Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:20 PM GMT

PDB ID	:	1OFR
Title	:	CRYSTAL STRUCTURE OF THE TYROSINE-REGULATED 3-DEOXY-D-ARABINO-HEPTULOSONATE-7-PHOSPHATE SYNTHASE FROM SACCHAROMYCES CEREVISIAE COMPLEXED WITH PHENYLALANINE AND MANGANESE
Authors	:	Koenig, V.; Pfeil, A.; Heinrich, G.; Braus, G.; Schneider, T.R.
Deposited on	:	2003-04-18
Resolution	:	2.70 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

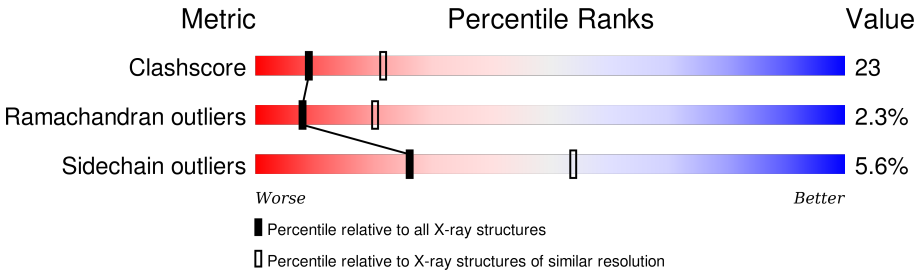
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.70 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	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	370	56% 33% 5% 5%
1	B	370	49% 42% • 6%
1	C	370	55% 35% • 6%
1	D	370	58% 34% • 5%
1	E	370	54% 34% • 8%
1	F	370	58% 33% • 6%
1	G	370	51% 37% 5% 7%

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Mol	Chain	Length	Quality of chain
1	H	370	

2 Entry composition (i)

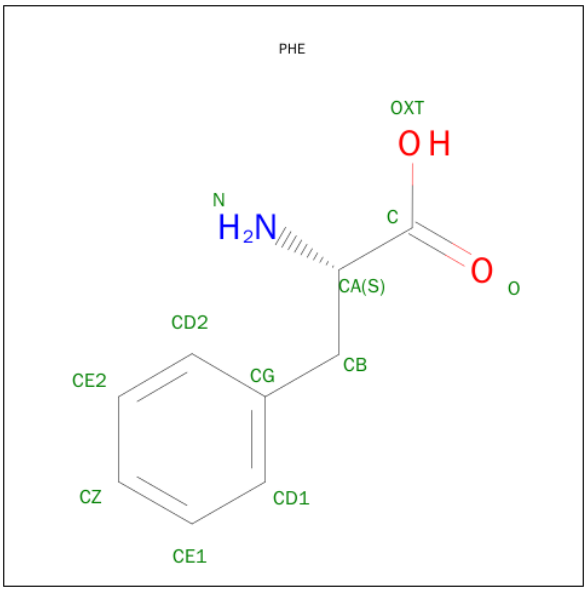
There are 4 unique types of molecules in this entry. The entry contains 20930 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	1
			2631	1636	474	511	10			
1	B	348	Total	C	N	O	S	0	0	1
			2618	1629	469	510	10			
1	C	349	Total	C	N	O	S	0	0	1
			2626	1634	471	511	10			
1	D	351	Total	C	N	O	S	0	0	1
			2623	1630	470	513	10			
1	E	339	Total	C	N	O	S	0	0	1
			2560	1591	460	499	10			
1	F	347	Total	C	N	O	S	0	0	1
			2604	1620	467	507	10			
1	G	344	Total	C	N	O	S	0	0	1
			2581	1605	462	504	10			
1	H	347	Total	C	N	O	S	0	0	1
			2599	1614	466	509	10			

- Molecule 2 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C N O 12 9 1 2	0	0
2	D	1	Total C N O 12 9 1 2	0	0
2	G	1	Total C N O 12 9 1 2	0	0
2	H	1	Total C N O 12 9 1 2	0	0

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Mn 1 1	0	0
3	D	1	Total Mn 1 1	0	0
3	E	1	Total Mn 1 1	0	0
3	H	1	Total Mn 1 1	0	0
3	B	1	Total Mn 1 1	0	0
3	C	1	Total Mn 1 1	0	0
3	A	1	Total Mn 1 1	0	0
3	F	1	Total Mn 1 1	0	0

- Molecule 4 is water.

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

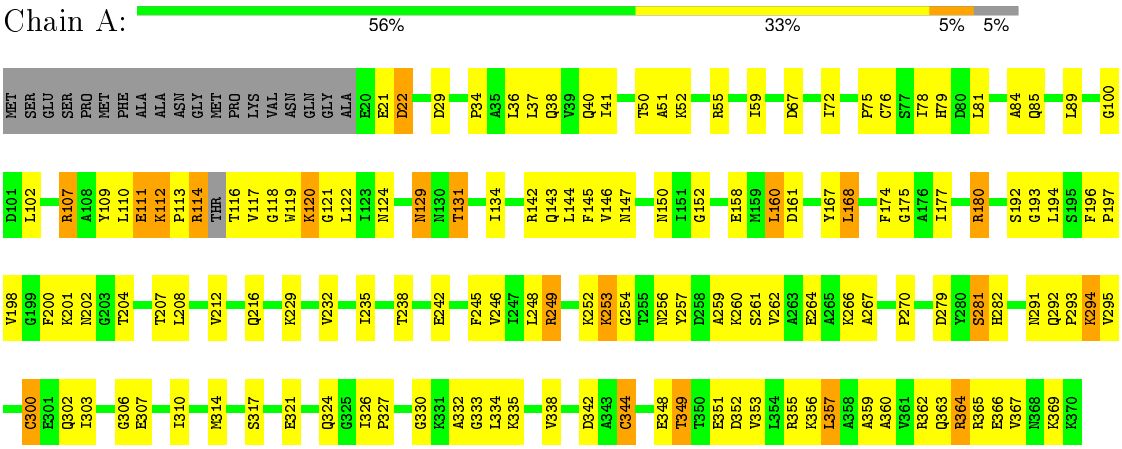
3 Residue-property plots (i)

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.

Note EDS was not executed.

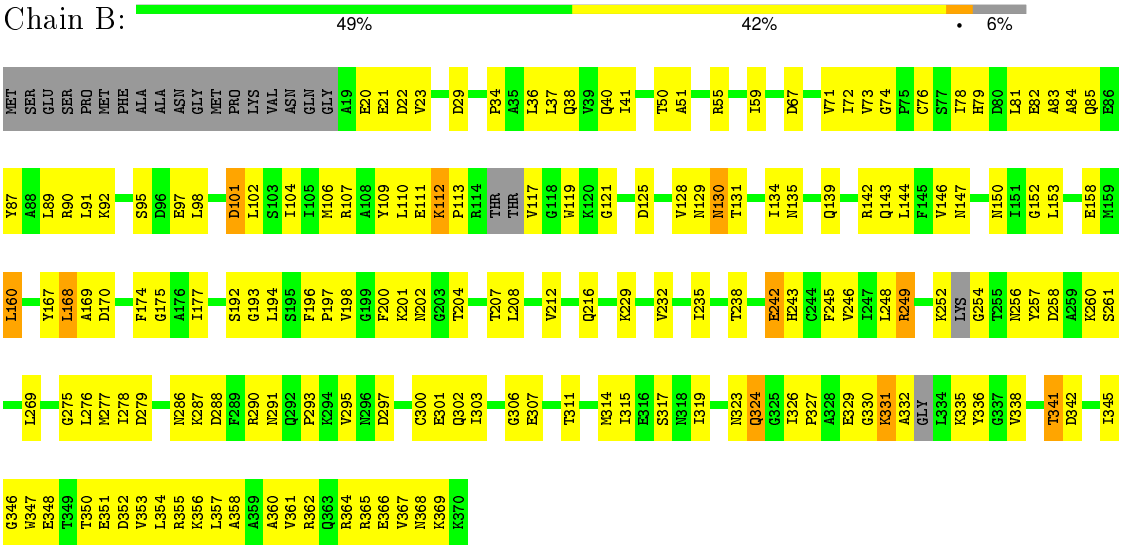
• Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE

Chain A:



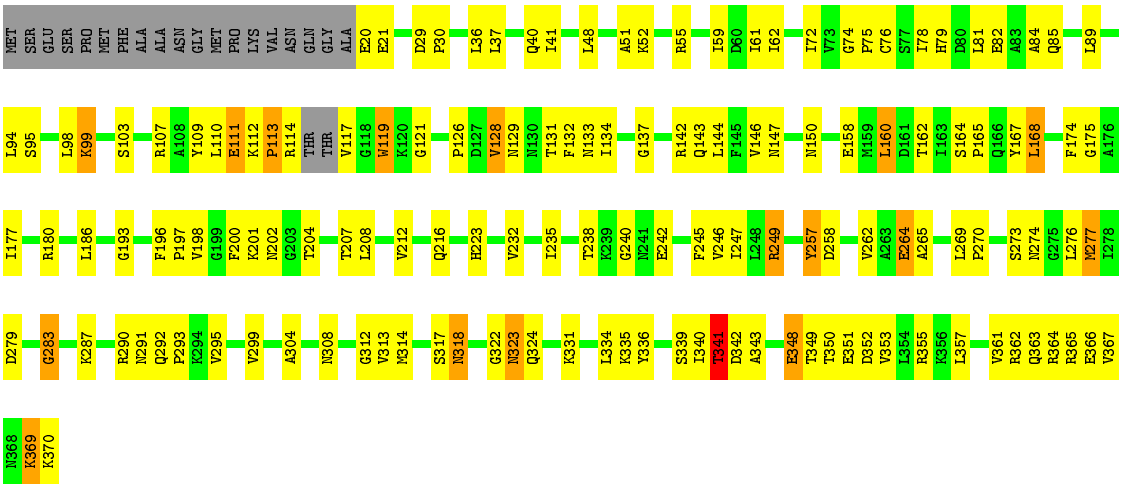
• Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE

Chain B:



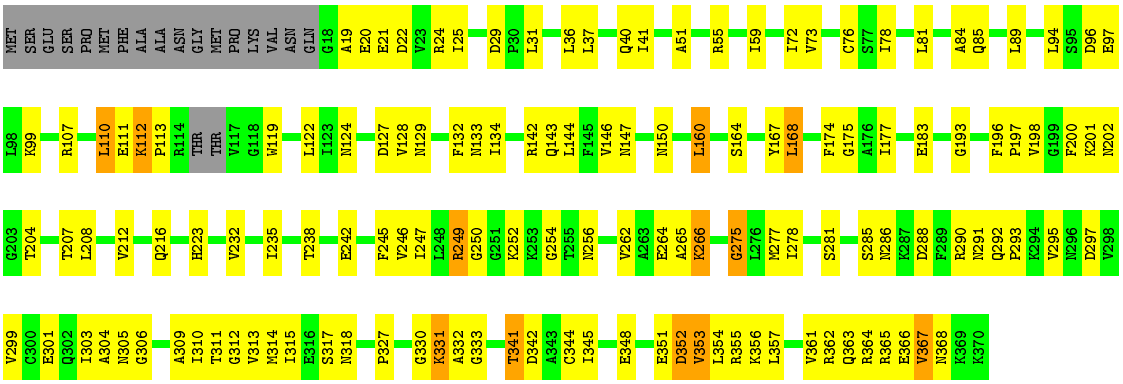
• Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE

Chain C:



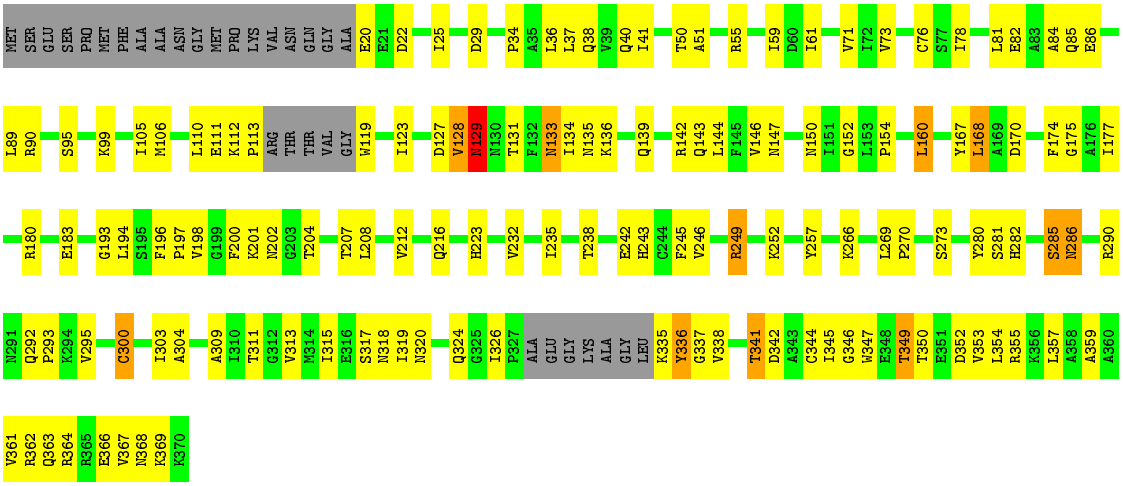
• Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE

Chain D:



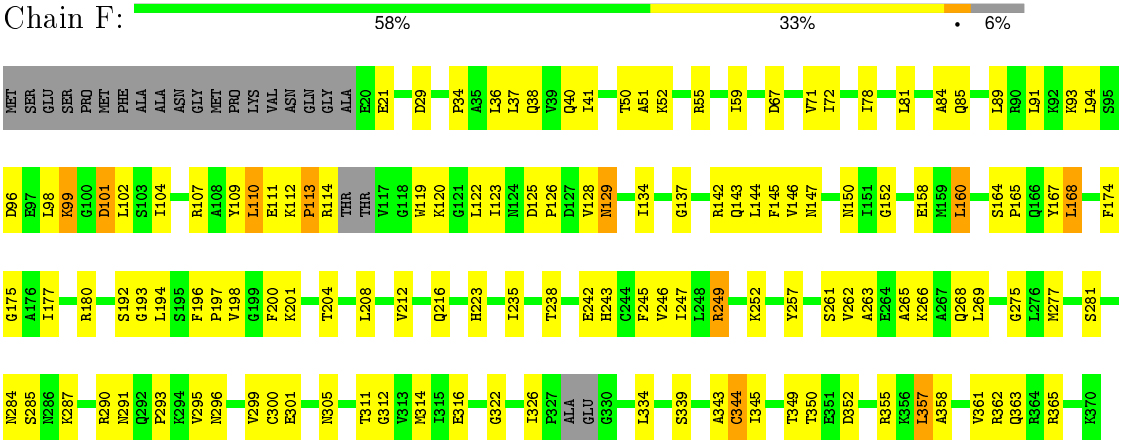
• Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE

Chain E:



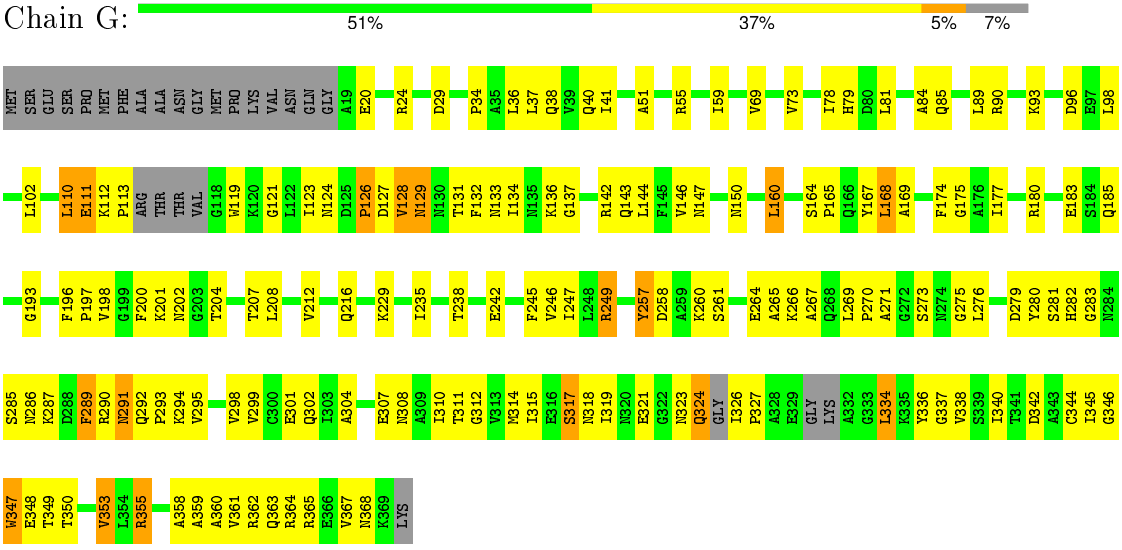
• Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE

