU
1	C	226	ARG
1	C	230	SER
1	C	232	LYS
1	C	254	LEU
1	C	255	VAL
1	C	269	GLU
1	C	302	LEU

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Mol	Chain	Res	Type
1	C	308	LEU
1	C	313	VAL
1	C	326	ASN
1	C	331	LEU
1	C	336	ASN
1	C	349	LYS
1	C	393	ASN
1	C	399	LYS
1	C	412	LEU
1	C	436	LEU
1	C	445	GLN
1	C	451	GLU
1	C	453	ASP
2	D	685	GLU
2	D	691	HIS
2	D	696	GLU
1	E	208	LYS
1	E	209	ARG
1	E	212	GLU
1	E	221	ASN
1	E	226	ARG
1	E	232	LYS
1	E	234	SER
1	E	236	ASN
1	E	254	LEU
1	E	257	LYS
1	E	265	ASN
1	E	289	GLU
1	E	313	VAL
1	E	326	ASN
1	E	345	LYS
1	E	387	ASP
1	E	394	VAL
1	E	414	SER
1	E	415	ASN
1	E	422	LEU
1	E	428	GLN
1	E	450	THR
1	E	451	GLU
1	E	459	LEU
1	E	461	GLN
2	F	685	GLU

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Mol	Chain	Res	Type
2	F	690	LEU
1	G	202	ASP
1	G	206	LEU
1	G	208	LYS
1	G	215	LEU
1	G	223	VAL
1	G	226	ARG
1	G	232	LYS
1	G	255	VAL
1	G	265	ASN
1	G	269	GLU
1	G	277	GLN
1	G	301	ASP
1	G	302	LEU
1	G	326	ASN
1	G	331	LEU
1	G	368	LEU
1	G	382	ILE
1	G	385	CYS
1	G	393	ASN
1	G	410	LEU
1	G	422	LEU
1	G	434	ARG
1	G	447	ILE
1	G	451	GLU
1	G	465	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	ASN
1	A	221	ASN
1	A	236	ASN
1	A	305	GLN
1	A	366	ASN
1	A	413	GLN
1	A	415	ASN
1	A	416	HIS
1	A	435	GLN
1	A	440	HIS
1	A	442	GLN
1	A	461	GLN

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Mol	Chain	Res	Type
2	B	691	HIS
2	B	695	GLN
1	C	235	ASN
1	C	242	HIS
1	C	299	ASN
1	C	326	ASN
1	C	336	ASN
1	C	393	ASN
1	C	396	HIS
1	C	413	GLN
1	C	416	HIS
1	C	440	HIS
1	C	457	HIS
1	C	461	GLN
2	D	691	HIS
2	D	695	GLN
1	E	217	ASN
1	E	219	ASN
1	E	221	ASN
1	E	261	ASN
1	E	277	GLN
1	E	299	ASN
1	E	326	ASN
1	E	415	ASN
1	E	416	HIS
1	E	457	HIS
1	E	461	GLN
2	F	691	HIS
2	F	695	GLN
1	G	261	ASN
1	G	265	ASN
1	G	277	GLN
1	G	299	ASN
1	G	305	GLN
1	G	326	ASN
1	G	336	ASN
1	G	445	GLN
2	H	695	GLN

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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	544	E	501	-	36,41,41	2.40	15 (41%)	41,55,55	1.57	3 (7%)
3	544	G	601	-	36,41,41	2.43	15 (41%)	41,55,55	1.67	4 (9%)
3	544	A	469	-	36,41,41	2.38	13 (36%)	41,55,55	1.72	5 (12%)
3	544	C	470	-	36,41,41	2.41	14 (38%)	41,55,55	1.64	4 (9%)

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	544	E	501	-	1/1/4/6	1/25/30/30	0/4/4/4
3	544	G	601	-	1/1/4/6	1/25/30/30	0/4/4/4
3	544	A	469	-	1/1/4/6	2/25/30/30	0/4/4/4
3	544	C	470	-	1/1/4/6	1/25/30/30	0/4/4/4

