



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:53 PM GMT

PDB ID : 2ACL  
Title : Liver X-Receptor alpha Ligand Binding Domain with SB313987  
Authors : Jaye, M.C.; Krawiec, J.A.; Campobasso, N.; Smallwood, A.; Qiu, C.; Lu, Q.;  
Kerrigan, J.J.  
Deposited on : 2005-07-19  
Resolution : 2.80 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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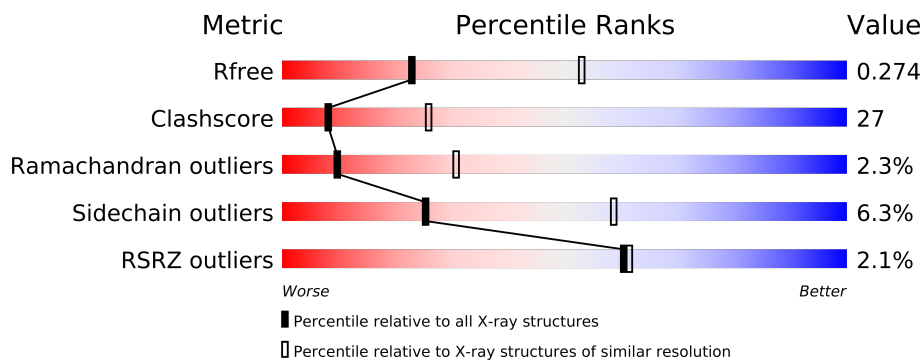
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	238	
1	C	238	
1	E	238	
1	G	238	
2	B	244	
2	D	244	
2	F	244	
2	H	244	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14858 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Retinoic acid receptor RXR-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1682	1078	289	305	10			
1	C	215	Total	C	N	O	S	0	0	0
			1689	1083	290	306	10			
1	E	214	Total	C	N	O	S	0	0	0
			1682	1078	289	305	10			
1	G	214	Total	C	N	O	S	0	0	0
			1682	1078	289	305	10			

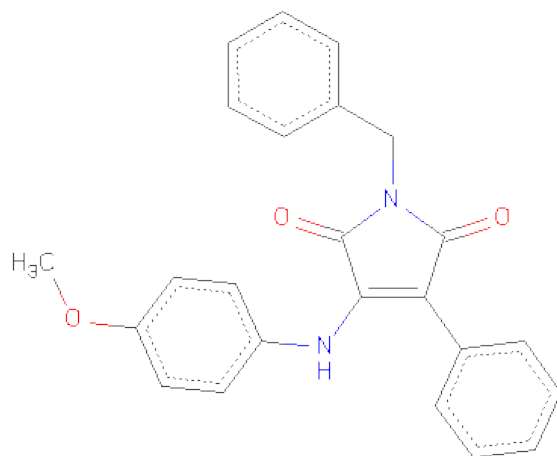
- Molecule 2 is a protein called Oxysterols receptor LXR-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	242	Total	C	N	O	S	0	0	0
			1966	1255	343	361	7			
2	D	242	Total	C	N	O	S	0	0	0
			1966	1255	343	361	7			
2	F	242	Total	C	N	O	S	0	0	0
			1966	1255	343	361	7			
2	H	244	Total	C	N	O	S	0	0	0
			1985	1266	347	365	7			

There are 8 discrepancies between the modelled and reference sequences:

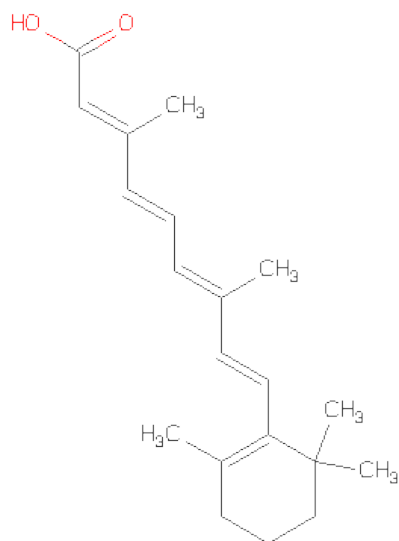
Chain	Residue	Modelled	Actual	Comment	Reference
B	202	VAL	-	CLONING ARTIFACT	UNP Q9Z0Y9
B	399	PRO	ARG	VARIANT	UNP Q9Z0Y9
D	202	VAL	-	CLONING ARTIFACT	UNP Q9Z0Y9
D	399	PRO	ARG	VARIANT	UNP Q9Z0Y9
F	202	VAL	-	CLONING ARTIFACT	UNP Q9Z0Y9
F	399	PRO	ARG	VARIANT	UNP Q9Z0Y9
H	202	VAL	-	CLONING ARTIFACT	UNP Q9Z0Y9
H	399	PRO	ARG	VARIANT	UNP Q9Z0Y9

- Molecule 3 is 1-BENZYL-3-(4-METHOXYPHENYLAMINO)-4-PHENYLPYRROLE-2,5-DIONE (three-letter code: L05) (formula:  $C_{24}H_{20}N_2O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			29	24	2	3		
3	D	1	Total	C	N	O	0	0
			29	24	2	3		
3	F	1	Total	C	N	O	0	0
			29	24	2	3		
3	H	1	Total	C	N	O	0	0
			29	24	2	3		

- Molecule 4 is RETINOIC ACID (three-letter code: REA) (formula:  $C_{20}H_{28}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	G	1	Total	C	O	0	0
			22	20	2		
4	A	1	Total	C	O	0	0
			22	20	2		
4	C	1	Total	C	O	0	0
			22	20	2		
4	E	1	Total	C	O	0	0
			22	20	2		

- Molecule 5 is water.

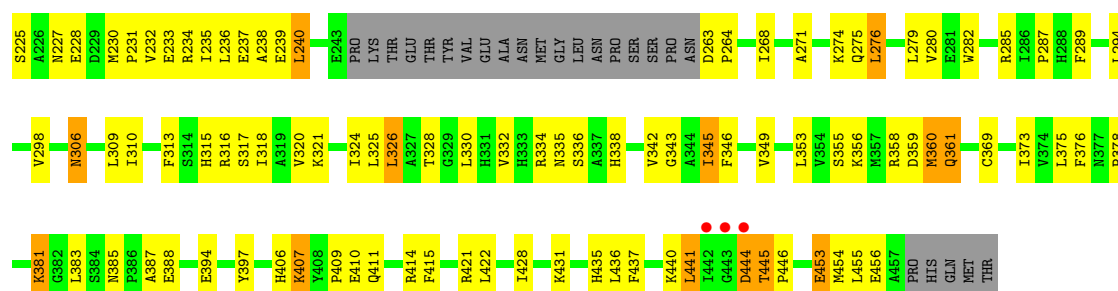
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	5	Total	O	0	0
			5	5		
5	B	4	Total	O	0	0
			4	4		
5	C	3	Total	O	0	0
			3	3		
5	D	7	Total	O	0	0
			7	7		
5	E	4	Total	O	0	0
			4	4		
5	F	6	Total	O	0	0
			6	6		
5	G	5	Total	O	0	0
			5	5		
5	H	2	Total	O	0	0
			2	2		

### 3 Residue-property plots

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

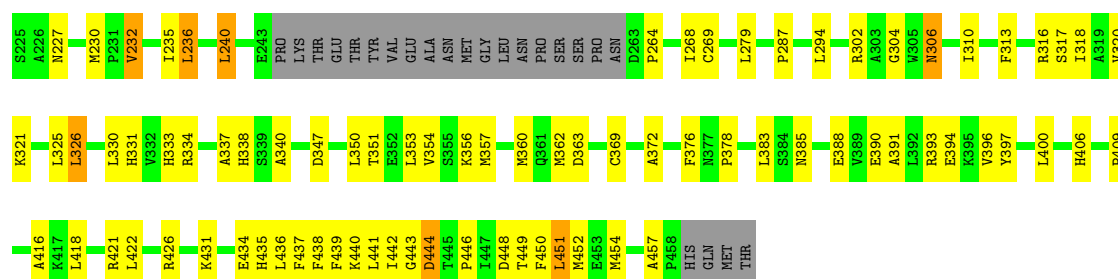
#### • Molecule 1: Retinoic acid receptor RXR-alpha

Chain A: 



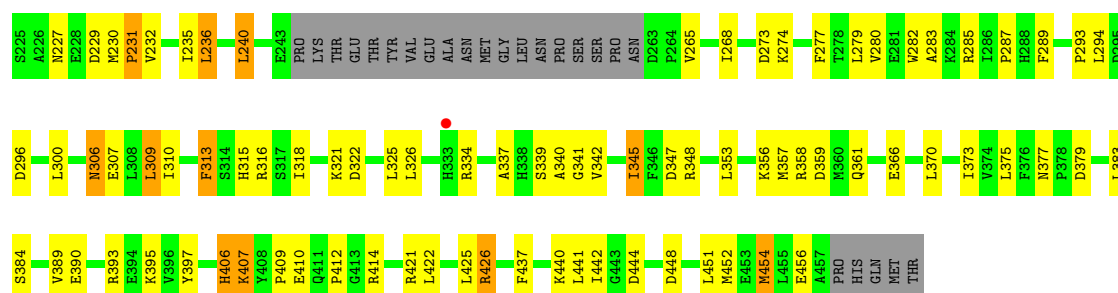
#### • Molecule 1: Retinoic acid receptor RXR-alpha

Chain C: 



#### • Molecule 1: Retinoic acid receptor RXR-alpha

Chain E: 



#### • Molecule 1: Retinoic acid receptor RXR-alpha

Frequency	Percentage
Daily	~2%
Weekly	~58%
Monthly	~35%
Quarterly	~4%
Other	~2%



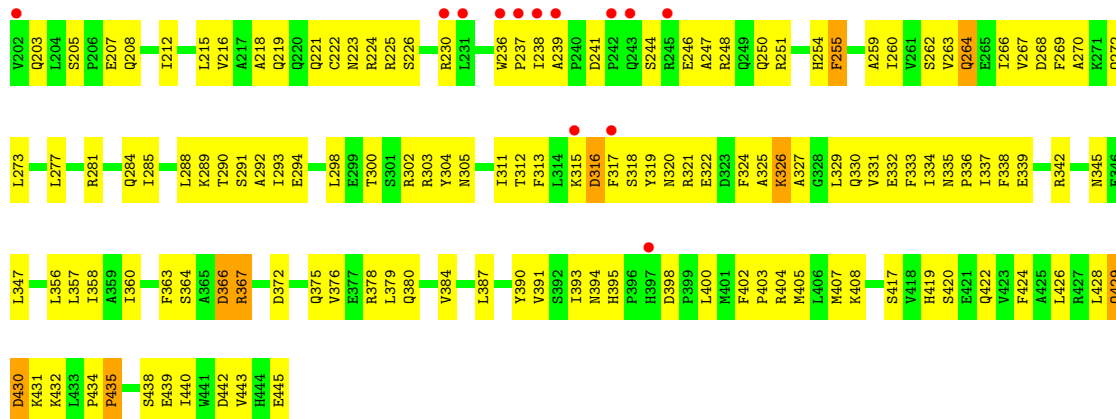
Response	Percentage
Yes, it is a crisis	95%
No, it is not a crisis	4%
I don't know	1%





● Molecule 2: Oxysterols receptor LXR-alpha

Chain H:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.77Å 81.95Å 111.44Å 88.98° 75.20° 78.27°	Depositor
Resolution (Å)	30.00 – 2.80 45.58 – 2.74	Depositor EDS
% Data completeness (in resolution range)	95.0 (30.00-2.80) 89.4 (45.58-2.74)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 2.73Å)	Xtriage
Refinement program	CNX	Depositor
R, $R_{free}$	0.210 , 0.280 0.209 , 0.274	Depositor DCC
$R_{free}$ test set	2310 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.6	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 16.6	EDS
Estimated twinning fraction	0.008 for -h,-k,-h+l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 50018 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	14858	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: L05, REA

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	0.39	0/1714	0.64	0/2317
1	C	0.42	0/1722	0.63	0/2329
1	E	0.37	0/1714	0.62	0/2317
1	G	0.40	0/1714	0.61	0/2317
2	B	0.40	0/2008	0.60	0/2721
2	D	0.42	0/2008	0.59	0/2721
2	F	0.38	0/2008	0.54	0/2721
2	H	0.39	0/2028	0.56	0/2748
All	All	0.39	0/14916	0.60	0/20191

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1682	0	1713	101	0
1	C	1689	0	1720	82	0
1	E	1682	0	1713	80	0
1	G	1682	0	1713	115	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1966	0	1973	108	0
2	D	1966	0	1973	129	0
2	F	1966	0	1973	94	0
2	H	1985	0	1986	154	0
3	B	29	0	20	0	0
3	D	29	0	20	2	0
3	F	29	0	20	1	0
3	H	29	0	20	1	0
4	A	22	0	27	0	0
4	C	22	0	27	0	0
4	E	22	0	27	0	0
4	G	22	0	27	0	0
5	A	5	0	0	0	0
5	B	4	0	0	1	0
5	C	3	0	0	1	0
5	D	7	0	0	0	0
5	E	4	0	0	0	0
5	F	6	0	0	2	0
5	G	5	0	0	0	0
5	H	2	0	0	2	0
All	All	14858	0	14952	793	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 27.