Chain F:



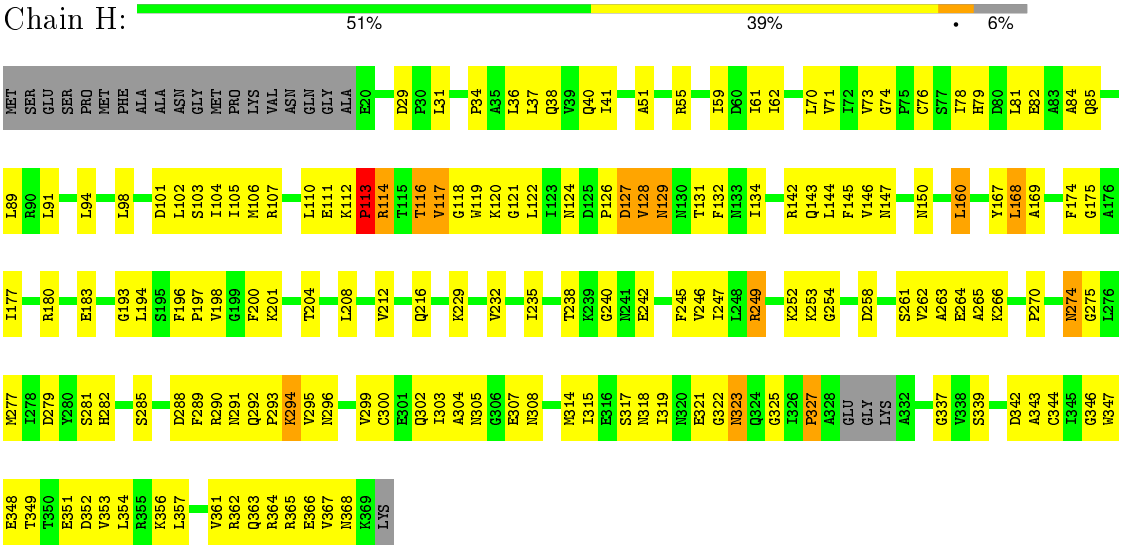
• Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE

Chain G:



• Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE

Chain H:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	82.29Å 94.03Å 105.12Å 65.14° 85.68° 75.73°	Depositor
Resolution (Å)	37.20 – 2.70	Depositor
% Data completeness (in resolution range)	85.9 (37.20-2.70)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.232 , 0.274	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	20930	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.42	0/2669	0.63	0/3613
1	B	0.42	0/2654	0.61	0/3590
1	C	0.42	0/2664	0.64	0/3605
1	D	0.43	0/2661	0.64	0/3605
1	E	0.39	0/2596	0.61	0/3513
1	F	0.41	0/2641	0.63	0/3575
1	G	0.40	0/2617	0.61	0/3544
1	H	0.39	0/2637	0.60	0/3577
All	All	0.41	0/21139	0.62	0/28622

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2631	0	2634	126	0
1	B	2618	0	2618	136	0
1	C	2626	0	2631	126	0
1	D	2623	0	2605	119	0
1	E	2560	0	2562	122	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2604	0	2596	105	0
1	G	2581	0	2564	146	0
1	H	2599	0	2576	132	0
2	C	12	0	8	0	0
2	D	12	0	8	0	0
2	G	12	0	8	1	0
2	H	12	0	8	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	6	0	0	1	0
4	B	4	0	0	0	0
4	C	5	0	0	1	0
4	D	5	0	0	1	0
4	E	2	0	0	0	0
4	F	4	0	0	1	0
4	G	3	0	0	0	0
4	H	3	0	0	0	0
All	All	20930	0	20818	964	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 23.