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	470	544	C1A-N	6.31	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	601	544	C1A-N	6.11	1.41	1.33
3	E	501	544	C1A-N	5.20	1.40	1.33
3	E	501	544	C3E-C3D	5.07	1.55	1.48
3	A	469	544	C3E-C3D	5.02	1.55	1.48
3	C	470	544	C3E-C3D	4.97	1.55	1.48
3	G	601	544	C3E-C3D	4.80	1.54	1.48
3	A	469	544	C1F-C1G	4.70	1.58	1.43
3	E	501	544	C1F-C1G	4.63	1.58	1.43
3	G	601	544	C1F-C1G	4.55	1.58	1.43
3	E	501	544	CE2-CZ	4.53	1.47	1.38
3	C	470	544	C1F-C1G	4.41	1.57	1.43
3	G	601	544	CE2-CZ	4.12	1.46	1.38
3	A	469	544	CE2-CZ	4.09	1.46	1.38
3	A	469	544	C1A-N	3.81	1.38	1.33
3	C	470	544	C1I-C1H	3.79	1.45	1.39
3	A	469	544	CA-N	3.71	1.53	1.45
3	E	501	544	C1I-C1H	3.70	1.45	1.39
3	C	470	544	CE2-CZ	3.69	1.46	1.38
3	G	601	544	C1I-C1H	3.66	1.45	1.39
3	G	601	544	CA-N	3.53	1.53	1.45
3	A	469	544	C1I-C1H	3.37	1.45	1.39
3	C	470	544	CA-N	3.35	1.52	1.45
3	C	470	544	C1M-C1H	3.33	1.45	1.39
3	E	501	544	C1M-C1H	3.30	1.45	1.39
3	A	469	544	C1H-C1G	-3.20	1.44	1.49
3	E	501	544	CA-N	3.16	1.52	1.45
3	A	469	544	C3K-C3J	3.11	1.43	1.36
3	G	601	544	C1M-C1H	3.07	1.44	1.39
3	A	469	544	C1M-C1H	2.96	1.44	1.39
3	C	470	544	CB-CA	2.77	1.60	1.54
3	E	501	544	CD1-CG	2.75	1.44	1.38
3	A	469	544	CD1-CG	2.73	1.44	1.38
3	G	601	544	C1H-C1G	-2.61	1.45	1.49
3	A	469	544	C3M-C3N	2.57	1.42	1.36
3	C	470	544	C3M-C3N	2.55	1.42	1.36
3	C	470	544	C1H-C1G	-2.50	1.45	1.49
3	E	501	544	C1H-C1G	-2.46	1.45	1.49
3	G	601	544	CD2-CG	2.42	1.44	1.38
3	C	470	544	C3K-C3J	2.40	1.42	1.36
3	A	469	544	C1B-C1A	2.40	1.54	1.50
3	G	601	544	C3K-C3J	2.38	1.42	1.36
3	A	469	544	CE1-CZ	2.34	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	501	544	C1B-C1A	2.30	1.54	1.50
3	E	501	544	C3M-C3N	2.30	1.41	1.36
3	E	501	544	C3K-C3J	2.28	1.41	1.36
3	E	501	544	O1-C	-2.27	1.23	1.30
3	G	601	544	CB-CA	2.27	1.59	1.54
3	C	470	544	CD2-CG	2.26	1.43	1.38
3	G	601	544	C1B-C1A	2.18	1.54	1.50
3	C	470	544	C1L-C1K	2.08	1.43	1.38
3	G	601	544	O1-C	-2.06	1.23	1.30
3	E	501	544	C3K-C3L	2.05	1.43	1.38
3	E	501	544	CD2-CG	2.05	1.43	1.38
3	C	470	544	OH-CZ	2.03	1.42	1.37
3	G	601	544	C3M-C3N	2.02	1.41	1.36
3	G	601	544	CD1-CG	2.02	1.43	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	469	544	C1F-C1A-N	-5.69	116.74	121.29
3	E	501	544	C1F-C1A-N	-5.57	116.83	121.29
3	G	601	544	C1B-C1A-N	5.57	125.06	118.82
3	C	470	544	C1B-C1A-N	5.52	125.00	118.82
3	G	601	544	C1F-C1A-N	-5.51	116.88	121.29
3	A	469	544	C1B-C1A-N	5.32	124.78	118.82
3	E	501	544	C1B-C1A-N	5.10	124.53	118.82
3	A	469	544	C-CA-N	4.85	122.03	110.55
3	C	470	544	C1F-C1A-N	-4.31	117.84	121.29
3	C	470	544	C-CA-N	4.17	120.43	110.55
3	G	601	544	C-CA-N	4.01	120.05	110.55
3	E	501	544	C-CA-N	3.83	119.61	110.55
3	C	470	544	CB-CA-C	3.67	119.25	110.42
3	A	469	544	CB-CA-C	2.83	117.23	110.42
3	G	601	544	CB-CA-C	2.36	116.10	110.42
3	A	469	544	C1A-C1F-C1G	2.15	129.21	124.22