All (793) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:385:ASN:HD22	1:A:388:GLU:HG3	1.31	0.95
2:H:387:LEU:O	2:H:391:VAL:HG22	1.69	0.91
1:E:454:MET:HE2	2:F:263:VAL:HG12	1.52	0.91
2:F:299:GLU:HG3	2:F:303:ARG:HH12	1.33	0.91
1:C:302:ARG:HH12	2:H:330:GLN:HE22	1.22	0.88
1:G:227:ASN:HD21	1:G:232:VAL:HG22	1.36	0.87
1:G:236:LEU:HD22	1:G:240:LEU:HD22	1.57	0.87
2:B:378:ARG:HH11	2:B:378:ARG:HB3	1.39	0.86
2:H:225:ARG:HH21	2:H:268:ASP:HB3	1.41	0.86
2:F:305:ASN:HD21	2:F:312:THR:HG23	1.37	0.85
1:G:380:SER:HB2	1:G:383:LEU:HD21	1.58	0.85
1:G:334:ARG:HD2	1:G:347:ASP:OD1	1.76	0.85
2:H:241:ASP:HB3	2:H:244:SER:HB2	1.59	0.84
1:A:385:ASN:ND2	1:A:388:GLU:HG3	1.91	0.84
1:A:274:LYS:HD3	1:A:275:GLN:HE21	1.43	0.84