All (964) 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:C:134:ILE:H	1:C:134:ILE:HD12	1.19	1.05
1:B:134:ILE:H	1:B:134:ILE:HD12	1.19	1.05
1:E:324:GLN:HE21	1:E:338:VAL:HB	1.18	1.01
1:G:355:ARG:HG3	1:G:355:ARG:HH11	1.28	0.94
1:C:208:LEU:HD11	1:C:246:VAL:HG11	1.50	0.94
1:H:208:LEU:HD11	1:H:246:VAL:HG11	1.49	0.94
1:G:208:LEU:HD11	1:G:246:VAL:HG11	1.51	0.92
1:A:208:LEU:HD11	1:A:246:VAL:HG11	1.52	0.92
1:B:208:LEU:HD11	1:B:246:VAL:HG11	1.51	0.92
1:D:208:LEU:HD11	1:D:246:VAL:HG11	1.49	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:208:LEU:HD11	1:E:246:VAL:HG11	1.52	0.91
1:G:257:TYR:CD2	1:G:295:VAL:HG13	2.06	0.91
1:F:208:LEU:HD11	1:F:246:VAL:HG11	1.51	0.89
1:H:319:ILE:H	1:H:319:ILE:HD12	1.37	0.88
1:B:95:SER:HA	1:B:104:ILE:HD12	1.54	0.88
1:H:308:ASN:HA	1:H:364:ARG:HH11	1.36	0.87
1:E:134:ILE:HD12	1:E:134:ILE:H	1.40	0.86
1:G:289:PHE:CE1	1:G:321:GLU:HB2	2.12	0.85
1:D:348:GLU:CD	1:D:348:GLU:H	1.77	0.85
1:G:289:PHE:HE1	1:G:321:GLU:HB2	1.41	0.84
1:H:357:LEU:O	1:H:361:VAL:HG23	1.77	0.84
1:G:359:ALA:HA	1:G:362:ARG:HD2	1.59	0.83
1:A:359:ALA:HA	1:A:362:ARG:NH1	1.91	0.83
1:B:355:ARG:HG2	1:B:355:ARG:HH11	1.44	0.83
1:H:290:ARG:O	1:H:293:PRO:HD2	1.79	0.82
1:C:349:THR:O	1:C:353:VAL:HG23	1.80	0.82
1:B:134:ILE:N	1:B:134:ILE:HD12	1.96	0.81
1:C:95:SER:O	1:C:99:LYS:HB3	1.81	0.81
1:B:134:ILE:H	1:B:134:ILE:CD1	1.92	0.80
1:E:317:SER:HA	1:E:344:CYS:HB3	1.63	0.80
1:H:308:ASN:HA	1:H:364:ARG:NH1	1.95	0.80
1:F:112:LYS:HD2	1:F:113:PRO:HD2	1.62	0.80
1:H:303:ILE:O	1:H:364:ARG:HB2	1.83	0.79
1:C:114:ARG:O	1:C:117:VAL:HG12	1.82	0.79
1:A:161:ASP:HB2	4:A:2001:HOH:O	1.82	0.78
1:G:257:TYR:CE2	1:G:295:VAL:HA	2.20	0.77
1:C:134:ILE:H	1:C:134:ILE:CD1	1.93	0.77
1:C:355:ARG:HH11	1:C:355:ARG:HG3	1.50	0.76
1:D:317:SER:HA	1:D:344:CYS:HB3	1.68	0.76
1:A:112:LYS:HZ3	1:A:114:ARG:HA	1.49	0.76
1:C:291:ASN:O	1:C:295:VAL:HG23	1.86	0.76
1:G:111:GLU:HB3	1:G:121:GLY:CA	2.15	0.75
1:H:112:LYS:HG2	1:H:113:PRO:HD2	1.68	0.75
1:A:160:LEU:HD22	1:A:160:LEU:H	1.51	0.74
1:H:348:GLU:CD	1:H:348:GLU:H	1.91	0.74
1:E:324:GLN:NE2	1:E:338:VAL:HB	1.99	0.74
1:G:269:LEU:HD11	1:G:276:LEU:HD21	1.70	0.74
1:B:160:LEU:H	1:B:160:LEU:HD22	1.52	0.73
1:A:359:ALA:HA	1:A:362:ARG:HH12	1.51	0.73
1:C:318:ASN:ND2	1:C:339:SER:HB2	2.03	0.73
1:C:160:LEU:H	1:C:160:LEU:HD22	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:160:LEU:HD22	1:F:160:LEU:H	1.54	0.73
1:H:160:LEU:H	1:H:160:LEU:HD22	1.53	0.72
1:H:319:ILE:N	1:H:319:ILE:HD12	2.04	0.72
1:E:134:ILE:HD13	1:F:235:ILE:HG21	1.71	0.72
1:D:110:LEU:HD22	1:D:110:LEU:H	1.54	0.72
1:A:110:LEU:HD21	1:A:145:PHE:CZ	2.25	0.72
1:G:324:GLN:HE22	1:G:334:LEU:HB3	1.54	0.72
1:G:291:ASN:HD22	1:G:291:ASN:N	1.86	0.71
1:G:160:LEU:HD22	1:G:160:LEU:H	1.53	0.71
1:E:160:LEU:H	1:E:160:LEU:HD22	1.55	0.71
1:C:331:LYS:O	1:C:331:LYS:HD3	1.89	0.71
1:H:124:ASN:HA	1:H:134:ILE:HD13	1.71	0.71
1:F:262:VAL:HG12	1:F:263:ALA:N	2.06	0.71
1:F:96:ASP:HA	1:F:99:LYS:HD2	1.72	0.71
1:A:21:GLU:OE1	1:B:169:ALA:HB3	1.91	0.71
1:E:292:GLN:HB2	1:E:293:PRO:HD3	1.73	0.71
1:B:297:ASP:OD1	1:B:356:LYS:HE2	1.90	0.71
1:D:160:LEU:HD22	1:D:160:LEU:H	1.54	0.70
1:G:111:GLU:HB3	1:G:121:GLY:HA2	1.72	0.70
1:F:93:LYS:HB2	1:F:93:LYS:NZ	2.07	0.70
1:H:304:ALA:C	1:H:305:ASN:HD22	1.95	0.70
1:A:114:ARG:HD3	1:A:114:ARG:H	1.57	0.70
1:G:308:ASN:OD1	1:G:364:ARG:HD2	1.93	0.69
1:E:183:GLU:HB3	1:F:180:ARG:HB3	1.74	0.69
1:C:277:MET:HE3	1:C:313:VAL:N	2.06	0.69
1:E:300:CYS:SG	1:E:357:LEU:HA	2.33	0.69
1:G:110:LEU:H	1:G:110:LEU:HD22	1.56	0.69
1:H:295:VAL:O	1:H:299:VAL:HG23	1.93	0.69
1:A:349:THR:HA	1:A:352:ASP:OD2	1.93	0.69
1:G:355:ARG:NH1	1:G:355:ARG:HG3	2.05	0.68
1:D:247:ILE:HD13	1:D:314:MET:HE1	1.73	0.68
1:G:185:GLN:OE1	1:H:114:ARG:HB3	1.93	0.68
1:E:20:GLU:HG2	1:F:52:LYS:HD3	1.74	0.68
1:B:355:ARG:HG2	1:B:355:ARG:NH1	2.08	0.68
1:D:291:ASN:O	1:D:295:VAL:HG23	1.93	0.68
1:H:319:ILE:H	1:H:319:ILE:CD1	2.07	0.68
1:E:134:ILE:N	1:E:134:ILE:HD12	2.09	0.68
1:H:98:LEU:HD13	1:H:102:LEU:HD22	1.76	0.67
1:G:302:GLN:O	1:G:307:GLU:HB3	1.94	0.67
1:E:304:ALA:O	1:E:363:GLN:HG3	1.94	0.67
1:G:90:ARG:HD3	1:G:347:TRP:NE1	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:134:ILE:CD1	1:E:134:ILE:H	2.08	0.67
1:D:247:ILE:HD13	1:D:314:MET:CE	2.24	0.67
1:G:291:ASN:O	1:G:295:VAL:HG23	1.93	0.67
1:G:290:ARG:O	1:G:293:PRO:HD2	1.95	0.67
1:A:117:VAL:HG12	1:A:118:GLY:N	2.09	0.67
1:A:307:GLU:HG2	1:A:310:ILE:HD12	1.77	0.67
1:A:300:CYS:SG	1:A:357:LEU:HA	2.35	0.67
1:H:261:SER:HA	1:H:264:GLU:OE1	1.94	0.67
1:E:119:TRP:NE1	1:E:128:VAL:HG22	2.09	0.67
1:G:294:LYS:NZ	1:G:294:LYS:HB2	2.10	0.67
1:B:76:CYS:SG	1:B:342:ASP:HB2	2.35	0.67
1:F:71:VAL:HG21	1:F:102:LEU:HD22	1.77	0.67
1:C:258:ASP:O	1:C:262:VAL:HG23	1.95	0.66
1:E:76:CYS:SG	1:E:342:ASP:HB2	2.35	0.66
1:C:349:THR:O	1:C:352:ASP:HB2	1.95	0.66