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	469	544	C1A
3	C	470	544	C1A
3	E	501	544	C1A
3	G	601	544	C1A

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	501	544	OH-C3A-C3B-C3C
3	C	470	544	C-CA-N-C1A
3	G	601	544	OH-C3A-C3B-C3C
3	A	469	544	C-CA-N-C1A
3	A	469	544	OH-C3A-C3B-C3C

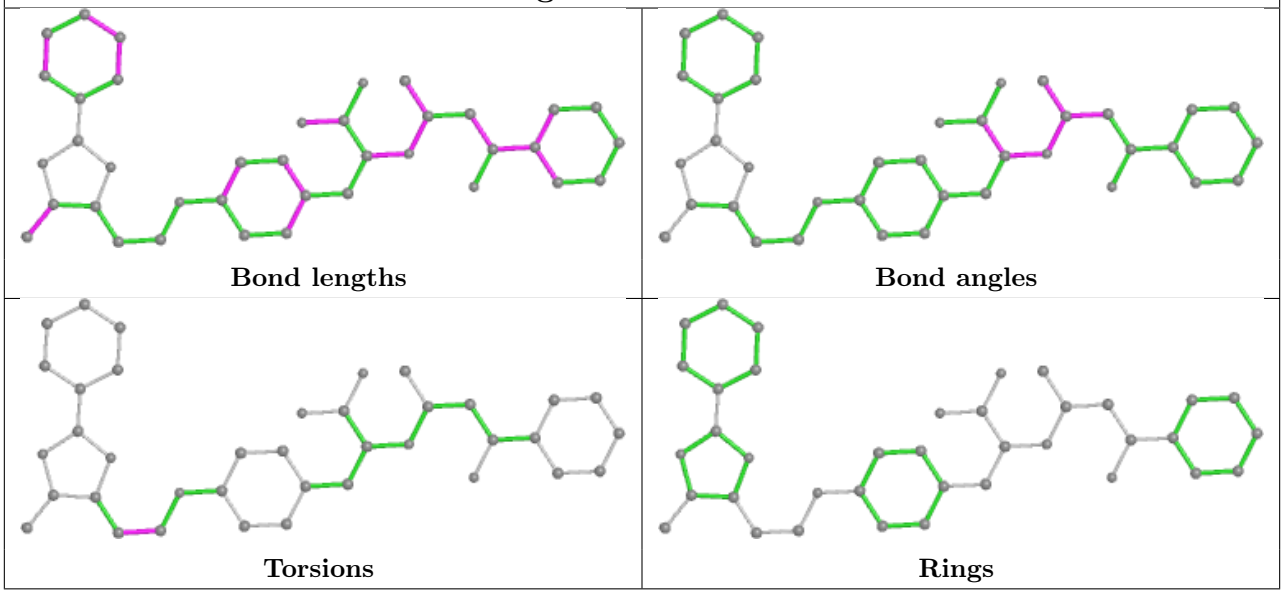
There are no ring outliers.