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:299:GLU:HG3	2:F:303:ARG:NH1	1.91	0.83
2:H:238:ILE:HG13	2:H:239:ALA:H	1.42	0.83
1:G:421:ARG:HA	1:G:421:ARG:HE	1.41	0.83
1:C:227:ASN:ND2	1:C:232:VAL:HG22	1.93	0.83
2:F:230:ARG:HG2	2:F:314:LEU:HD13	1.59	0.82
2:D:243:GLN:HE21	1:G:294:LEU:H	1.27	0.82
2:D:219:GLN:NE2	2:D:302:ARG:HH22	1.77	0.82
1:A:446:PRO:HB3	2:B:443:VAL:HB	1.60	0.82
1:A:385:ASN:HD21	1:A:387:ALA:HB3	1.44	0.82
2:H:241:ASP:CB	2:H:244:SER:HB2	2.11	0.81
1:C:230:MET:HE3	1:C:235:ILE:HD11	1.62	0.81
1:A:356:LYS:HG3	1:A:421:ARG:NH1	1.96	0.81
2:F:374:LEU:HD12	2:F:378:ARG:NH1	1.96	0.80
2:D:243:GLN:NE2	1:G:294:LEU:H	1.78	0.80
1:A:355:SER:HA	1:A:358:ARG:NH1	1.96	0.80
1:E:307:GLU:HG2	1:E:425:LEU:HG	1.62	0.80
1:G:394:GLU:HA	1:G:397:TYR:CD2	2.16	0.80
2:F:294:GLU:HG2	2:F:412:LEU:HB3	1.62	0.80
2:H:375:GLN:HA	2:H:378:ARG:HE	1.45	0.80
2:D:229:ASP:O	2:D:232:ARG:HG2	1.82	0.80
1:G:325:LEU:HD13	1:G:331:HIS:CE1	2.18	0.79
1:A:230:MET:CE	1:A:235:ILE:HD11	2.12	0.79
1:G:421:ARG:NE	1:G:421:ARG:HA	1.96	0.79
2:B:248:ARG:HH12	2:B:431:LYS:HE2	1.47	0.79
1:A:233:GLU:O	1:A:237:GLU:HG3	1.83	0.79
2:H:315:LYS:O	2:H:316:ASP:HB2	1.82	0.79
1:G:441:LEU:HB2	2:H:445:GLU:OE1	1.81	0.79
1:E:306:ASN:H	1:E:306:ASN:HD22	1.31	0.79
2:F:204:LEU:H	2:F:393:ILE:HD11	1.48	0.78
1:C:269:CYS:HB3	2:H:445:GLU:OE2	1.84	0.78
2:H:375:GLN:HB2	2:H:378:ARG:HH21	1.48	0.78
2:H:380:GLN:O	2:H:384:VAL:HG23	1.84	0.78
2:F:219:GLN:NE2	2:F:302:ARG:HH22	1.82	0.77
1:C:347:ASP:O	1:C:351:THR:HG23	1.85	0.77
2:H:320:ASN:HD21	2:H:322:GLU:HB3	1.49	0.77
1:C:357:MET:HG2	1:C:362:MET:HE3	1.64	0.77
2:B:300:THR:HG22	2:B:311:ILE:HD13	1.67	0.77
1:E:410:GLU:O	1:E:412:PRO:HD3	1.84	0.77
2:H:262:SER:O	2:H:266:ILE:HG13	1.83	0.77
1:A:397:TYR:OH	2:B:407:MET:HG3	1.84	0.77
1:E:227:ASN:HD21	1:E:232:VAL:HG22	1.49	0.77
2:B:430:ASP:HB2	1:E:280:VAL:HG11	1.66	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:342:ARG:HB3	2:D:342:ARG:NH1	2.01	0.76
2:H:387:LEU:HD21	2:H:405:MET:HE2	1.65	0.76
1:A:394:GLU:HA	1:A:397:TYR:CD2	2.20	0.76
1:E:321:LYS:HE3	1:E:322:ASP:OD2	1.85	0.76
1:C:227:ASN:HD21	1:C:232:VAL:H	1.34	0.75
2:H:400:LEU:O	2:H:403:PRO:HD2	1.86	0.75
2:D:330:GLN:N	2:D:330:GLN:HE21	1.84	0.75
1:C:304:GLY:HA2	5:C:23:HOH:O	1.86	0.75
1:C:356:LYS:O	1:C:360:MET:HG2	1.86	0.75
2:D:437:LEU:O	2:D:440:ILE:HD13	1.87	0.75
2:H:356:LEU:HD13	2:H:387:LEU:HA	1.67	0.75
2:H:429:GLN:O	2:H:430:ASP:HB3	1.87	0.75
2:F:387:LEU:O	2:F:391:VAL:HG22	1.88	0.74
2:F:434:PRO:HD2	2:F:437:LEU:HD12	1.70	0.74
1:G:347:ASP:O	1:G:351:THR:HG23	1.86	0.73
2:B:243:GLN:HG3	2:B:248:ARG:HD2	1.70	0.73
2:F:256:THR:O	2:F:260:ILE:HG12	1.88	0.73
1:C:227:ASN:HD21	1:C:232:VAL:HG22	1.54	0.73
1:A:227:ASN:HD21	1:A:232:VAL:HG22	1.52	0.73
2:B:227:PHE:CE1	2:B:315:LYS:HG3	2.24	0.72
1:G:356:LYS:HG3	1:G:421:ARG:NH1	2.04	0.72
2:D:428:LEU:H	2:D:428:LEU:HD22	1.55	0.72
2:H:305:ASN:HD21	2:H:312:THR:HG23	1.53	0.72
2:F:280:SER:OG	2:F:282:GLU:HG2	1.89	0.71
1:C:357:MET:HG2	1:C:362:MET:CE	2.20	0.71
2:B:330:GLN:HG3	2:B:332:GLU:HG2	1.72	0.71
1:C:236:LEU:HD22	1:C:240:LEU:HD22	1.69	0.71
2:B:400:LEU:O	2:B:403:PRO:HD2	1.90	0.71
2:B:300:THR:CG2	2:B:311:ILE:HD13	2.21	0.71
2:B:402:PHE:HB3	2:B:403:PRO:HD3	1.73	0.71
2:D:260:ILE:HG23	2:D:436:LEU:HD23	1.71	0.71
1:C:230:MET:CE	1:C:235:ILE:HD11	2.21	0.71
1:E:282:TRP:CZ3	1:E:375:LEU:HD22	2.25	0.71
1:C:390:GLU:O	1:C:394:GLU:HG3	1.90	0.71
1:E:230:MET:CE	1:E:235:ILE:HD11	2.21	0.71
2:D:219:GLN:HE22	2:D:302:ARG:HH22	1.38	0.70
2:F:387:LEU:HD21	2:F:405:MET:HE3	1.73	0.70
2:H:364:SER:HB2	2:H:367:ARG:HH11	1.57	0.70
1:A:385:ASN:ND2	1:A:387:ALA:HB3	2.06	0.70
2:D:333:PHE:CE2	2:D:337:ILE:HD11	2.27	0.69
1:G:353:LEU:O	1:G:357:MET:HG3	1.93	0.69
1:G:334:ARG:HD3	1:G:350:LEU:HD12	1.75	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:421:ARG:HA	1:A:421:ARG:NE	2.06	0.69
1:A:349:VAL:HG13	1:A:353:LEU:HD12	1.73	0.69
1:C:422:LEU:HD12	2:D:407:MET:CE	2.23	0.69
1:C:454:MET:HE1	2:D:264:GLN:HB2	1.74	0.69
2:F:374:LEU:HD12	2:F:378:ARG:HH12	1.57	0.69
1:C:422:LEU:HD12	2:D:407:MET:HE3	1.73	0.69
1:A:415:PHE:HE2	2:B:403:PRO:HG3	1.57	0.69
2:B:254:HIS:HE2	2:B:319:TYR:HH	1.40	0.69
2:D:330:GLN:CA	2:D:330:GLN:HE21	2.06	0.68
2:H:364:SER:CB	2:H:367:ARG:HH11	2.06	0.68
1:G:392:LEU:O	1:G:396:VAL:HG23	1.94	0.68
1:C:443:GLY:HA3	2:D:443:VAL:HG11	1.76	0.68
2:D:241:ASP:H	2:D:242:PRO:HD3	1.58	0.67
1:E:236:LEU:HD22	1:E:240:LEU:CD2	2.24	0.67
1:E:334:ARG:NH1	1:E:347:ASP:OD1	2.28	0.67
1:C:227:ASN:ND2	1:C:232:VAL:H	1.91	0.67
1:C:440:LYS:HG3	1:G:266:THR:HG23	1.76	0.67
1:G:381:LYS:HD2	1:G:381:LYS:N	2.10	0.66
1:A:230:MET:HE2	1:A:235:ILE:HD11	1.76	0.66
1:G:315:HIS:CG	1:G:367:LEU:HD22	2.30	0.66
1:C:443:GLY:HA3	2:D:443:VAL:CG1	2.25	0.66
2:B:237:PRO:HG3	2:B:250:GLN:HB3	1.77	0.66
2:B:287:LEU:O	2:B:291:SER:HB3	1.95	0.66
2:H:342:ARG:O	2:H:345:ASN:HB3	1.95	0.66
1:G:446:PRO:O	1:G:447:ILE:HG13	1.96	0.66
1:A:355:SER:HA	1:A:358:ARG:HH12	1.59	0.66
2:D:254:HIS:NE2	2:D:319:TYR:OH	2.27	0.66
2:F:428:LEU:HD22	2:F:428:LEU:H	1.61	0.66
1:G:334:ARG:HD3	1:G:350:LEU:CD1	2.26	0.65
2:B:231:LEU:O	2:B:231:LEU:HD23	1.96	0.65
1:G:380:SER:HB2	1:G:383:LEU:CD2	2.26	0.65
2:F:230:ARG:CG	2:F:314:LEU:HD13	2.27	0.65
2:B:203:GLN:HG2	2:B:204:LEU:H	1.61	0.65
1:C:230:MET:CE	1:C:396:VAL:HG22	2.26	0.65
1:G:356:LYS:HG3	1:G:421:ARG:HH11	1.59	0.65
2:D:350:ASN:OD1	2:D:353:GLU:HG3	1.97	0.65
2:F:312:THR:HG22	2:F:318:SER:HB2	1.79	0.65
1:A:385:ASN:ND2	1:A:388:GLU:H	1.95	0.65
1:G:316:ARG:HG2	1:G:316:ARG:HH11	1.61	0.65
1:A:271:ALA:CB	1:A:326:LEU:HD12	2.27	0.65
1:A:349:VAL:O	1:A:353:LEU:HB2	1.97	0.64
2:B:248:ARG:NE	1:E:294:LEU:HD23	2.12	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:236:LEU:HD22	1:G:240:LEU:CD2	2.26	0.64
2:F:387:LEU:HD11	2:F:405:MET:HE1	1.79	0.64
2:B:335:ASN:HB2	2:B:336:PRO:HD3	1.79	0.64
2:H:289:LYS:NZ	2:H:440:ILE:HA	2.11	0.64
2:B:204:LEU:HD12	2:B:208:GLN:OE1	1.97	0.64
2:F:322:GLU:HG2	2:F:326:LYS:HE3	1.79	0.64
2:H:330:GLN:OE1	2:H:422:GLN:HB2	1.96	0.64
2:H:237:PRO:HB2	2:H:251:ARG:NH1	2.12	0.64
1:G:230:MET:CE	1:G:235:ILE:HD11	2.27	0.64
1:G:264:PRO:HG2	1:G:336:SER:HB3	1.80	0.64
2:H:303:ARG:HD3	2:H:312:THR:O	1.98	0.64
2:F:303:ARG:HD3	2:F:312:THR:O	1.98	0.63
1:G:380:SER:O	1:G:383:LEU:HD23	1.98	0.63
2:D:219:GLN:HE22	2:D:302:ARG:NH2	1.96	0.63
1:G:348:ARG:O	1:G:352:GLU:HB2	1.99	0.63
2:D:364:SER:O	2:D:367:ARG:HG2	1.99	0.63
1:E:318:ILE:HG23	1:E:358:ARG:HG3	1.80	0.63
2:F:333:PHE:CE2	2:F:337:ILE:HD11	2.34	0.63
2:F:204:LEU:N	2:F:393:ILE:HD11	2.13	0.63
2:H:400:LEU:CB	2:H:404:ARG:HH21	2.12	0.62
2:D:330:GLN:O	2:D:334:ILE:HG13	1.98	0.62
1:C:334:ARG:HD2	1:C:347:ASP:OD1	1.98	0.62
2:D:428:LEU:HD11	1:G:276:LEU:HD21	1.81	0.62
1:E:397:TYR:OH	2:F:407:MET:HG3	2.00	0.62
1:C:302:ARG:HH22	2:H:330:GLN:HE21	1.47	0.62
1:G:422:LEU:HD12	2:H:407:MET:HE3	1.81	0.62
2:H:400:LEU:HB2	2:H:404:ARG:HH21	1.65	0.62
2:B:238:ILE:HD12	2:B:238:ILE:H	1.64	0.62
1:C:333:HIS:HD2	1:C:334:ARG:N	1.97	0.62
2:B:320:ASN:ND2	2:B:323:ASP:H	1.97	0.62
2:H:402:PHE:HB3	2:H:403:PRO:HD3	1.82	0.62
1:E:422:LEU:HD12	2:F:407:MET:HE3	1.82	0.62
2:F:238:ILE:O	2:F:240:PRO:HD3	1.99	0.62
2:B:238:ILE:N	2:B:238:ILE:HD12	2.14	0.62
2:H:225:ARG:NH2	2:H:268:ASP:HB3	2.15	0.61
2:D:237:PRO:HG2	2:D:250:GLN:CB	2.30	0.61
1:C:302:ARG:HH12	2:H:330:GLN:NE2	1.95	0.61
2:D:235:PRO:O	2:D:237:PRO:HD3	1.99	0.61
2:F:219:GLN:NE2	2:F:302:ARG:NH2	2.47	0.61
2:B:254:HIS:NE2	2:B:319:TYR:OH	2.31	0.61
1:C:325:LEU:HD13	1:C:331:HIS:CE1	2.35	0.61
2:H:221:GLN:O	2:H:225:ARG:HG3	2.01	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:210:GLY:O	2:D:214:LYS:HG2	2.00	0.61
1:G:431:LYS:HZ3	1:G:442:ILE:HB	1.64	0.61
1:E:315:HIS:O	1:E:318:ILE:HG13	2.01	0.61
2:F:300:THR:HG23	2:F:311:ILE:HD13	1.82	0.61
1:A:328:THR:OG1	1:A:330:LEU:HD23	2.01	0.61
2:B:320:ASN:C	2:B:320:ASN:HD22	2.03	0.61
1:A:455:LEU:HB3	2:B:281:ARG:HH21	1.64	0.61
2:F:292:ALA:O	2:F:296:MET:HG3	2.01	0.61
2:D:320:ASN:C	2:D:320:ASN:HD22	2.03	0.61
1:E:306:ASN:HD22	1:E:306:ASN:N	1.97	0.60
1:E:282:TRP:HZ3	1:E:375:LEU:HD22	1.66	0.60
2:F:262:SER:O	2:F:266:ILE:HG13	2.01	0.60
2:H:312:THR:HG22	2:H:318:SER:HA	1.82	0.60
2:B:330:GLN:HG2	2:B:422:GLN:OE1	2.00	0.60
1:C:431:LYS:O	1:C:434:GLU:HB2	2.01	0.60
1:G:431:LYS:NZ	1:G:442:ILE:HB	2.16	0.60
2:B:214:LYS:O	2:B:217:ALA:HB3	2.01	0.60
1:G:227:ASN:O	1:G:231:PRO:HA	2.01	0.60
1:A:227:ASN:HD21	1:A:232:VAL:CG2	2.13	0.60
2:F:230:ARG:HD3	2:F:314:LEU:HD22	1.83	0.60
1:E:383:LEU:HD21	1:E:389:VAL:HG21	1.84	0.60
1:E:316:ARG:NH1	1:E:325:LEU:O	2.34	0.60
2:F:356:LEU:O	2:F:360:ILE:HG13	2.01	0.59
1:E:454:MET:CE	2:F:263:VAL:HG12	2.27	0.59
1:G:234:ARG:O	1:G:237:GLU:HB2	2.02	0.59
2:B:248:ARG:NH1	2:B:248:ARG:HB3	2.17	0.59
2:D:230:ARG:HH11	2:D:314:LEU:HD23	1.67	0.59
2:H:289:LYS:HZ3	2:H:440:ILE:HA	1.67	0.59
2:H:428:LEU:HD22	2:H:428:LEU:H	1.68	0.59
2:F:312:THR:HG22	2:F:318:SER:CB	2.33	0.59
2:F:302:ARG:HH21	2:F:354:PHE:HB3	1.67	0.59
2:B:230:ARG:HH11	2:B:230:ARG:HG2	1.68	0.59
1:G:421:ARG:CA	1:G:421:ARG:HE	2.15	0.59
1:C:446:PRO:HB3	2:D:443:VAL:HG23	1.83	0.59
2:B:393:ILE:O	2:B:396:PRO:HD3	2.01	0.59
1:C:353:LEU:O	1:C:357:MET:HG3	2.02	0.59
2:H:400:LEU:C	2:H:403:PRO:HD2	2.22	0.59
2:H:254:HIS:HE2	2:H:319:TYR:HH	1.48	0.59
1:G:264:PRO:CG	1:G:336:SER:HB3	2.32	0.59
1:A:359:ASP:C	1:A:361:GLN:H	2.06	0.59
2:H:212:ILE:O	2:H:215:LEU:HB2	2.03	0.59
2:H:330:GLN:O	2:H:334:ILE:HG13	2.02	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:406:HIS:O	1:E:409:PRO:HD3	2.04	0.58
2:B:441:TRP:O	2:B:443:VAL:N	2.36	0.58
2:B:248:ARG:HH12	2:B:431:LYS:CE	2.15	0.58
1:G:447:ILE:HD12	1:G:447:ILE:N	2.18	0.58
2:F:324:PHE:HD1	2:F:329:LEU:HD12	1.67	0.58
1:G:294:LEU:O	1:G:298:VAL:HG23	2.03	0.58
2:B:400:LEU:C	2:B:403:PRO:HD2	2.24	0.58
2:B:237:PRO:HB3	2:B:250:GLN:NE2	2.19	0.58
2:D:400:LEU:O	2:D:404:ARG:HG3	2.03	0.58
2:F:330:GLN:HG2	2:F:422:GLN:HE22	1.67	0.58
1:A:320:VAL:HG22	1:A:321:LYS:N	2.18	0.58
2:B:378:ARG:NH1	2:B:378:ARG:HB3	2.13	0.58
2:D:356:LEU:HD13	2:D:387:LEU:HA	1.86	0.58
2:B:210:GLY:O	2:B:214:LYS:HE2	2.04	0.58
1:A:436:LEU:HD23	1:A:436:LEU:O	2.04	0.58
1:E:437:PHE:O	1:E:441:LEU:HB2	2.04	0.57
2:F:406:LEU:O	2:F:409:LEU:HB2	2.04	0.57
1:E:353:LEU:O	1:E:357:MET:HG3	2.04	0.57
2:B:427:ARG:NH2	1:E:273:ASP:OD1	2.37	0.57
2:H:321:ARG:HG3	2:H:338:PHE:CE2	2.38	0.57
2:H:219:GLN:NE2	2:H:302:ARG:HH12	2.03	0.57
2:F:293:ILE:HG22	5:F:7:HOH:O	2.04	0.57
2:B:219:GLN:HG2	2:B:269:PHE:CE1	2.39	0.57
1:C:302:ARG:NH1	2:H:330:GLN:HE22	1.97	0.57
2:D:243:GLN:HE21	1:G:294:LEU:HD23	1.68	0.57
2:H:394:ASN:HD22	2:H:395:HIS:CE1	2.22	0.57
2:D:309:GLU:OE1	2:D:321:ARG:NH2	2.37	0.57
2:F:395:HIS:N	2:F:396:PRO:HD3	2.20	0.57
2:B:243:GLN:HG3	2:B:248:ARG:CD	2.35	0.57
1:C:397:TYR:OH	2:D:407:MET:HG3	2.05	0.57
2:D:237:PRO:HG3	2:D:250:GLN:OE1	2.05	0.57
2:F:330:GLN:O	2:F:334:ILE:HG13	2.04	0.57
1:E:306:ASN:O	1:E:310:ILE:HG13	2.05	0.57
1:C:357:MET:CG	1:C:362:MET:HE3	2.35	0.57
2:D:240:PRO:O	2:D:241:ASP:HB3	2.04	0.56
1:A:394:GLU:O	1:A:397:TYR:HB2	2.05	0.56
2:H:237:PRO:HG3	2:H:250:GLN:HB3	1.86	0.56
2:D:237:PRO:HG2	2:D:250:GLN:HB3	1.87	0.56
2:D:251:ARG:HH11	2:D:251:ARG:HG2	1.70	0.56
1:A:422:LEU:HD12	2:B:407:MET:HE1	1.87	0.56
1:C:236:LEU:HD22	1:C:240:LEU:CD2	2.36	0.56
1:A:338:HIS:ND1	1:A:343:GLY:HA3	2.21	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:281:ARG:HD2	2:D:284:GLN:HE22	1.70	0.56
2:B:438:SER:O	2:B:442:ASP:HB2	2.05	0.56
2:B:418:VAL:O	2:B:421:GLU:HB2	2.05	0.56
1:C:356:LYS:HG3	1:C:421:ARG:NH1	2.21	0.56
2:B:315:LYS:O	2:B:316:ASP:HB2	2.05	0.56
1:C:236:LEU:O	1:C:240:LEU:HD22	2.06	0.56
2:D:212:ILE:O	2:D:216:VAL:HG23	2.06	0.56
1:E:441:LEU:HD12	1:E:442:ILE:H	1.71	0.56
2:F:363:PHE:CE1	2:F:379:LEU:HD13	2.41	0.56