1:C:264:GLU:HG3	1:C:265:ALA:N	2.10	0.66
1:G:257:TYR:HD2	1:G:295:VAL:HG13	1.56	0.66
1:A:260:LYS:O	1:A:264:GLU:HG3	1.95	0.66
1:F:357:LEU:O	1:F:361:VAL:HG23	1.95	0.66
1:A:253:LYS:HG2	1:A:253:LYS:O	1.93	0.66
1:C:348:GLU:CD	1:C:348:GLU:H	1.99	0.66
1:C:292:GLN:HB2	1:C:293:PRO:HD3	1.78	0.66
1:C:134:ILE:N	1:C:134:ILE:HD12	2.04	0.66
1:A:114:ARG:O	1:A:116:THR:HA	1.96	0.66
1:A:207:THR:HG21	1:B:252:LYS:NZ	2.11	0.66
1:B:129:ASN:O	1:B:131:THR:HG23	1.96	0.65
1:E:22:ASP:HB3	1:E:25:ILE:HB	1.78	0.65
1:H:318:ASN:HD21	1:H:339:SER:HB3	1.61	0.65
1:G:319:ILE:HB	1:G:337:GLY:HA3	1.78	0.65
1:C:308:ASN:OD1	1:C:364:ARG:HD2	1.96	0.65
1:G:321:GLU:HA	1:G:344:CYS:O	1.95	0.65
1:G:129:ASN:HD22	1:G:129:ASN:H	1.45	0.65
1:H:293:PRO:O	1:H:296:ASN:HB3	1.96	0.65
1:E:129:ASN:HD22	1:E:129:ASN:N	1.92	0.65
1:C:323:ASN:HB3	1:C:343:ALA:HA	1.77	0.65
1:F:129:ASN:HD22	1:F:129:ASN:H	1.43	0.65
1:G:257:TYR:HE2	1:G:295:VAL:HA	1.60	0.64
1:G:51:ALA:O	1:G:55:ARG:HG3	1.97	0.64
1:C:269:LEU:HD11	1:C:276:LEU:CD1	2.28	0.64
1:D:55:ARG:O	1:D:59:ILE:HG13	1.98	0.64
1:F:275:GLY:HA3	1:F:311:THR:CG2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:291:ASN:O	1:H:295:VAL:HG23	1.98	0.64
1:E:303:ILE:O	1:E:364:ARG:HB2	1.97	0.64
1:D:51:ALA:O	1:D:55:ARG:HG3	1.98	0.64
1:E:51:ALA:O	1:E:55:ARG:HG3	1.98	0.64
1:F:277:MET:HA	1:F:312:GLY:O	1.97	0.64
1:G:123:ILE:O	1:G:137:GLY:HA3	1.98	0.64
1:H:55:ARG:O	1:H:59:ILE:HG13	1.98	0.64
1:G:349:THR:O	1:G:353:VAL:HG22	1.98	0.63
1:G:20:GLU:HG3	1:G:20:GLU:O	1.97	0.63
1:B:366:GLU:O	1:B:369:LYS:N	2.30	0.63
1:F:51:ALA:O	1:F:55:ARG:HG3	1.98	0.63
1:E:112:LYS:HB3	1:E:341:THR:HG21	1.80	0.63
1:B:72:ILE:HG12	1:B:277:MET:CE	2.29	0.63
1:C:362:ARG:O	1:C:365:ARG:HB2	1.98	0.63
1:E:324:GLN:NE2	1:E:335:LYS:HB2	2.14	0.63
1:A:294:LYS:N	1:A:294:LYS:HD2	2.14	0.63
1:C:363:GLN:O	1:C:367:VAL:HG23	1.98	0.63
1:H:289:PHE:CD1	1:H:343:ALA:HB1	2.33	0.63
1:D:281:SER:HA	1:D:285:SER:HB3	1.81	0.63
1:B:71:VAL:HG21	1:B:102:LEU:HD22	1.81	0.62
1:A:112:LYS:HZ2	1:A:114:ARG:HB3	1.64	0.62
1:A:216:GLN:NE2	1:A:270:PRO:HG3	2.14	0.62
1:D:327:PRO:HG2	1:D:333:GLY:O	1.99	0.62
1:H:294:LYS:N	1:H:294:LYS:HD2	2.14	0.62
1:D:313:VAL:HG21	1:D:357:LEU:HD11	1.82	0.62
1:G:111:GLU:HB3	1:G:121:GLY:HA3	1.80	0.62
1:F:263:ALA:HA	1:F:266:LYS:HD3	1.80	0.62
1:A:327:PRO:HG3	1:A:333:GLY:O	1.99	0.62
1:D:128:VAL:HB	1:D:331:LYS:HB2	1.81	0.62
1:E:90:ARG:NH1	1:E:319:ILE:HG23	2.12	0.62
1:D:97:GLU:CD	1:D:355:ARG:HH12	2.03	0.62
1:G:216:GLN:NE2	1:G:270:PRO:HG3	2.15	0.61
1:F:110:LEU:N	1:F:110:LEU:HD22	2.15	0.61
1:C:52:LYS:HD3	1:D:20:GLU:HG3	1.81	0.61
1:G:112:LYS:HG3	1:G:113:PRO:HD2	1.81	0.61
1:E:326:ILE:HD12	1:E:326:ILE:N	2.15	0.61
1:B:101:ASP:HB3	1:B:361:VAL:HG11	1.81	0.61
1:H:116:THR:HG23	1:H:117:VAL:HG23	1.82	0.61
1:F:322:GLY:O	1:F:343:ALA:HA	1.99	0.61
1:B:51:ALA:O	1:B:55:ARG:HG3	2.00	0.61
1:A:279:ASP:HA	1:A:314:MET:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:110:LEU:HD21	1:F:145:PHE:HZ	1.66	0.61
1:B:82:GLU:OE2	1:B:82:GLU:N	2.34	0.61
1:D:212:VAL:O	1:D:216:GLN:HG2	2.01	0.61
1:D:262:VAL:O	1:D:266:LYS:HG3	2.01	0.61
1:H:124:ASN:HA	1:H:134:ILE:CD1	2.31	0.61
1:G:281:SER:HA	1:G:285:SER:HB2	1.82	0.60
1:A:110:LEU:O	1:A:111:GLU:HB3	2.00	0.60
1:A:110:LEU:HD21	1:A:145:PHE:HZ	1.63	0.60
1:G:126:PRO:HB3	1:G:137:GLY:HA2	1.83	0.60
1:G:249:ARG:O	1:G:283:GLY:HA3	2.01	0.60
1:C:357:LEU:O	1:C:361:VAL:HG23	2.01	0.60
1:C:82:GLU:HA	1:C:82:GLU:OE1	2.01	0.60
1:G:291:ASN:ND2	1:G:291:ASN:N	2.49	0.60
1:B:212:VAL:O	1:B:216:GLN:HG2	2.02	0.60
1:A:21:GLU:OE2	1:B:170:ASP:HB3	2.02	0.60
1:E:280:TYR:O	1:E:292:GLN:HG2	2.00	0.60
1:H:51:ALA:O	1:H:55:ARG:HG3	2.01	0.60
1:A:76:CYS:SG	1:A:342:ASP:HB2	2.42	0.60
1:B:326:ILE:HD12	1:B:326:ILE:N	2.16	0.60
1:G:308:ASN:HA	1:G:364:ARG:NH1	2.16	0.60
1:A:281:SER:OG	1:A:282:HIS:N	2.34	0.60
1:G:275:GLY:HA3	1:G:311:THR:CG2	2.32	0.60
1:C:111:GLU:HB3	1:C:121:GLY:CA	2.31	0.60
1:B:73:VAL:HG23	1:B:315:ILE:HB	1.83	0.60
1:C:269:LEU:HD11	1:C:276:LEU:HD11	1.83	0.60
1:B:72:ILE:HG12	1:B:277:MET:HE1	1.84	0.60
1:B:257:TYR:CD1	1:B:295:VAL:HG13	2.38	0.59
1:D:295:VAL:O	1:D:299:VAL:HG23	2.02	0.59
1:G:260:LYS:O	1:G:264:GLU:HG3	2.02	0.59
1:H:299:VAL:O	1:H:303:ILE:HG13	2.03	0.59
1:C:143:GLN:HG3	1:C:147:ASN:HD21	1.68	0.59
1:H:317:SER:HA	1:H:344:CYS:HB3	1.84	0.59
1:C:48:LEU:HD13	1:D:19:ALA:HB2	1.83	0.59
1:E:349:THR:O	1:E:353:VAL:HG23	2.02	0.59
1:G:364:ARG:O	1:G:368:ASN:ND2	2.36	0.59
1:A:232:VAL:HG21	1:D:232:VAL:HG21	1.85	0.59
1:C:111:GLU:HB3	1:C:121:GLY:HA2	1.84	0.59
1:C:51:ALA:O	1:C:55:ARG:HG3	2.02	0.59
1:B:232:VAL:HG21	1:C:232:VAL:HG21	1.85	0.59
1:H:201:LYS:HD3	1:H:249:ARG:HG2	1.84	0.59
1:H:319:ILE:HD13	1:H:337:GLY:HA2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:129:ASN:HD22	1:G:129:ASN:N	2.00	0.58
1:G:299:VAL:HG13	1:G:310:ILE:HD13	1.85	0.58
1:E:143:GLN:HG3	1:E:147:ASN:HD21	1.68	0.58