2 monomers are involved in 3 short contacts:

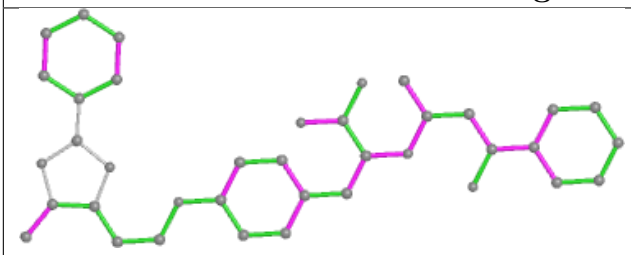
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	469	544	1	0
3	C	470	544	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

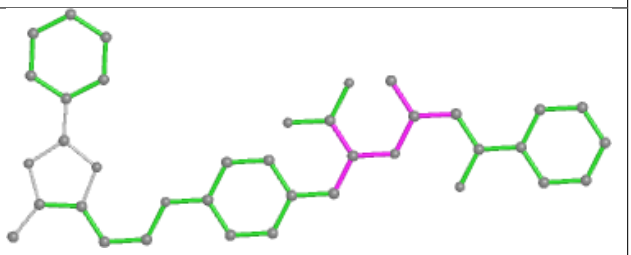
Ligand 544 E 501



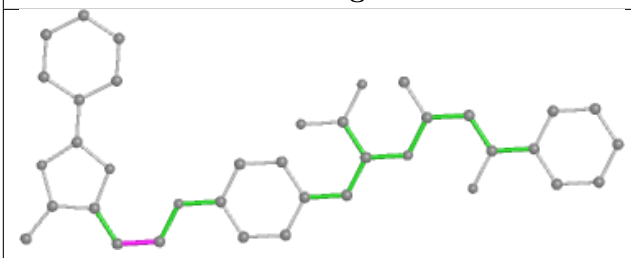
Ligand 544 G 601



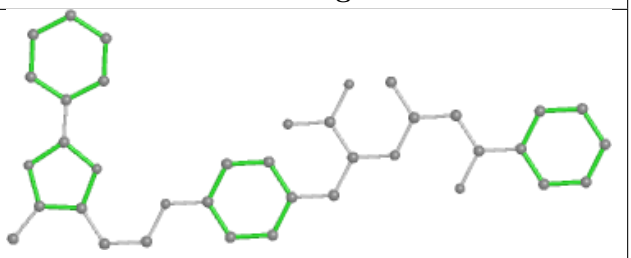
Bond lengths



Bond angles