2:D:292:ALA:O	2:D:296:MET:HG3	2.06	0.56
2:B:233:VAL:HA	2:B:257:GLU:OE2	2.06	0.55
2:H:321:ARG:HG3	2:H:338:PHE:CD2	2.41	0.55
2:F:289:LYS:NZ	2:F:443:VAL:HG11	2.20	0.55
2:D:221:GLN:HA	2:D:224:ARG:NH1	2.22	0.55
1:C:448:ASP:O	1:C:452:MET:HG3	2.06	0.55
1:A:407:LYS:HE2	1:A:407:LYS:HA	1.88	0.55
1:G:264:PRO:O	1:G:267:ASN:HB2	2.07	0.55
1:C:437:PHE:HD2	1:C:438:PHE:CD2	2.24	0.55
2:B:374:LEU:HB3	2:B:378:ARG:NH2	2.21	0.55
2:H:219:GLN:HG2	2:H:269:PHE:CE1	2.41	0.55
2:F:290:THR:O	2:F:290:THR:HG22	2.06	0.55
2:F:315:LYS:O	2:F:316:ASP:HB2	2.07	0.55
2:B:293:ILE:HG23	2:B:294:GLU:N	2.22	0.55
1:A:410:GLU:OE2	1:A:410:GLU:N	2.34	0.55
1:G:231:PRO:CG	1:G:234:ARG:HD3	2.37	0.55
1:C:333:HIS:CD2	1:C:334:ARG:N	2.73	0.55
2:F:270:ALA:HA	2:F:273:LEU:HD12	1.88	0.55
1:A:225:SER:HB3	1:A:228:GLU:CD	2.27	0.55
2:H:375:GLN:CB	2:H:378:ARG:HH21	2.19	0.55
2:H:320:ASN:ND2	2:H:322:GLU:HB3	2.18	0.55
1:G:337:ALA:HB1	1:G:342:VAL:HG23	1.89	0.55
2:F:402:PHE:HB3	2:F:403:PRO:CD	2.37	0.55
2:H:305:ASN:ND2	2:H:312:THR:HG23	2.22	0.54
1:A:263:ASP:HB2	1:A:264:PRO:HD2	1.88	0.54
1:A:415:PHE:CE2	2:B:403:PRO:HG3	2.39	0.54
1:C:310:ILE:HA	1:C:313:PHE:CE2	2.42	0.54
2:D:315:LYS:HE3	2:D:315:LYS:HA	1.90	0.54
1:G:397:TYR:OH	2:H:407:MET:HG3	2.08	0.54
1:A:349:VAL:HG22	1:A:428:ILE:HD13	1.89	0.54
2:F:300:THR:CG2	2:F:311:ILE:HD13	2.37	0.54
2:D:221:GLN:HE22	2:D:225:ARG:HH21	1.56	0.54
1:A:315:HIS:O	1:A:318:ILE:HG13	2.08	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:230:MET:SD	1:E:287:PRO:HB2	2.48	0.54
1:G:359:ASP:O	1:G:361:GLN:HG3	2.06	0.54
2:D:342:ARG:HH11	2:D:342:ARG:HB3	1.72	0.54
2:B:243:GLN:CD	2:B:248:ARG:HE	2.11	0.54
2:H:218:ALA:HB2	2:H:272:GLN:HG2	1.89	0.54
2:D:387:LEU:HD11	2:D:405:MET:HE1	1.90	0.54
2:H:439:GLU:O	2:H:439:GLU:HG2	2.07	0.54
2:H:263:VAL:O	2:H:267:VAL:HG23	2.08	0.54
1:G:378:PRO:HG3	1:G:390:GLU:HG2	1.89	0.54
2:H:372:ASP:O	2:H:376:VAL:HG23	2.08	0.54
2:B:256:THR:O	2:B:260:ILE:HG12	2.07	0.54
1:A:369:CYS:O	1:A:373:ILE:HG13	2.08	0.54
2:B:203:GLN:HG2	2:B:204:LEU:N	2.23	0.53
1:G:359:ASP:C	1:G:361:GLN:H	2.11	0.53
2:F:243:GLN:O	2:F:245:ARG:N	2.42	0.53
2:D:283:ASP:OD2	2:D:371:GLN:HB3	2.07	0.53
2:F:375:GLN:CD	2:F:378:ARG:HH21	2.12	0.53
1:G:422:LEU:HD12	2:H:407:MET:CE	2.38	0.53
2:F:267:VAL:HG22	2:F:288:LEU:HD13	1.90	0.53
2:B:333:PHE:CZ	2:B:337:ILE:HD11	2.43	0.53
1:G:306:ASN:HD22	1:G:433:LEU:HD11	1.74	0.53
1:E:274:LYS:O	1:E:277:PHE:HD1	1.91	0.53
2:D:333:PHE:C	2:D:336:PRO:HD2	2.28	0.53
2:F:342:ARG:O	2:F:345:ASN:HB3	2.09	0.53
1:E:406:HIS:ND1	1:E:407:LYS:N	2.56	0.53
2:F:401:MET:O	2:F:405:MET:HG3	2.07	0.53
2:H:251:ARG:HD2	2:H:326:LYS:O	2.08	0.53
1:G:441:LEU:HD21	2:H:443:VAL:HG21	1.91	0.53
2:B:426:LEU:C	2:B:428:LEU:H	2.12	0.53
1:A:338:HIS:CE1	1:A:343:GLY:HA3	2.42	0.53
2:B:304:TYR:CE1	2:B:342:ARG:HA	2.44	0.53
1:G:231:PRO:HG3	1:G:234:ARG:HD3	1.90	0.53
2:H:320:ASN:O	2:H:324:PHE:HD2	1.92	0.53
2:D:332:GLU:CD	2:D:332:GLU:H	2.11	0.53
1:E:421:ARG:HA	1:E:421:ARG:NE	2.24	0.53
1:A:411:GLN:HE22	1:A:414:ARG:HH11	1.57	0.53
1:E:356:LYS:HE3	2:F:377:GLU:OE2	2.08	0.53
2:H:237:PRO:HB2	2:H:251:ARG:CZ	2.39	0.53
2:B:263:VAL:O	2:B:267:VAL:HG23	2.09	0.53
1:E:268:ILE:HA	1:E:326:LEU:HD21	1.91	0.53
2:D:431:LYS:O	2:D:432:LYS:HD3	2.10	0.52
2:B:222:CYS:SG	2:B:268:ASP:HB3	2.49	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:320:ASN:ND2	2:D:323:ASP:H	2.08	0.52
1:C:406:HIS:O	1:C:409:PRO:HD3	2.09	0.52
2:H:255:PHE:HE1	3:H:104:L05:H23	1.75	0.52
2:H:329:LEU:HD22	2:H:329:LEU:N	2.24	0.52
2:D:240:PRO:O	2:D:241:ASP:CB	2.57	0.52
1:A:231:PRO:HB2	1:A:234:ARG:HG2	1.90	0.52
2:D:222:CYS:SG	2:D:268:ASP:HB3	2.50	0.52
2:D:358:ILE:O	2:D:362:ILE:HG13	2.08	0.52
2:D:291:SER:O	2:D:295:VAL:HG23	2.09	0.52
1:C:230:MET:HE2	1:C:396:VAL:HG22	1.91	0.52
1:A:271:ALA:HB2	1:A:326:LEU:HD12	1.90	0.52
1:C:317:SER:O	1:C:320:VAL:HG12	2.08	0.52
1:G:345:ILE:HA	1:G:348:ARG:HG3	1.90	0.52
2:D:317:PHE:H	2:D:317:PHE:HD2	1.57	0.52
1:G:283:ALA:HB1	1:G:289:PHE:CE2	2.45	0.52
2:H:224:ARG:C	2:H:226:SER:H	2.13	0.52
2:B:305:ASN:HB3	2:B:308:SER:HB3	1.92	0.52
1:G:345:ILE:HD13	1:G:431:LYS:HG2	1.91	0.52
1:G:242:VAL:HG11	1:G:282:TRP:HB2	1.91	0.52
2:H:244:SER:O	2:H:248:ARG:HB2	2.10	0.52
2:H:311:ILE:HD12	2:H:311:ILE:N	2.25	0.51
2:D:266:ILE:HG12	2:D:295:VAL:HG11	1.91	0.51
2:B:414:THR:O	2:B:418:VAL:HG23	2.10	0.51
1:E:348:ARG:HH11	1:E:348:ARG:HG2	1.76	0.51
1:E:279:LEU:HD11	1:E:309:LEU:HD13	1.91	0.51
2:H:244:SER:HB3	2:H:247:ALA:HB3	1.92	0.51
1:G:419:LEU:HD22	2:H:407:MET:HE3	1.92	0.51
1:A:453:GLU:O	1:A:456:GLU:N	2.38	0.51
2:F:241:ASP:CG	2:F:242:PRO:HD2	2.31	0.51
1:E:236:LEU:HD22	1:E:240:LEU:HD22	1.92	0.51
1:C:320:VAL:HG22	1:C:321:LYS:N	2.26	0.51
2:D:391:VAL:HG11	2:D:405:MET:HE1	1.93	0.51
2:D:313:PHE:CE1	3:D:102:L05:H13	2.46	0.51
2:D:360:ILE:HG23	2:D:380:GLN:HE21	1.75	0.51
2:F:205:SER:HB2	2:F:206:PRO:CD	2.41	0.51
2:H:330:GLN:HG2	2:H:422:GLN:OE1	2.10	0.51
2:F:324:PHE:O	2:F:329:LEU:HB2	2.11	0.51
2:B:230:ARG:HG2	2:B:230:ARG:NH1	2.26	0.51
1:C:306:ASN:O	1:C:310:ILE:HG13	2.11	0.51
1:E:454:MET:HE3	2:F:264:GLN:HA	1.93	0.51
2:D:243:GLN:NE2	1:G:294:LEU:N	2.56	0.51
2:D:317:PHE:CD2	2:D:317:PHE:N	2.77	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:306:ASN:HD22	1:A:306:ASN:N	2.08	0.51
1:A:236:LEU:CD1	1:A:240:LEU:HD22	2.40	0.51
2:H:405:MET:O	2:H:408:LYS:HB2	2.11	0.51
1:E:409:PRO:HG2	1:E:410:GLU:H	1.75	0.51
1:E:236:LEU:O	1:E:240:LEU:HD22	2.11	0.51
1:G:446:PRO:C	1:G:447:ILE:HG13	2.30	0.51
1:A:326:LEU:N	1:A:326:LEU:CD2	2.74	0.51
2:H:438:SER:O	2:H:442:ASP:HB2	2.11	0.51
2:H:225:ARG:HH21	2:H:268:ASP:CB	2.19	0.50
1:A:326:LEU:HD23	1:A:330:LEU:O	2.11	0.50
2:H:212:ILE:O	2:H:216:VAL:HG23	2.11	0.50
1:A:225:SER:HB3	1:A:228:GLU:HB2	1.93	0.50
1:A:334:ARG:HA	1:A:346:PHE:CE1	2.46	0.50
1:A:385:ASN:ND2	1:A:388:GLU:N	2.58	0.50
2:D:333:PHE:CZ	2:D:337:ILE:HD11	2.46	0.50
1:G:315:HIS:CB	1:G:367:LEU:HD22	2.41	0.50
2:H:428:LEU:HD22	2:H:428:LEU:N	2.25	0.50
2:D:281:ARG:HD2	2:D:284:GLN:NE2	2.26	0.50
2:H:387:LEU:HD11	2:H:405:MET:CE	2.42	0.50
2:D:400:LEU:HB2	2:D:404:ARG:HH12	1.76	0.50
1:A:356:LYS:NZ	2:B:377:GLU:OE1	2.44	0.50
1:G:357:MET:HE2	1:G:367:LEU:HD13	1.93	0.50
1:A:326:LEU:HD21	1:A:332:VAL:HG23	1.92	0.50
1:C:385:ASN:ND2	1:C:388:GLU:H	2.10	0.50
1:A:437:PHE:CZ	1:A:441:LEU:HD22	2.47	0.50
2:H:298:LEU:HD21	2:H:357:LEU:HD23	1.92	0.50
2:H:230:ARG:HG2	2:H:230:ARG:O	2.11	0.50
1:G:307:GLU:HG2	1:G:425:LEU:HG	1.93	0.50
1:A:444:ASP:O	1:A:446:PRO:N	2.44	0.50
2:H:269:PHE:CE2	2:H:273:LEU:HD21	2.47	0.50
2:B:294:GLU:CD	2:B:367:ARG:HH22	2.14	0.50
2:F:335:ASN:HB2	2:F:336:PRO:HD3	1.94	0.50
1:A:345:ILE:HD11	1:A:428:ILE:HG23	1.93	0.50
1:A:406:HIS:O	1:A:409:PRO:HD3	2.12	0.50
2:D:330:GLN:HB2	2:D:422:GLN:OE1	2.12	0.50
2:H:325:ALA:C	2:H:327:ALA:H	2.14	0.50
1:A:276:LEU:HD23	1:A:279:LEU:HD12	1.93	0.50
2:H:356:LEU:HD13	2:H:387:LEU:CA	2.39	0.49
2:D:237:PRO:CG	2:D:250:GLN:HB3	2.42	0.49
1:C:436:LEU:HD23	1:C:436:LEU:O	2.12	0.49
2:D:402:PHE:N	2:D:403:PRO:HD2	2.26	0.49
1:G:441:LEU:HD23	1:G:441:LEU:C	2.32	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:227:PHE:CD1	2:B:315:LYS:HG3	2.47	0.49
2:B:320:ASN:ND2	2:B:320:ASN:C	2.65	0.49
2:B:260:ILE:HG23	2:B:436:LEU:HD23	1.95	0.49
2:B:292:ALA:HB3	5:B:14:HOH:O	2.13	0.49
1:C:310:ILE:HA	1:C:313:PHE:CD2	2.48	0.49
2:D:320:ASN:HD22	2:D:323:ASP:H	1.60	0.49
1:C:451:LEU:HD12	2:D:285:ILE:HG23	1.94	0.49
2:H:224:ARG:HB2	2:H:224:ARG:NH1	2.27	0.49
2:F:205:SER:OG	2:F:208:GLN:HG3	2.12	0.49
1:A:230:MET:SD	1:A:287:PRO:HB2	2.52	0.49
2:F:360:ILE:HD13	2:F:384:VAL:HG22	1.94	0.49
1:C:230:MET:SD	1:C:287:PRO:HB2	2.53	0.49
2:F:387:LEU:HD21	2:F:405:MET:CE	2.42	0.49
1:G:381:LYS:HD2	1:G:381:LYS:H	1.78	0.49
2:D:401:MET:O	2:D:405:MET:HG3	2.12	0.49
2:D:313:PHE:HE1	3:D:102:L05:H13	1.77	0.49
2:B:322:GLU:OE2	2:B:326:LYS:HE3	2.13	0.49
2:D:308:SER:O	2:D:309:GLU:C	2.49	0.49
2:B:294:GLU:OE2	2:B:367:ARG:NH1	2.45	0.49
1:C:306:ASN:HD22	1:C:306:ASN:H	1.61	0.49
1:G:236:LEU:O	1:G:240:LEU:HD22	2.13	0.49
2:H:238:ILE:HG13	2:H:239:ALA:N	2.21	0.49
1:E:230:MET:HE1	1:E:235:ILE:HD11	1.93	0.49
1:A:440:LYS:O	1:A:441:LEU:C	2.50	0.49
1:E:227:ASN:ND2	1:E:232:VAL:HG13	2.28	0.48
2:H:364:SER:HB2	2:H:367:ARG:HD3	1.93	0.48
1:G:230:MET:HE2	1:G:235:ILE:HD11	1.95	0.48
2:H:277:LEU:HA	2:H:284:GLN:NE2	2.28	0.48
2:D:232:ARG:HH11	2:D:232:ARG:HG3	1.78	0.48
2:F:204:LEU:HG	2:F:393:ILE:HD12	1.95	0.48
2:H:219:GLN:O	2:H:223:ASN:HB2	2.13	0.48
2:D:221:GLN:NE2	2:D:225:ARG:HH21	2.11	0.48
1:A:294:LEU:O	1:A:298:VAL:HG23	2.13	0.48
1:E:296:ASP:OD2	1:E:384:SER:HB3	2.13	0.48
1:G:366:GLU:HG2	1:G:418:LEU:HD11	1.95	0.48
1:C:326:LEU:HB2	1:C:330:LEU:O	2.13	0.48
1:G:325:LEU:HD13	1:G:331:HIS:NE2	2.26	0.48
2:D:335:ASN:HB2	2:D:336:PRO:HD3	1.96	0.48
2:H:290:THR:OG1	2:H:367:ARG:HG3	2.13	0.48
1:G:264:PRO:HB3	1:G:332:VAL:HG13	1.96	0.48
2:D:237:PRO:HG2	2:D:250:GLN:HB2	1.94	0.48
1:C:437:PHE:HE1	1:G:272:ALA:HB3	1.78	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:310:ILE:HA	1:E:313:PHE:CD2	2.49	0.48
2:B:316:ASP:O	2:B:317:PHE:HB2	2.14	0.48
1:C:388:GLU:O	1:C:391:ALA:HB3	2.13	0.48
2:B:237:PRO:HG3	2:B:250:GLN:CB	2.42	0.48
2:B:253:ALA:O	2:B:257:GLU:HG3	2.14	0.48
2:H:305:ASN:HD21	2:H:312:THR:CG2	2.23	0.48
1:A:268:ILE:HA	1:A:326:LEU:HD11	1.95	0.48
2:D:216:VAL:HG22	2:D:352:ALA:HA	1.96	0.48
2:B:294:GLU:OE2	2:B:367:ARG:NH2	2.47	0.48
1:A:225:SER:O	1:A:228:GLU:HG3	2.13	0.48
2:D:344:MET:HB3	2:D:344:MET:HE2	1.81	0.48
1:G:449:THR:HB	2:H:439:GLU:OE2	2.13	0.48
2:B:205:SER:HB3	2:B:208:GLN:HG3	1.96	0.47
2:B:248:ARG:CZ	1:E:294:LEU:HD23	2.44	0.47
2:F:282:GLU:CD	2:F:282:GLU:H	2.17	0.47
1:E:422:LEU:HD12	2:F:407:MET:CE	2.43	0.47
2:D:312:THR:O	2:D:312:THR:HG23	2.14	0.47
2:B:387:LEU:HD11	2:B:405:MET:SD	2.53	0.47
1:G:352:GLU:CD	2:H:366:ASP:HB3	2.33	0.47
1:C:317:SER:O	1:C:318:ILE:C	2.53	0.47
1:C:449:THR:HG22	1:C:450:PHE:N	2.29	0.47
1:E:307:GLU:HG2	1:E:425:LEU:CG	2.38	0.47
1:C:418:LEU:O	1:C:421:ARG:HB2	2.14	0.47
1:A:227:ASN:ND2	1:A:232:VAL:HG22	2.27	0.47
2:B:427:ARG:HH22	1:E:273:ASP:CG	2.17	0.47
1:A:376:PHE:O	1:A:378:PRO:HD3	2.14	0.47
2:H:387:LEU:HD11	2:H:405:MET:HE1	1.96	0.47
2:D:437:LEU:HA	2:D:440:ILE:CD1	2.44	0.47
1:E:230:MET:HG2	1:E:395:LYS:HB3	1.97	0.47
1:A:326:LEU:HD22	1:A:326:LEU:N	2.29	0.47
1:C:302:ARG:HH22	2:H:330:GLN:NE2	2.10	0.47
1:A:320:VAL:HG22	1:A:321:LYS:H	1.79	0.47
1:A:264:PRO:HG3	1:A:336:SER:OG	2.14	0.47
2:D:243:GLN:HG3	1:G:294:LEU:HD23	1.96	0.47
2:D:332:GLU:N	2:D:332:GLU:CD	2.67	0.47
1:A:345:ILE:HG12	1:A:431:LYS:HG2	1.96	0.47
1:A:360:MET:O	1:A:361:GLN:C	2.53	0.47
1:E:366:GLU:CD	1:E:414:ARG:HH21	2.17	0.47
1:G:316:ARG:HG2	1:G:316:ARG:NH1	2.29	0.47
2:H:224:ARG:CB	2:H:224:ARG:HH11	2.27	0.47
2:H:331:VAL:CG2	2:H:335:ASN:HD22	2.27	0.47
2:H:333:PHE:O	2:H:337:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:243:GLN:HG3	1:G:294:LEU:CD2	2.45	0.47
1:C:378:PRO:HG3	1:C:390:GLU:OE2	2.15	0.47
2:D:332:GLU:O	2:D:336:PRO:HG2	2.15	0.47
2:H:254:HIS:NE2	2:H:319:TYR:OH	2.41	0.47
1:A:385:ASN:HD22	1:A:388:GLU:CG	2.16	0.46
2:B:439:GLU:O	2:B:443:VAL:HG23	2.14	0.46
2:D:208:GLN:O	2:D:212:ILE:HG13	2.14	0.46
1:A:294:LEU:HD12	2:F:243:GLN:HA	1.97	0.46
1:G:394:GLU:HA	1:G:397:TYR:HD2	1.77	0.46
1:G:449:THR:HB	2:H:439:GLU:CD	2.35	0.46
2:H:360:ILE:HG23	2:H:380:GLN:HE21	1.80	0.46
2:H:237:PRO:CG	2:H:250:GLN:HB3	2.45	0.46
1:G:442:ILE:HG12	1:G:443:GLY:N	2.30	0.46
2:D:314:LEU:HD12	2:D:317:PHE:CZ	2.50	0.46
1:C:416:ALA:HB2	2:D:402:PHE:HE2	1.79	0.46
2:H:293:ILE:HG22	5:H:19:HOH:O	2.15	0.46
1:E:448:ASP:HA	2:F:439:GLU:CD	2.35	0.46
2:B:330:GLN:O	2:B:334:ILE:HG13	2.16	0.46
2:H:219:GLN:HG2	2:H:269:PHE:HE1	1.80	0.46
2:B:350:ASN:C	2:B:350:ASN:OD1	2.54	0.46
1:A:239:GLU:OE2	1:A:282:TRP:NE1	2.49	0.46