1:G:98:LEU:HD13	1:G:358:ALA:HB2	1.85	0.58
1:E:110:LEU:HD13	1:E:123:ILE:HD11	1.84	0.58
1:H:36:LEU:O	1:H:40:GLN:HG3	2.03	0.58
1:E:90:ARG:HH12	1:E:319:ILE:HG23	1.68	0.58
1:F:291:ASN:O	1:F:295:VAL:HG23	2.03	0.58
1:E:55:ARG:O	1:E:59:ILE:HG13	2.03	0.58
1:G:323:ASN:HA	1:G:338:VAL:HG12	1.86	0.58
1:D:330:GLY:O	1:D:332:ALA:N	2.37	0.58
1:A:117:VAL:HG12	1:A:118:GLY:H	1.69	0.58
1:C:76:CYS:SG	1:C:342:ASP:HB2	2.43	0.58
1:C:112:LYS:HD2	1:C:113:PRO:HD2	1.85	0.58
1:A:51:ALA:O	1:A:55:ARG:HG3	2.03	0.58
1:G:201:LYS:HD3	1:G:249:ARG:HG2	1.86	0.58
1:F:212:VAL:O	1:F:216:GLN:HG2	2.04	0.58
1:G:212:VAL:O	1:G:216:GLN:HG2	2.05	0.57
1:G:264:GLU:O	1:G:267:ALA:HB3	2.04	0.57
1:B:106:MET:HB2	1:B:153:LEU:HD21	1.85	0.57
1:H:212:VAL:O	1:H:216:GLN:HG2	2.04	0.57
1:F:110:LEU:HD21	1:F:145:PHE:CZ	2.39	0.57
1:A:212:VAL:O	1:A:216:GLN:HG2	2.04	0.57
1:F:129:ASN:H	1:F:129:ASN:ND2	2.02	0.57
1:E:281:SER:HA	1:E:285:SER:HB2	1.85	0.57
1:E:170:ASP:HB3	1:F:21:GLU:CD	2.23	0.57
1:C:30:PRO:HA	4:C:2001:HOH:O	2.04	0.57
1:E:20:GLU:O	1:E:20:GLU:HG3	2.05	0.57
1:H:175:GLY:O	1:H:198:VAL:HA	2.05	0.57
1:D:247:ILE:HG12	1:D:277:MET:HB3	1.86	0.57
1:D:266:LYS:HE2	1:D:309:ALA:HB2	1.86	0.57
1:C:55:ARG:O	1:C:59:ILE:HG13	2.04	0.57
1:C:110:LEU:HD22	1:C:110:LEU:N	2.20	0.57
1:E:335:LYS:O	1:E:336:TYR:HB2	2.04	0.57
1:C:72:ILE:HG22	1:C:107:ARG:HG3	1.87	0.57
1:G:350:THR:HA	1:G:353:VAL:CG2	2.35	0.57
1:G:143:GLN:HG3	1:G:147:ASN:HD21	1.70	0.57
1:D:297:ASP:OD1	1:D:356:LYS:HE3	2.05	0.57
1:A:67:ASP:OD1	1:A:365:ARG:NE	2.37	0.57
1:A:143:GLN:HG3	1:A:147:ASN:HD21	1.69	0.57
1:H:325:GLY:O	1:H:327:PRO:HD3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:VAL:HG23	1:D:315:ILE:HB	1.86	0.57
1:A:120:LYS:HE3	1:A:120:LYS:HA	1.86	0.56
1:D:20:GLU:O	1:D:21:GLU:HG2	2.05	0.56
1:A:55:ARG:O	1:A:59:ILE:HG13	2.05	0.56
1:D:22:ASP:HB3	1:D:25:ILE:HB	1.85	0.56
1:E:257:TYR:CD1	1:E:295:VAL:HG13	2.40	0.56
1:C:257:TYR:CD2	1:C:295:VAL:HG13	2.40	0.56
1:F:101:ASP:HB3	1:F:361:VAL:HB	1.87	0.56
1:G:55:ARG:O	1:G:59:ILE:HG13	2.06	0.56
1:F:55:ARG:O	1:F:59:ILE:HG13	2.06	0.56
1:H:91:LEU:HA	1:H:347:TRP:HH2	1.70	0.56
1:E:212:VAL:O	1:E:216:GLN:HG2	2.05	0.56
1:A:201:LYS:HD3	1:A:249:ARG:HG2	1.86	0.56
1:C:212:VAL:O	1:C:216:GLN:HG2	2.05	0.56
1:C:324:GLN:HE22	1:C:335:LYS:H	1.54	0.56
1:E:317:SER:CA	1:E:344:CYS:HB3	2.34	0.56
1:B:143:GLN:HG3	1:B:147:ASN:HD21	1.71	0.56
1:E:204:THR:HA	1:E:249:ARG:HH12	1.71	0.56
1:A:112:LYS:NZ	1:A:114:ARG:HA	2.18	0.56
1:A:102:LEU:HD21	1:A:357:LEU:HD13	1.87	0.56
1:D:143:GLN:HG3	1:D:147:ASN:HD21	1.70	0.56
1:D:306:GLY:HA2	1:D:364:ARG:HG3	1.88	0.56
1:B:257:TYR:CZ	1:B:295:VAL:HG22	2.41	0.56
1:F:36:LEU:O	1:F:40:GLN:HG3	2.05	0.56
1:B:79:HIS:HB3	1:B:119:TRP:CH2	2.41	0.56
1:A:204:THR:HA	1:A:249:ARG:HH12	1.71	0.56
1:A:36:LEU:O	1:A:40:GLN:HG3	2.06	0.56
1:A:72:ILE:HG22	1:A:107:ARG:HG2	1.87	0.56
1:D:367:VAL:O	1:D:367:VAL:HG12	2.06	0.56
1:E:129:ASN:ND2	1:E:131:THR:HB	2.21	0.55
1:B:55:ARG:O	1:B:59:ILE:HG13	2.06	0.55
1:E:201:LYS:HD3	1:E:249:ARG:HG2	1.88	0.55
1:E:232:VAL:HG21	1:H:232:VAL:CG2	2.36	0.55
1:H:127:ASP:OD1	1:H:131:THR:HB	2.07	0.55
1:B:74:GLY:HA3	1:B:107:ARG:HB2	1.89	0.55
1:B:125:ASP:OD2	1:B:128:VAL:HA	2.06	0.55
1:B:101:ASP:HB3	1:B:361:VAL:CG1	2.36	0.55
1:F:290:ARG:O	1:F:293:PRO:HD2	2.06	0.55
1:C:36:LEU:O	1:C:40:GLN:HG3	2.06	0.55
1:H:82:GLU:CD	1:H:82:GLU:N	2.59	0.55
1:D:76:CYS:SG	1:D:342:ASP:HB2	2.46	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:307:GLU:HA	1:G:307:GLU:OE2	2.05	0.55
1:H:294:LYS:CD	1:H:294:LYS:H	2.20	0.55
1:H:208:LEU:CD2	1:H:265:ALA:HA	2.37	0.55
1:G:257:TYR:CD2	1:G:295:VAL:HA	2.41	0.55
1:G:275:GLY:HA3	1:G:311:THR:HG21	1.88	0.55
1:D:175:GLY:O	1:D:198:VAL:HA	2.06	0.55
1:D:201:LYS:HD3	1:D:249:ARG:HG2	1.89	0.55
1:E:232:VAL:HG21	1:H:232:VAL:HG21	1.87	0.55
1:A:207:THR:HG21	1:B:252:LYS:HZ2	1.70	0.55
1:H:143:GLN:HG3	1:H:147:ASN:HD21	1.72	0.55
1:B:36:LEU:O	1:B:40:GLN:HG3	2.07	0.55
1:B:204:THR:HA	1:B:249:ARG:HH12	1.72	0.55
1:B:232:VAL:CG2	1:C:232:VAL:HG21	2.37	0.55
1:D:330:GLY:C	1:D:332:ALA:H	2.09	0.55
1:G:363:GLN:O	1:G:367:VAL:HG23	2.07	0.55
1:G:235:ILE:HD13	1:H:134:ILE:HB	1.89	0.54
1:F:201:LYS:HD3	1:F:249:ARG:HG2	1.90	0.54
1:G:169:ALA:HB1	2:H:1002:PHE:OXT	2.07	0.54
1:F:345:ILE:HG13	1:F:345:ILE:O	2.07	0.54
1:E:357:LEU:O	1:E:361:VAL:HG23	2.06	0.54
1:G:204:THR:HA	1:G:249:ARG:HH12	1.72	0.54
1:F:263:ALA:HB2	4:F:2004:HOH:O	2.07	0.54
1:A:324:GLN:HE21	1:A:338:VAL:HB	1.73	0.54
1:F:247:ILE:HD13	1:F:314:MET:CE	2.38	0.54
1:G:281:SER:HA	1:G:285:SER:CB	2.37	0.54
1:A:262:VAL:O	1:A:266:LYS:HG3	2.07	0.54
1:F:143:GLN:HG3	1:F:147:ASN:HD21	1.71	0.54
1:E:324:GLN:HB3	1:E:335:LYS:HD3	1.90	0.54
1:B:324:GLN:HE21	1:B:338:VAL:HB	1.73	0.54
1:H:352:ASP:OD1	1:H:356:LYS:NZ	2.39	0.54
1:H:302:GLN:O	1:H:307:GLU:HB3	2.07	0.54
1:G:317:SER:HA	1:G:344:CYS:HB3	1.89	0.54