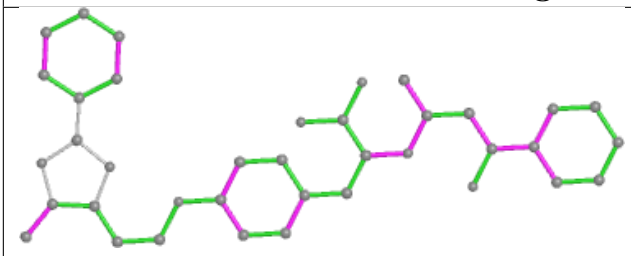


Torsions

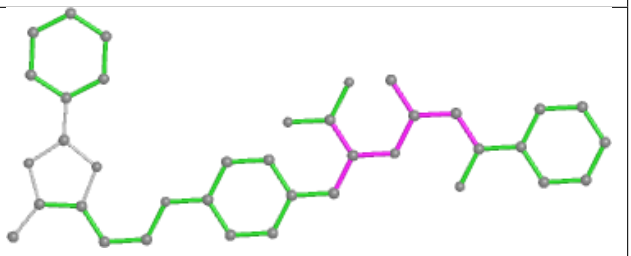


Rings

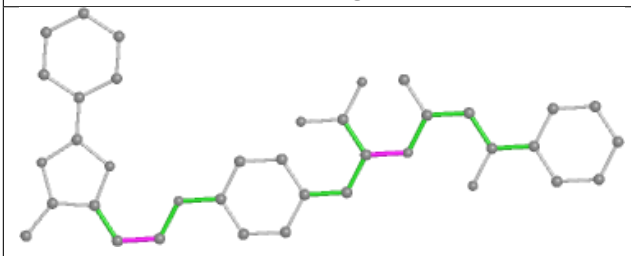
Ligand 544 A 469



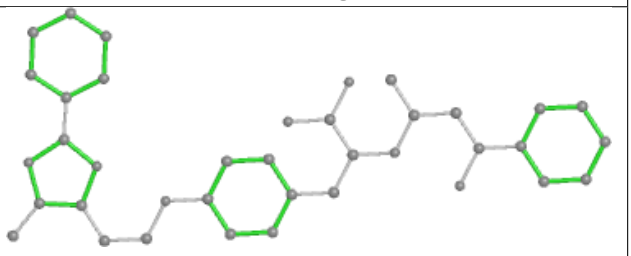
Bond lengths



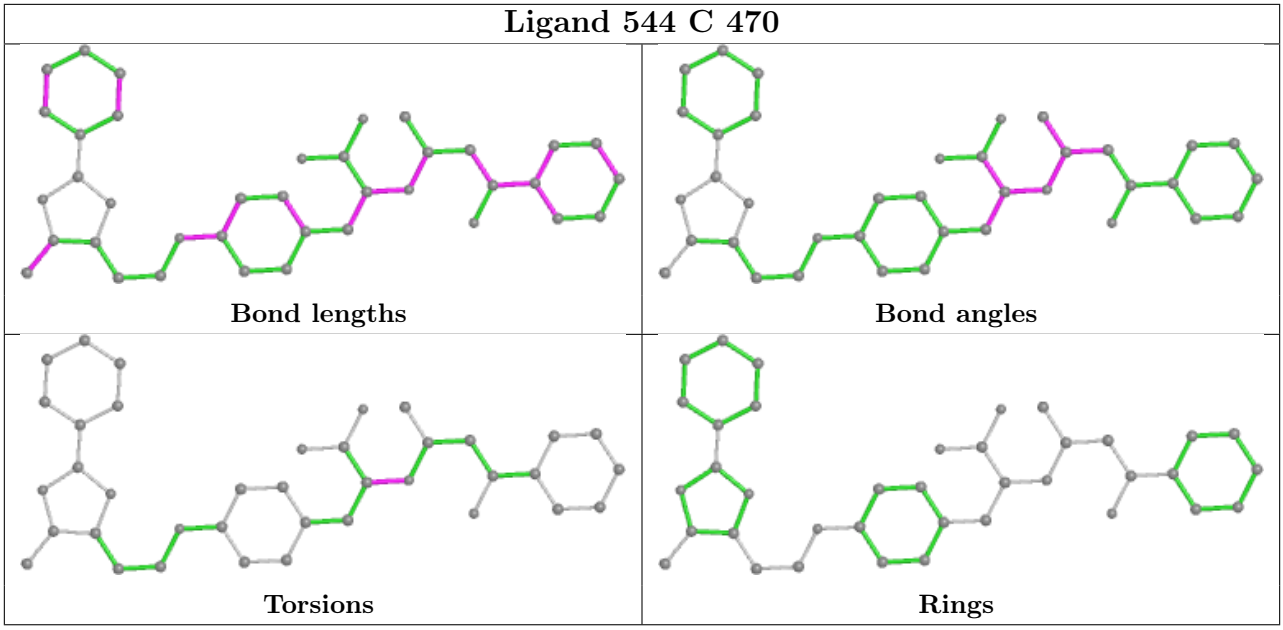
Bond angles



Torsions



Rings



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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.