1:G:422:LEU:N	1:G:423:PRO:HD2	2.30	0.46
2:B:208:GLN:O	2:B:211:MET:N	2.48	0.46
2:D:339:GLU:OE2	2:D:342:ARG:NH1	2.41	0.46
2:D:289:LYS:HG2	2:D:440:ILE:HA	1.97	0.46
2:D:350:ASN:O	2:D:351:ASP:C	2.54	0.46
1:A:236:LEU:HD13	1:A:240:LEU:HD22	1.96	0.46
2:H:303:ARG:HG3	2:H:303:ARG:HH11	1.81	0.46
1:A:435:HIS:N	1:A:435:HIS:CD2	2.84	0.46
1:G:441:LEU:HD21	2:H:443:VAL:CG2	2.45	0.46
2:F:276:PHE:CE2	2:F:284:GLN:HG2	2.50	0.46
1:C:457:ALA:O	2:D:271:LYS:NZ	2.49	0.46
1:E:230:MET:N	1:E:231:PRO:HD3	2.30	0.45
2:D:314:LEU:CB	2:D:317:PHE:HE2	2.29	0.45
2:H:312:THR:HG22	2:H:318:SER:CA	2.45	0.45
1:A:236:LEU:C	1:A:236:LEU:HD13	2.37	0.45
2:D:333:PHE:O	2:D:336:PRO:HD2	2.16	0.45
1:G:378:PRO:HD2	1:G:393:ARG:NH1	2.31	0.45
1:A:306:ASN:H	1:A:306:ASN:HD22	1.63	0.45
2:B:401:MET:HG3	2:B:405:MET:HE3	1.99	0.45
1:G:409:PRO:HG2	1:G:410:GLU:H	1.81	0.45
1:G:333:HIS:CD2	1:G:335:ASN:H	2.34	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:320:ASN:ND2	2:D:320:ASN:C	2.70	0.45
2:H:224:ARG:C	2:H:226:SER:N	2.70	0.45
2:H:246:GLU:HA	2:H:246:GLU:OE2	2.16	0.45
2:B:299:GLU:CD	2:B:302:ARG:HH21	2.20	0.45
2:B:202:VAL:HG22	2:B:203:GLN:N	2.31	0.45
2:F:368:PRO:HG2	5:F:9:HOH:O	2.15	0.45
2:D:241:ASP:N	2:D:242:PRO:HD3	2.25	0.45
2:D:263:VAL:O	2:D:267:VAL:HG23	2.17	0.45
2:F:303:ARG:HH11	2:F:303:ARG:HG3	1.81	0.45
2:D:314:LEU:HB2	2:D:317:PHE:HE2	1.82	0.45
2:D:205:SER:OG	2:D:208:GLN:HG3	2.17	0.45
2:H:360:ILE:HD13	2:H:384:VAL:HG22	1.98	0.45
2:D:363:PHE:CE1	2:D:379:LEU:HD13	2.52	0.45
2:B:441:TRP:O	2:B:442:ASP:C	2.55	0.45
1:E:307:GLU:CG	1:E:425:LEU:HG	2.40	0.45
1:A:268:ILE:HA	1:A:326:LEU:CD1	2.47	0.45
2:D:227:PHE:HA	2:D:230:ARG:HD2	1.98	0.45
2:B:387:LEU:O	2:B:391:VAL:HG23	2.17	0.45
2:D:427:ARG:NE	1:G:277:PHE:CE2	2.85	0.45
2:F:301:SER:HB2	2:F:344:MET:HB2	1.98	0.45
2:F:230:ARG:CD	2:F:314:LEU:HB3	2.47	0.44
1:E:409:PRO:HG2	1:E:410:GLU:N	2.32	0.44
1:A:335:ASN:O	1:A:338:HIS:N	2.50	0.44
1:E:268:ILE:HA	1:E:326:LEU:CD2	2.47	0.44
1:G:227:ASN:ND2	1:G:232:VAL:HG13	2.33	0.44
1:C:294:LEU:HD12	2:H:248:ARG:HE	1.82	0.44
2:D:437:LEU:HA	2:D:440:ILE:HD12	1.99	0.44
2:F:280:SER:OG	2:F:283:ASP:HB2	2.17	0.44
2:B:423:VAL:O	2:B:426:LEU:HB2	2.17	0.44
2:H:300:THR:CG2	2:H:311:ILE:HG12	2.46	0.44
2:D:427:ARG:HG2	2:D:427:ARG:H	1.42	0.44
2:B:310:SER:OG	2:B:318:SER:HB2	2.17	0.44
2:D:243:GLN:HE21	1:G:294:LEU:CD2	2.30	0.44
1:E:370:LEU:O	1:E:373:ILE:HB	2.17	0.44
2:H:264:GLN:HE21	2:H:264:GLN:C	2.21	0.44
2:H:298:LEU:CD2	2:H:357:LEU:HD23	2.47	0.44
2:H:333:PHE:CE2	2:H:337:ILE:HD11	2.53	0.44
1:G:349:VAL:HG22	1:G:428:ILE:HD13	2.00	0.44
1:G:276:LEU:O	1:G:276:LEU:HD23	2.17	0.44
1:G:321:LYS:H	1:G:321:LYS:HD3	1.82	0.44
1:G:404:CYS:SG	1:G:414:ARG:HG2	2.58	0.44
1:E:306:ASN:H	1:E:306:ASN:ND2	2.09	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:287:LEU:O	2:B:291:SER:CB	2.65	0.44
1:A:326:LEU:CD2	1:A:332:VAL:HG23	2.48	0.44
2:F:289:LYS:HZ1	2:F:443:VAL:HG11	1.82	0.44
1:G:404:CYS:SG	1:G:414:ARG:CG	3.05	0.44
1:G:367:LEU:O	1:G:371:ARG:HG3	2.18	0.44
2:H:219:GLN:NE2	2:H:358:ILE:HD12	2.32	0.44
1:G:310:ILE:HA	1:G:313:PHE:CD2	2.51	0.44
1:A:381:LYS:CD	1:A:381:LYS:H	2.30	0.44
2:B:427:ARG:C	2:B:428:LEU:HD22	2.37	0.44
2:H:325:ALA:C	2:H:327:ALA:N	2.72	0.44
2:H:331:VAL:CG2	2:H:335:ASN:ND2	2.81	0.44
1:E:441:LEU:HD12	1:E:442:ILE:N	2.33	0.43
2:H:270:ALA:HA	2:H:273:LEU:HD12	1.98	0.43
2:F:275:GLY:HA3	2:F:379:LEU:HD21	2.00	0.43
2:F:290:THR:CG2	2:F:367:ARG:HD2	2.47	0.43
1:G:227:ASN:O	1:G:231:PRO:CA	2.64	0.43
1:C:416:ALA:HB2	2:D:402:PHE:CE2	2.53	0.43
2:F:262:SER:HB2	3:F:103:L05:H13	1.99	0.43
2:F:230:ARG:CD	2:F:314:LEU:HD13	2.47	0.43
1:G:437:PHE:CE1	2:H:445:GLU:OE2	2.72	0.43
2:B:341:SER:O	2:B:342:ARG:C	2.57	0.43
2:B:222:CYS:SG	2:B:268:ASP:CB	3.06	0.43
1:A:231:PRO:HB2	1:A:234:ARG:CG	2.48	0.43
1:C:435:HIS:O	1:C:439:PHE:HB2	2.17	0.43
2:D:430:ASP:HB2	1:G:280:VAL:HG11	2.00	0.43
2:B:339:GLU:HA	2:B:339:GLU:OE1	2.19	0.43
2:H:347:LEU:HD23	2:H:347:LEU:HA	1.77	0.43
1:E:454:MET:HE1	2:F:264:GLN:HG2	1.99	0.43
1:G:445:THR:HA	1:G:446:PRO:HD3	1.75	0.43
2:F:311:ILE:HD12	2:F:324:PHE:CE2	2.54	0.43
1:C:363:ASP:OD1	1:C:363:ASP:C	2.57	0.43
1:C:444:ASP:O	2:D:443:VAL:HG21	2.18	0.43
2:D:360:ILE:HG23	2:D:380:GLN:NE2	2.34	0.43
1:G:316:ARG:NH1	1:G:325:LEU:O	2.51	0.43
2:D:342:ARG:CZ	2:D:342:ARG:HB3	2.47	0.43
2:H:237:PRO:HG2	2:H:251:ARG:HG3	2.00	0.43
1:A:411:GLN:NE2	1:A:414:ARG:HH11	2.17	0.43
2:D:312:THR:HA	2:D:318:SER:HA	1.99	0.43
2:H:424:PHE:C	2:H:426:LEU:H	2.20	0.43
1:C:426:ARG:NH1	2:D:414:THR:OG1	2.52	0.43
1:E:227:ASN:HD21	1:E:232:VAL:CG2	2.27	0.43
1:C:394:GLU:O	1:C:397:TYR:HB2	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:315:LYS:NZ	2:F:315:LYS:HB2	2.34	0.43
2:F:242:PRO:C	2:F:244:SER:H	2.21	0.43
1:G:453:GLU:OE2	1:G:454:MET:N	2.52	0.43
2:B:248:ARG:HH11	2:B:248:ARG:HB3	1.84	0.43
1:G:435:HIS:CD2	1:G:437:PHE:HB3	2.53	0.43
2:F:320:ASN:ND2	2:F:322:GLU:H	2.16	0.43
2:B:426:LEU:C	2:B:428:LEU:N	2.71	0.43
2:D:245:ARG:HH11	2:D:245:ARG:HG3	1.84	0.43
1:C:441:LEU:HD12	1:C:442:ILE:H	1.84	0.43
1:G:317:SER:OG	1:G:324:ILE:HA	2.18	0.43
1:C:421:ARG:HA	1:C:421:ARG:NE	2.34	0.42
1:G:446:PRO:C	1:G:447:ILE:CG1	2.86	0.42
2:F:311:ILE:HD12	2:F:324:PHE:CZ	2.54	0.42
2:H:398:ASP:C	2:H:400:LEU:H	2.22	0.42
1:E:296:ASP:O	1:E:300:LEU:HG	2.19	0.42
2:H:331:VAL:HG23	2:H:335:ASN:ND2	2.34	0.42
2:H:222:CYS:SG	2:H:268:ASP:HB3	2.59	0.42
2:F:230:ARG:HD2	2:F:314:LEU:HB3	2.00	0.42
1:C:230:MET:HE1	1:C:396:VAL:HG22	1.99	0.42
1:E:294:LEU:HD12	1:E:294:LEU:HA	1.78	0.42
1:A:359:ASP:C	1:A:361:GLN:N	2.71	0.42
2:B:357:LEU:HD13	2:B:405:MET:HG2	2.00	0.42
1:G:313:PHE:C	1:G:313:PHE:CD1	2.92	0.42
2:B:259:ALA:HB3	2:B:437:LEU:HD11	2.01	0.42
1:E:265:VAL:HG23	1:E:340:ALA:HB1	2.01	0.42
1:G:415:PHE:HE2	2:H:403:PRO:HG3	1.83	0.42
2:D:330:GLN:NE2	2:D:330:GLN:CA	2.77	0.42
2:H:304:TYR:CE1	2:H:342:ARG:HA	2.54	0.42
2:H:212:ILE:HD13	2:H:390:TYR:CD1	2.55	0.42
2:H:333:PHE:C	2:H:336:PRO:HD2	2.39	0.42
2:H:335:ASN:O	2:H:339:GLU:HG3	2.19	0.42
1:C:264:PRO:O	1:C:268:ILE:HG13	2.20	0.42
1:E:318:ILE:CG2	1:E:358:ARG:HG3	2.48	0.42
2:D:374:LEU:HD12	2:D:374:LEU:HA	1.85	0.42
1:E:307:GLU:OE1	1:E:426:ARG:HA	2.19	0.42
2:H:294:GLU:CD	2:H:367:ARG:NH2	2.73	0.42
1:G:312:SER:OG	1:G:371:ARG:NH1	2.53	0.42
2:H:224:ARG:CB	2:H:224:ARG:NH1	2.83	0.42
1:C:422:LEU:HD12	2:D:407:MET:HE1	1.98	0.42
2:H:294:GLU:CD	2:H:367:ARG:HH22	2.22	0.42
2:H:363:PHE:CE1	2:H:379:LEU:HD13	2.54	0.42
2:H:288:LEU:HA	2:H:291:SER:OG	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:375:GLN:HB2	2:H:378:ARG:NH2	2.26	0.42
1:C:376:PHE:HB3	1:C:393:ARG:HB2	2.01	0.42
2:H:236:TRP:HE3	2:H:254:HIS:CD2	2.38	0.42
1:A:359:ASP:O	1:A:361:GLN:N	2.52	0.42
2:H:335:ASN:HB2	2:H:336:PRO:HD3	2.01	0.42
2:H:419:HIS:ND1	5:H:37:HOH:O	2.26	0.42
2:H:260:ILE:HD11	2:H:434:PRO:HB2	2.00	0.42
2:B:243:GLN:NE2	2:B:248:ARG:HE	2.17	0.42
1:E:316:ARG:O	1:E:316:ARG:HG3	2.19	0.42
1:E:326:LEU:N	1:E:326:LEU:HD12	2.35	0.42
1:A:234:ARG:NE	1:A:234:ARG:HA	2.34	0.42
1:E:293:PRO:HB2	1:E:296:ASP:OD2	2.20	0.42
2:H:205:SER:OG	2:H:208:GLN:HG3	2.19	0.42
1:C:369:CYS:HB3	1:C:400:LEU:HD22	2.02	0.42
1:E:345:ILE:HD13	1:E:345:ILE:O	2.19	0.42
2:B:374:LEU:O	2:B:378:ARG:HG2	2.20	0.42
2:D:219:GLN:NE2	2:D:302:ARG:NH2	2.52	0.42
1:G:357:MET:HE2	1:G:362:MET:SD	2.60	0.42
2:B:294:GLU:HG2	2:B:412:LEU:HB3	2.02	0.42
2:B:333:PHE:CE2	2:B:337:ILE:HD11	2.55	0.42
1:E:359:ASP:C	1:E:361:GLN:H	2.23	0.42
1:A:445:THR:HG22	1:A:445:THR:O	2.20	0.41
2:D:331:VAL:CG1	2:D:335:ASN:ND2	2.83	0.41
1:A:453:GLU:O	1:A:455:LEU:N	2.53	0.41
1:A:263:ASP:HB2	1:A:264:PRO:CD	2.50	0.41
2:H:387:LEU:CD2	2:H:405:MET:HE2	2.43	0.41
2:F:203:GLN:O	2:F:204:LEU:C	2.58	0.41
1:A:349:VAL:HG22	1:A:428:ILE:HG21	2.02	0.41
2:B:202:VAL:HG22	2:B:203:GLN:H	1.85	0.41
1:G:377:ASN:HA	1:G:378:PRO:HD2	1.94	0.41
1:A:437:PHE:O	1:A:441:LEU:HB2	2.20	0.41
2:D:388:HIS:HB2	2:D:402:PHE:CZ	2.55	0.41
1:G:451:LEU:HB3	2:H:285:ILE:HD12	2.03	0.41
1:C:378:PRO:HD2	1:C:393:ARG:NH1	2.36	0.41
1:E:230:MET:HE2	1:E:235:ILE:HD11	2.01	0.41
2:D:281:ARG:HA	2:D:284:GLN:NE2	2.35	0.41
2:H:417:SER:O	2:H:420:SER:HB3	2.20	0.41
1:E:339:SER:C	1:E:341:GLY:H	2.23	0.41
1:A:444:ASP:O	1:A:445:THR:C	2.58	0.41
2:D:256:THR:O	2:D:260:ILE:HG13	2.20	0.41
2:D:300:THR:CG2	2:D:311:ILE:HG12	2.50	0.41
1:G:406:HIS:C	1:G:406:HIS:CD2	2.94	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:285:ARG:HD3	1:G:285:ARG:HA	1.91	0.41
2:H:398:ASP:C	2:H:400:LEU:N	2.73	0.41
2:H:424:PHE:C	2:H:426:LEU:N	2.73	0.41
1:C:337:ALA:O	1:C:340:ALA:HB3	2.20	0.41
1:A:317:SER:OG	1:A:324:ILE:HA	2.21	0.41
1:G:356:LYS:CG	1:G:421:ARG:HH11	2.29	0.41
2:H:300:THR:HG22	2:H:311:ILE:HG12	2.02	0.41
1:E:448:ASP:O	1:E:452:MET:HG3	2.20	0.41
2:B:355:ALA:O	2:B:356:LEU:C	2.58	0.41
2:D:331:VAL:HG13	2:D:335:ASN:ND2	2.36	0.41
1:C:437:PHE:CD2	1:C:438:PHE:CD2	3.06	0.41
1:A:238:ALA:HA	1:A:285:ARG:HD2	2.03	0.41
1:A:289:PHE:CD1	1:A:375:LEU:HD21	2.55	0.41
2:F:426:LEU:HD22	2:F:431:LYS:HG3	2.03	0.41
1:C:372:ALA:HB3	1:C:396:VAL:HG11	2.02	0.41
2:D:330:GLN:HG2	1:G:302:ARG:NH1	2.35	0.41
2:D:428:LEU:CD2	2:D:428:LEU:H	2.29	0.41
1:C:442:ILE:CD1	1:G:266:THR:HG21	2.51	0.41
2:B:426:LEU:O	2:B:428:LEU:N	2.53	0.41
2:D:226:SER:OG	2:D:265:GLU:HG3	2.21	0.41
2:H:207:GLU:HA	2:H:207:GLU:OE2	2.21	0.41
1:A:316:ARG:HD2	1:A:325:LEU:O	2.21	0.41
2:F:314:LEU:HB2	2:F:317:PHE:HD2	1.85	0.41
1:E:313:PHE:CD1	1:E:313:PHE:C	2.94	0.41
1:E:306:ASN:ND2	1:E:306:ASN:N	2.67	0.41
2:H:259:ALA:O	2:H:262:SER:HB3	2.20	0.41
2:D:329:LEU:C	2:D:330:GLN:HE21	2.23	0.41
1:A:330:LEU:N	1:A:330:LEU:HD22	2.36	0.41
1:A:326:LEU:HD21	1:A:332:VAL:CG2	2.50	0.41
2:D:320:ASN:ND2	2:D:323:ASP:OD2	2.53	0.41
2:F:330:GLN:HB2	2:F:422:GLN:OE1	2.21	0.41
2:B:364:SER:O	2:B:367:ARG:HG2	2.21	0.41
2:H:331:VAL:HG13	2:H:332:GLU:N	2.35	0.41
2:B:350:ASN:OD1	2:B:352:ALA:N	2.54	0.41
1:E:341:GLY:O	1:E:440:LYS:HE2	2.21	0.41
2:F:209:LEU:HD13	2:F:209:LEU:C	2.42	0.41
2:B:371:GLN:HA	2:B:371:GLN:NE2	2.36	0.41
2:F:230:ARG:HA	2:F:233:VAL:HG23	2.03	0.41
2:H:236:TRP:CH2	2:H:251:ARG:HB3	2.56	0.41
1:A:225:SER:HB3	1:A:228:GLU:OE2	2.20	0.41
1:E:337:ALA:HB1	1:E:342:VAL:HG23	2.03	0.41
2:F:255:PHE:O	2:F:258:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:313:PHE:O	2:H:317:PHE:HB2	2.21	0.41
2:H:291:SER:O	2:H:292:ALA:C	2.59	0.40
1:A:342:VAL:O	1:A:342:VAL:HG23	2.21	0.40
2:H:203:GLN:HA	2:H:393:ILE:HD11	2.03	0.40
2:F:353:GLU:OE2	2:F:390:TYR:HE2	2.04	0.40
1:A:320:VAL:CG2	1:A:321:LYS:N	2.85	0.40
1:G:359:ASP:C	1:G:361:GLN:N	2.72	0.40
2:H:313:PHE:O	2:H:317:PHE:HD2	2.04	0.40
1:E:283:ALA:O	1:E:289:PHE:HB3	2.22	0.40
2:F:281:ARG:HH11	2:F:281:ARG:HG3	1.87	0.40
1:G:239:GLU:OE2	1:G:371:ARG:NE	2.53	0.40
1:G:439:PHE:O	1:G:442:ILE:HG22	2.20	0.40
2:B:293:ILE:CG2	2:B:294:GLU:N	2.85	0.40
1:C:320:VAL:CG2	1:C:321:LYS:N	2.82	0.40
2:H:333:PHE:CZ	2:H:337:ILE:HD11	2.57	0.40
1:E:377:ASN:OD1	1:E:379:ASP:N	2.50	0.40
1:A:310:ILE:HA	1:A:313:PHE:CE2	2.56	0.40
1:C:338:HIS:NE2	1:C:347:ASP:OD2	2.54	0.40
2:H:215:LEU:O	2:H:218:ALA:N	2.55	0.40
2:B:333:PHE:O	2:B:337:ILE:HG13	2.20	0.40
1:E:348:ARG:HG2	1:E:348:ARG:NH1	2.36	0.40
1:E:310:ILE:HA	1:E:313:PHE:CE2	2.56	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	210/238 (88%)	181 (86%)	23 (11%)	6 (3%)	7	23
1	C	211/238 (89%)	191 (90%)	19 (9%)	1 (0%)	38	76
1	E	210/238 (88%)	189 (90%)	18 (9%)	3 (1%)	16	49
1	G	210/238 (88%)	185 (88%)	21 (10%)	4 (2%)	12	37
2	B	240/244 (98%)	206 (86%)	24 (10%)	10 (4%)	4	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	240/244 (98%)	220 (92%)	16 (7%)	4 (2%)	14	42
2	F	240/244 (98%)	209 (87%)	23 (10%)	8 (3%)	6	19
2	H	242/244 (99%)	206 (85%)	31 (13%)	5 (2%)	11	33
All	All	1803/1928 (94%)	1587 (88%)	175 (10%)	41 (2%)	10	31