1:B:128:VAL:CG2	1:B:331:LYS:HE3	2.37	0.54
1:A:366:GLU:OE2	1:A:369:LYS:HE2	2.08	0.54
1:G:90:ARG:HD3	1:G:347:TRP:CD1	2.43	0.54
1:E:207:THR:HG21	1:F:252:LYS:NZ	2.23	0.54
1:C:201:LYS:HD3	1:C:249:ARG:HG2	1.89	0.54
1:C:175:GLY:O	1:C:198:VAL:HA	2.08	0.53
1:H:120:LYS:HE3	1:H:132:PHE:CZ	2.43	0.53
1:G:257:TYR:CG	1:G:257:TYR:O	2.61	0.53
1:E:282:HIS:N	1:E:285:SER:HB2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:263:ALA:HA	1:H:266:LYS:HD3	1.90	0.53
1:C:247:ILE:HD13	1:C:314:MET:CE	2.38	0.53
1:A:252:LYS:C	1:A:254:GLY:H	2.11	0.53
1:B:248:LEU:HB2	1:B:278:ILE:HD13	1.90	0.53
1:H:111:GLU:HB3	1:H:121:GLY:HA3	1.91	0.53
1:H:294:LYS:CD	1:H:294:LYS:N	2.71	0.53
1:G:110:LEU:N	1:G:110:LEU:HD22	2.22	0.53
1:G:175:GLY:O	1:G:198:VAL:HA	2.08	0.53
1:H:362:ARG:HH11	1:H:362:ARG:HG3	1.74	0.53
1:G:350:THR:HA	1:G:353:VAL:HG22	1.90	0.53
1:E:113:PRO:HG3	1:E:180:ARG:NH1	2.23	0.53
1:G:261:SER:O	1:G:264:GLU:HB2	2.08	0.53
1:A:204:THR:HA	1:A:249:ARG:NH1	2.23	0.53
1:E:36:LEU:O	1:E:40:GLN:HG3	2.09	0.53
1:E:320:ASN:ND2	1:E:337:GLY:HA3	2.24	0.53
1:G:36:LEU:O	1:G:40:GLN:HG3	2.09	0.53
1:G:93:LYS:HB2	1:G:93:LYS:NZ	2.23	0.53
1:B:362:ARG:O	1:B:365:ARG:HB3	2.08	0.53
1:H:300:CYS:SG	1:H:357:LEU:HA	2.49	0.53
1:A:324:GLN:NE2	1:A:335:LYS:HB2	2.23	0.53
1:H:204:THR:HA	1:H:249:ARG:HH12	1.74	0.52
1:B:269:LEU:HD11	1:B:276:LEU:CD2	2.39	0.52
1:G:355:ARG:CG	1:G:355:ARG:HH11	2.09	0.52
1:G:355:ARG:NH1	1:G:355:ARG:CG	2.71	0.52
1:G:324:GLN:O	1:G:326:ILE:N	2.42	0.52
1:E:204:THR:HA	1:E:249:ARG:NH1	2.23	0.52
1:C:366:GLU:HA	1:C:369:LYS:HG2	1.90	0.52
1:A:75:PRO:HA	1:A:317:SER:O	2.09	0.52
1:B:201:LYS:HD3	1:B:249:ARG:HG2	1.91	0.52
1:E:336:TYR:CD1	1:E:337:GLY:N	2.78	0.52
1:B:269:LEU:HD11	1:B:276:LEU:HD21	1.92	0.52
1:D:36:LEU:O	1:D:40:GLN:HG3	2.09	0.52
1:E:134:ILE:HD13	1:F:235:ILE:CG2	2.38	0.52
1:A:307:GLU:HG2	1:A:310:ILE:CD1	2.40	0.52
1:A:232:VAL:HG21	1:D:232:VAL:CG2	2.39	0.52
1:B:335:LYS:CE	1:B:338:VAL:HG21	2.40	0.52
1:E:175:GLY:O	1:E:198:VAL:HA	2.10	0.52
1:E:266:LYS:HE2	1:E:309:ALA:HB2	1.91	0.52
1:G:308:ASN:HA	1:G:364:ARG:HH11	1.74	0.52
1:G:204:THR:HA	1:G:249:ARG:NH1	2.25	0.52
1:A:175:GLY:O	1:A:198:VAL:HA	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:THR:HA	1:C:249:ARG:HH12	1.75	0.52
1:B:248:LEU:HD12	1:B:278:ILE:HD11	1.91	0.52
1:H:110:LEU:HD22	1:H:110:LEU:N	2.25	0.52
1:G:167:TYR:C	1:G:168:LEU:HG	2.30	0.52
1:A:303:ILE:HG22	1:A:360:ALA:O	2.10	0.52
1:G:180:ARG:HB3	1:H:183:GLU:HB3	1.92	0.52
1:F:111:GLU:HB2	1:F:160:LEU:HD11	1.92	0.51
1:H:81:LEU:HG	1:H:144:LEU:HD13	1.91	0.51
1:F:144:LEU:HA	1:F:147:ASN:HD22	1.75	0.51
1:B:324:GLN:HE22	1:B:335:LYS:H	1.58	0.51
1:C:109:TYR:CD2	1:C:158:GLU:HB2	2.45	0.51
1:B:358:ALA:O	1:B:361:VAL:HB	2.11	0.51
1:C:340:ILE:O	1:C:341:THR:HG23	2.10	0.51
1:F:94:LEU:HD11	1:F:98:LEU:HD11	1.92	0.51
1:D:266:LYS:HB3	1:D:266:LYS:NZ	2.26	0.51
1:C:340:ILE:HG13	1:C:340:ILE:O	2.11	0.51
1:H:349:THR:O	1:H:353:VAL:HG23	2.10	0.51
1:F:355:ARG:HH11	1:F:355:ARG:HG2	1.74	0.51
1:A:257:TYR:CD1	1:A:295:VAL:HG13	2.46	0.51
1:E:110:LEU:HD13	1:E:123:ILE:CD1	2.40	0.51
1:H:71:VAL:HG11	1:H:354:LEU:HD21	1.91	0.51
1:C:177:ILE:HG13	1:C:200:PHE:CE1	2.46	0.51
1:D:292:GLN:N	1:D:293:PRO:CD	2.74	0.51
1:A:248:LEU:HB3	1:A:256:ASN:OD1	2.10	0.51
1:E:105:ILE:HG12	1:E:154:PRO:HB2	1.92	0.51
1:A:134:ILE:HD12	1:A:134:ILE:H	1.75	0.51
1:F:110:LEU:HD22	1:F:110:LEU:H	1.74	0.51
1:F:72:ILE:HG22	1:F:107:ARG:HG3	1.92	0.51
1:C:167:TYR:C	1:C:168:LEU:HG	2.30	0.51
1:D:81:LEU:HG	1:D:144:LEU:HD13	1.92	0.51
1:D:167:TYR:C	1:D:168:LEU:HG	2.30	0.51
1:E:235:ILE:HB	1:F:29:ASP:HB2	1.93	0.51
1:C:355:ARG:NH1	1:C:355:ARG:HG3	2.21	0.51
1:A:72:ILE:HG22	1:A:107:ARG:CG	2.40	0.51
1:B:67:ASP:OD1	1:B:365:ARG:NH2	2.44	0.51
1:F:355:ARG:O	1:F:358:ALA:HB3	2.11	0.51
1:D:177:ILE:HG13	1:D:200:PHE:CE1	2.46	0.51
1:A:359:ALA:CA	1:A:362:ARG:HH12	2.22	0.51
1:H:292:GLN:HB2	1:H:293:PRO:HD3	1.92	0.51
1:A:100:GLY:O	1:A:365:ARG:NH2	2.44	0.51
1:B:204:THR:HA	1:B:249:ARG:NH1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:304:ALA:O	1:G:367:VAL:HG21	2.11	0.51
1:B:175:GLY:O	1:B:198:VAL:HA	2.10	0.51
1:F:93:LYS:HZ3	1:F:93:LYS:HB2	1.76	0.50
1:B:252:LYS:O	1:B:254:GLY:N	2.44	0.50
1:F:204:THR:HA	1:F:249:ARG:HH12	1.76	0.50
1:B:258:ASP:OD2	1:B:260:LYS:HB3	2.11	0.50
1:D:204:THR:HA	1:D:249:ARG:HH12	1.77	0.50
1:D:72:ILE:HG22	1:D:107:ARG:HG3	1.94	0.50
1:C:204:THR:HA	1:C:249:ARG:NH1	2.26	0.50
1:G:146:VAL:O	1:G:150:ASN:HB2	2.11	0.50
1:F:175:GLY:O	1:F:198:VAL:HA	2.11	0.50
1:D:250:GLY:N	1:D:256:ASN:OD1	2.41	0.50
1:F:129:ASN:ND2	1:F:129:ASN:N	2.60	0.50
1:E:113:PRO:HG3	1:E:180:ARG:HH11	1.76	0.50
1:B:167:TYR:C	1:B:168:LEU:HG	2.32	0.50
1:E:85:GLN:O	1:E:89:LEU:HD23	2.12	0.50
1:A:122:LEU:O	1:A:122:LEU:HG	2.10	0.50
1:B:117:VAL:O	1:B:117:VAL:HG23	2.10	0.50
1:H:216:GLN:NE2	1:H:270:PRO:HG3	2.27	0.50