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	441	LEU
1	A	454	MET
2	B	314	LEU
2	D	203	GLN
2	D	240	PRO
1	E	406	HIS
2	F	242	PRO
2	F	316	ASP
1	G	442	ILE
1	G	447	ILE
2	H	316	ASP
2	B	230	ARG
2	B	244	SER
2	B	315	LYS
2	B	442	ASP
1	C	354	VAL
2	D	241	ASP
1	E	407	LYS
2	F	207	GLU
2	F	244	SER
1	G	354	VAL
1	G	443	GLY
1	A	360	MET
1	A	445	THR
1	A	453	GLU
2	B	209	LEU
2	B	427	ARG
2	B	435	PRO
2	D	242	PRO
1	E	231	PRO
2	F	204	LEU
2	F	235	PRO
2	F	237	PRO

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Mol	Chain	Res	Type
2	F	206	PRO
2	H	326	LYS
2	H	430	ASP
2	H	435	PRO
1	A	361	GLN
2	B	425	ALA
2	H	431	LYS
2	B	393	ILE

### 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	182/205 (89%)	171 (94%)	11 (6%)	27	61
1	C	183/205 (89%)	172 (94%)	11 (6%)	27	61
1	E	182/205 (89%)	167 (92%)	15 (8%)	17	43
1	G	182/205 (89%)	170 (93%)	12 (7%)	24	56
2	B	219/221 (99%)	201 (92%)	18 (8%)	17	43
2	D	219/221 (99%)	204 (93%)	15 (7%)	22	54
2	F	219/221 (99%)	208 (95%)	11 (5%)	34	70
2	H	221/221 (100%)	213 (96%)	8 (4%)	47	82
All	All	1607/1704 (94%)	1506 (94%)	101 (6%)	25	59

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	240	LEU
1	A	276	LEU
1	A	280	VAL
1	A	306	ASN
1	A	309	LEU
1	A	326	LEU
1	A	345	ILE
1	A	381	LYS
1	A	383	LEU

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Mol	Chain	Res	Type
1	A	407	LYS
1	A	444	ASP
2	B	214	LYS
2	B	224	ARG
2	B	230	ARG
2	B	250	GLN
2	B	255	PHE
2	B	262	SER
2	B	281	ARG
2	B	309	GLU
2	B	312	THR
2	B	317	PHE
2	B	320	ASN
2	B	375	GLN
2	B	377	GLU
2	B	378	ARG
2	B	388	HIS
2	B	416	SER
2	B	435	PRO
2	B	442	ASP
1	C	232	VAL
1	C	236	LEU
1	C	240	LEU
1	C	279	LEU
1	C	306	ASN
1	C	316	ARG
1	C	326	LEU
1	C	350	LEU
1	C	383	LEU
1	C	444	ASP
1	C	451	LEU
2	D	238	ILE
2	D	243	GLN
2	D	255	PHE
2	D	281	ARG
2	D	290	THR
2	D	293	ILE
2	D	316	ASP
2	D	317	PHE
2	D	320	ASN
2	D	330	GLN
2	D	354	PHE

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Mol	Chain	Res	Type
2	D	385	GLU
2	D	398	ASP
2	D	435	PRO
2	D	440	ILE
1	E	229	ASP
1	E	236	LEU
1	E	240	LEU
1	E	285	ARG
1	E	306	ASN
1	E	309	LEU
1	E	313	PHE
1	E	345	ILE
1	E	390	GLU
1	E	393	ARG
1	E	426	ARG
1	E	444	ASP
1	E	451	LEU
1	E	454	MET
1	E	456	GLU
2	F	220	GLN
2	F	237	PRO
2	F	241	ASP
2	F	243	GLN
2	F	246	GLU
2	F	281	ARG
2	F	282	GLU
2	F	315	LYS
2	F	351	ASP
2	F	374	LEU
2	F	428	LEU
1	G	236	LEU
1	G	240	LEU
1	G	263	ASP
1	G	266	THR
1	G	274	LYS
1	G	276	LEU
1	G	313	PHE
1	G	321	LYS
1	G	348	ARG
1	G	351	THR
1	G	426	ARG
1	G	447	ILE

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Mol	Chain	Res	Type
2	H	255	PHE
2	H	264	GLN
2	H	281	ARG
2	H	366	ASP
2	H	367	ARG
2	H	429	GLN
2	H	432	LYS
2	H	435	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	227	ASN
1	A	275	GLN
1	A	306	ASN
1	A	333	HIS
1	A	385	ASN
1	A	406	HIS
1	A	411	GLN
1	A	435	HIS
2	B	221	GLN
2	B	223	ASN
2	B	305	ASN
2	B	320	ASN
2	B	330	GLN
2	B	345	ASN
2	B	371	GLN
1	C	227	ASN
1	C	270	GLN
1	C	306	ASN
1	C	331	HIS
1	C	333	HIS
1	C	335	ASN
1	C	385	ASN
2	D	219	GLN
2	D	221	GLN
2	D	243	GLN
2	D	249	GLN
2	D	284	GLN
2	D	305	ASN
2	D	320	ASN
2	D	330	GLN

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Mol	Chain	Res	Type
2	D	335	ASN
2	D	380	GLN
1	E	227	ASN
1	E	267	ASN
1	E	275	GLN
1	E	306	ASN
1	E	335	ASN
2	F	219	GLN
2	F	249	GLN
2	F	305	ASN
2	F	335	ASN
2	F	345	ASN
2	F	371	GLN
2	F	419	HIS
1	G	227	ASN
1	G	267	ASN
1	G	270	GLN
1	G	306	ASN
1	G	333	HIS
1	G	335	ASN
1	G	361	GLN
1	G	406	HIS
1	G	435	HIS
2	H	219	GLN
2	H	249	GLN
2	H	264	GLN
2	H	305	ASN
2	H	320	ASN
2	H	330	GLN
2	H	380	GLN
2	H	394	ASN
2	H	429	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	REA	A	502	-	22,22,22	1.93	5 (22%)	30,30,30	1.27	3 (10%)
3	L05	B	101	-	32,32,32	1.65	8 (25%)	44,44,44	0.83	1 (2%)
4	REA	C	503	-	22,22,22	1.70	4 (18%)	30,30,30	1.38	4 (13%)
3	L05	D	102	-	32,32,32	1.52	7 (21%)	44,44,44	0.82	1 (2%)
4	REA	E	504	-	22,22,22	1.59	3 (13%)	30,30,30	1.25	4 (13%)
3	L05	F	103	-	32,32,32	1.69	9 (28%)	44,44,44	0.87	2 (4%)
4	REA	G	501	-	22,22,22	1.57	4 (18%)	30,30,30	1.30	4 (13%)
3	L05	H	104	-	32,32,32	1.58	8 (25%)	44,44,44	0.84	2 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	REA	A	502	-	-	0/15/32/32	0/1/1/1
3	L05	B	101	-	-	0/14/34/34	0/4/4/4
4	REA	C	503	-	-	0/15/32/32	0/1/1/1
3	L05	D	102	-	-	0/14/34/34	0/4/4/4
4	REA	E	504	-	-	0/15/32/32	0/1/1/1
3	L05	F	103	-	-	0/14/34/34	0/4/4/4
4	REA	G	501	-	-	0/15/32/32	0/1/1/1
3	L05	H	104	-	-	0/14/34/34	0/4/4/4

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	REA	C1-C6	5.69	1.62	1.53
4	C	503	REA	C1-C6	4.60	1.60	1.53
4	G	501	REA	C1-C6	4.13	1.59	1.53
4	E	504	REA	C1-C6	3.79	1.59	1.53
4	E	504	REA	C5-C6	3.78	1.40	1.34
4	C	503	REA	C5-C6	3.56	1.40	1.34
4	A	502	REA	C5-C6	3.55	1.40	1.34
4	G	501	REA	C5-C6	3.32	1.39	1.34
3	F	103	L05	C5-C6	3.22	1.44	1.39
3	B	101	L05	C5-C6	2.98	1.44	1.39
3	D	102	L05	C5-C6	2.76	1.43	1.39
4	G	501	REA	C20-C13	2.61	1.55	1.51
3	B	101	L05	C23-C22	2.60	1.43	1.39
3	H	104	L05	C5-C6	2.60	1.43	1.39
3	D	102	L05	C23-C22	2.59	1.43	1.39
4	C	503	REA	C20-C13	2.57	1.55	1.51
3	B	101	L05	C27-C22	2.54	1.43	1.39
3	F	103	L05	C19-C14	2.53	1.44	1.38
3	F	103	L05	C23-C22	2.52	1.43	1.39
3	F	103	L05	C27-C22	2.51	1.43	1.39
4	A	502	REA	C20-C13	2.46	1.55	1.51
4	E	504	REA	C20-C13	2.45	1.55	1.51
3	D	102	L05	C29-C3	2.44	1.43	1.38
4	A	502	REA	C19-C9	2.40	1.55	1.51
3	H	104	L05	C23-C22	2.39	1.43	1.39
3	F	103	L05	C28-C6	2.38	1.43	1.39
3	H	104	L05	C19-C14	2.37	1.44	1.38
3	D	102	L05	C27-C22	2.36	1.43	1.39
3	B	101	L05	C15-C14	2.34	1.44	1.38
3	D	102	L05	C29-C28	2.33	1.43	1.38
3	F	103	L05	C5-C4	2.29	1.43	1.38
3	B	101	L05	C19-C14	2.26	1.44	1.38
3	F	103	L05	C29-C3	2.25	1.43	1.38
4	C	503	REA	C19-C9	2.24	1.54	1.51
3	F	103	L05	C29-C28	2.19	1.43	1.38
3	B	101	L05	C4-C3	2.18	1.43	1.38
3	H	104	L05	C27-C22	2.17	1.43	1.39
3	H	104	L05	C28-C6	2.15	1.42	1.39
3	F	103	L05	C15-C14	2.15	1.43	1.38
3	D	102	L05	C28-C6	2.12	1.42	1.39
3	H	104	L05	C29-C28	2.11	1.42	1.38
3	D	102	L05	C19-C14	2.09	1.43	1.38
3	B	101	L05	C29-C3	2.08	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	101	L05	C29-C28	2.04	1.42	1.38
4	A	502	REA	C18-C5	2.04	1.54	1.51
3	H	104	L05	C15-C14	2.03	1.43	1.38
4	G	501	REA	C19-C9	2.03	1.54	1.51
3	H	104	L05	C29-C3	2.01	1.42	1.38

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	503	REA	C18-C5-C6	4.24	129.32	124.51
4	A	502	REA	C18-C5-C6	3.66	128.66	124.51
4	E	504	REA	C18-C5-C6	3.47	128.44	124.51
4	G	501	REA	C18-C5-C6	3.36	128.31	124.51
4	G	501	REA	C18-C5-C4	-2.59	108.58	113.34
4	E	504	REA	C18-C5-C4	-2.47	108.81	113.34
4	C	503	REA	C7-C8-C9	2.41	129.82	126.22
4	E	504	REA	O2-C15-C14	2.41	121.03	113.59
4	G	501	REA	O2-C15-C14	2.40	121.00	113.59
4	A	502	REA	O2-C15-C14	2.39	120.98	113.59
4	C	503	REA	C18-C5-C4	-2.37	108.98	113.34
3	D	102	L05	O11-C10-C9	-2.36	124.64	129.00
3	F	103	L05	O11-C10-C9	-2.30	124.74	129.00
3	F	103	L05	C6-N7-C8	2.28	133.47	128.16
3	B	101	L05	O11-C10-C9	-2.21	124.91	129.00
4	G	501	REA	C7-C8-C9	2.20	129.50	126.22
4	C	503	REA	O2-C15-C14	2.15	120.24	113.59
3	H	104	L05	O11-C10-C9	-2.13	125.06	129.00
4	E	504	REA	O1-C15-C14	-2.06	117.50	124.10
3	H	104	L05	C6-N7-C8	2.05	132.93	128.16
4	A	502	REA	C18-C5-C4	-2.01	109.65	113.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 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	214/238 (89%)	-0.39	3 (1%) 72 72	12, 33, 58, 84	0
1	C	215/238 (90%)	-0.61	0 100 100	9, 28, 48, 54	0
1	E	214/238 (89%)	-0.46	1 (0%) 88 90	16, 36, 54, 64	0
1	G	214/238 (89%)	-0.30	2 (0%) 81 81	15, 37, 61, 82	0
2	B	242/244 (99%)	-0.21	8 (3%) 44 45	13, 36, 76, 99	0
2	D	242/244 (99%)	-0.43	2 (0%) 83 83	9, 30, 64, 90	0
2	F	242/244 (99%)	-0.17	10 (4%) 35 36	16, 40, 100, 110	0
2	H	244/244 (100%)	-0.12	13 (5%) 25 26	21, 43, 94, 104	0
All	All	1827/1928 (94%)	-0.33	39 (2%) 60 61	9, 36, 76, 110	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	202	VAL	6.8
2	H	231	LEU	4.9
1	A	442	ILE	4.9
2	D	202	VAL	4.5
1	G	443	GLY	4.4
1	A	443	GLY	4.3
2	H	242	PRO	4.3
2	B	231	LEU	4.1
1	G	442	ILE	4.0
2	F	231	LEU	3.3
2	B	315	LYS	3.3
2	B	241	ASP	3.3
2	H	245	ARG	3.2
2	F	235	PRO	3.1
2	F	315	LYS	3.0
2	H	397	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	238	ILE	2.6
2	B	243	GLN	2.5
2	F	230	ARG	2.4
2	H	315	LYS	2.4
2	H	230	ARG	2.4
2	H	239	ALA	2.4
2	F	236	TRP	2.3
2	B	242	PRO	2.3
2	H	243	GLN	2.3
2	H	236	TRP	2.3
2	H	238	ILE	2.2
2	F	228	SER	2.2
2	D	243	GLN	2.2
2	H	317	PHE	2.2
1	A	444	ASP	2.1
2	F	242	PRO	2.1
2	F	227	PHE	2.1
2	H	202	VAL	2.1
2	F	319	TYR	2.1
2	B	240	PRO	2.1
2	H	237	PRO	2.1
1	E	333	HIS	2.0
2	B	397	HIS	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	REA	C	503	22/22	0.17	1.63	6,19,20,21	0
3	L05	F	103	29/29	0.21	1.03	37,42,49,52	0
4	REA	A	502	22/22	0.19	0.84	23,28,31,32	0
3	L05	H	104	29/29	0.17	0.45	30,35,43,49	0
4	REA	E	504	22/22	0.17	0.25	11,16,23,25	0
4	REA	G	501	22/22	0.17	0.20	11,20,25,26	0
3	L05	D	102	29/29	0.15	0.15	8,14,21,24	0
3	L05	B	101	29/29	0.15	0.06	22,25,31,32	0

## 6.5 Other polymers

There are no such residues in this entry.