1:F:128:VAL:HG12	1:F:128:VAL:O	2.11	0.50
1:A:177:ILE:HG13	1:A:200:PHE:CE1	2.47	0.50
1:G:177:ILE:HG13	1:G:200:PHE:CE1	2.47	0.50
1:C:348:GLU:CD	1:C:348:GLU:N	2.64	0.50
1:D:356:LYS:O	1:D:356:LYS:HG3	2.11	0.50
1:A:144:LEU:HA	1:A:147:ASN:HD22	1.76	0.50
1:B:345:ILE:HD11	1:B:350:THR:OG1	2.11	0.50
1:F:262:VAL:O	1:F:265:ALA:HB3	2.12	0.50
1:G:280:TYR:CD2	1:G:315:ILE:HG12	2.47	0.50
1:E:281:SER:CA	1:E:285:SER:HB2	2.42	0.50
1:H:204:THR:HA	1:H:249:ARG:NH1	2.27	0.49
1:F:293:PRO:O	1:F:296:ASN:HB3	2.12	0.49
1:E:366:GLU:CD	1:E:366:GLU:H	2.15	0.49
1:H:144:LEU:HA	1:H:147:ASN:HD22	1.76	0.49
1:H:177:ILE:HG13	1:H:200:PHE:CE1	2.47	0.49
1:G:90:ARG:HB3	1:G:347:TRP:CZ2	2.47	0.49
1:D:266:LYS:HZ3	1:D:266:LYS:HB3	1.76	0.49
1:F:247:ILE:HD13	1:F:314:MET:HE1	1.94	0.49
1:C:174:PHE:HE1	1:C:245:PHE:CZ	2.31	0.49
1:E:112:LYS:HG2	1:E:113:PRO:HD2	1.94	0.49
1:H:321:GLU:HB3	1:H:346:GLY:N	2.27	0.49
1:F:265:ALA:O	1:F:268:GLN:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:LYS:HG2	1:B:341:THR:CG2	2.43	0.49
1:B:81:LEU:HG	1:B:144:LEU:HD13	1.94	0.49
1:A:229:LYS:NZ	1:B:21:GLU:OE2	2.33	0.49
1:G:289:PHE:N	1:G:289:PHE:CD2	2.80	0.49
1:G:129:ASN:ND2	1:G:129:ASN:N	2.61	0.49
1:B:303:ILE:O	1:B:364:ARG:HB2	2.12	0.49
1:A:327:PRO:HD2	1:A:334:LEU:HD21	1.94	0.49
1:H:252:LYS:C	1:H:254:GLY:H	2.15	0.49
1:E:95:SER:O	1:E:99:LYS:HB2	2.11	0.49
1:A:129:ASN:HD22	1:A:129:ASN:C	2.16	0.49
1:F:134:ILE:HD12	1:F:134:ILE:H	1.78	0.49
1:B:347:TRP:O	1:B:350:THR:HB	2.13	0.49
1:B:302:GLN:O	1:B:307:GLU:HB3	2.12	0.49
1:D:96:ASP:O	1:D:99:LYS:HG2	2.11	0.49
1:E:129:ASN:HD21	1:E:131:THR:HB	1.76	0.49
1:G:247:ILE:HD13	1:G:314:MET:CE	2.42	0.49
1:E:177:ILE:HG13	1:E:200:PHE:CE1	2.48	0.49
1:C:81:LEU:HG	1:C:144:LEU:HD13	1.95	0.49
1:B:85:GLN:O	1:B:89:LEU:HD23	2.13	0.49
1:B:177:ILE:HG13	1:B:200:PHE:CE1	2.47	0.49
1:D:164:SER:HB2	4:D:2003:HOH:O	2.12	0.49
1:E:82:GLU:N	1:E:82:GLU:OE1	2.38	0.49
1:D:94:LEU:HD11	1:D:351:GLU:HG3	1.95	0.49
1:E:324:GLN:CD	1:E:335:LYS:HB2	2.32	0.49
1:B:112:LYS:HD3	1:B:342:ASP:OD2	2.13	0.49
1:F:257:TYR:CD1	1:F:295:VAL:HG13	2.48	0.49
1:B:335:LYS:HE3	1:B:338:VAL:HG21	1.95	0.49
1:E:167:TYR:C	1:E:168:LEU:HG	2.33	0.49
1:E:324:GLN:CB	1:E:335:LYS:HD3	2.43	0.48
1:G:129:ASN:ND2	1:G:131:THR:OG1	2.47	0.48
1:G:144:LEU:HA	1:G:147:ASN:HD22	1.78	0.48
1:C:249:ARG:O	1:C:283:GLY:HA3	2.13	0.48
1:E:78:ILE:HG23	1:E:84:ALA:HB2	1.95	0.48
1:H:304:ALA:HB1	1:H:363:GLN:HG2	1.95	0.48
1:E:304:ALA:O	1:E:367:VAL:HG21	2.13	0.48
1:A:134:ILE:HD13	1:B:235:ILE:HG21	1.94	0.48
1:E:345:ILE:HG13	1:E:350:THR:OG1	2.13	0.48
1:A:78:ILE:HG23	1:A:84:ALA:HB2	1.95	0.48
1:D:304:ALA:C	1:D:306:GLY:H	2.17	0.48
1:A:110:LEU:N	1:A:110:LEU:HD22	2.28	0.48
1:D:204:THR:HA	1:D:249:ARG:NH1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:349:THR:O	1:F:352:ASP:HB3	2.12	0.48
1:A:146:VAL:O	1:A:150:ASN:HB2	2.13	0.48
1:F:67:ASP:OD1	1:F:365:ARG:NE	2.47	0.48
1:C:78:ILE:HG23	1:C:84:ALA:HB2	1.95	0.48
1:A:79:HIS:HB3	1:A:119:TRP:CH2	2.48	0.48
1:C:304:ALA:O	1:C:367:VAL:HG21	2.14	0.48
1:B:144:LEU:HA	1:B:147:ASN:HD22	1.78	0.48
1:A:134:ILE:HB	1:B:235:ILE:HD13	1.95	0.48
1:G:174:PHE:HE1	1:G:245:PHE:CZ	2.32	0.48
1:G:85:GLN:O	1:G:89:LEU:HD23	2.13	0.48
1:H:361:VAL:HG12	1:H:365:ARG:HH12	1.79	0.48
1:F:262:VAL:CG1	1:F:263:ALA:N	2.77	0.48
1:F:275:GLY:HA3	1:F:311:THR:HG21	1.94	0.48
1:F:122:LEU:HD12	1:F:126:PRO:HA	1.95	0.48
1:G:280:TYR:O	1:G:285:SER:HB2	2.14	0.48
1:H:78:ILE:HG23	1:H:84:ALA:HB2	1.95	0.48
1:D:366:GLU:C	1:D:368:ASN:H	2.16	0.48
1:G:362:ARG:O	1:G:365:ARG:HB2	2.13	0.48
1:A:113:PRO:HB2	1:A:180:ARG:CZ	2.44	0.48
1:D:110:LEU:N	1:D:110:LEU:HD22	2.26	0.48
1:D:76:CYS:HA	1:D:107:ARG:HH21	1.78	0.48
1:B:291:ASN:O	1:B:295:VAL:HG23	2.14	0.48
1:F:204:THR:HA	1:F:249:ARG:NH1	2.28	0.48
1:H:74:GLY:CA	1:H:107:ARG:HB2	2.43	0.48
1:F:112:LYS:HD2	1:F:113:PRO:CD	2.37	0.48
1:H:363:GLN:HE21	1:H:367:VAL:HG23	1.78	0.48
1:E:112:LYS:HB3	1:E:341:THR:CG2	2.42	0.48
1:E:144:LEU:HA	1:E:147:ASN:HD22	1.79	0.48
1:B:146:VAL:O	1:B:150:ASN:HB2	2.14	0.48
1:E:146:VAL:O	1:E:150:ASN:HB2	2.14	0.48
1:E:359:ALA:HA	1:E:362:ARG:CZ	2.44	0.48
1:D:277:MET:SD	1:D:314:MET:HE2	2.54	0.48
1:F:71:VAL:CG2	1:F:102:LEU:HD22	2.43	0.48
1:A:363:GLN:O	1:A:365:ARG:N	2.47	0.48
1:C:369:LYS:HG3	1:C:370:LYS:N	2.28	0.48
1:D:290:ARG:O	1:D:293:PRO:HD2	2.14	0.48
1:G:29:ASP:HB2	1:H:235:ILE:HB	1.96	0.48
1:D:112:LYS:C	1:D:112:LYS:HD3	2.34	0.48
1:G:78:ILE:HG23	1:G:84:ALA:HB2	1.95	0.48
1:F:112:LYS:O	1:F:114:ARG:N	2.47	0.47
1:C:277:MET:HE3	1:C:313:VAL:CA	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:VAL:HG23	1:B:331:LYS:HE3	1.96	0.47
1:D:94:LEU:CD1	1:D:351:GLU:HG3	2.44	0.47
1:H:74:GLY:HA3	1:H:107:ARG:HB2	1.95	0.47
1:F:119:TRP:HB2	1:F:326:ILE:CD1	2.44	0.47
1:A:292:GLN:HB2	1:A:293:PRO:HD3	1.94	0.47
1:B:348:GLU:H	1:B:348:GLU:CD	2.18	0.47
1:C:295:VAL:O	1:C:299:VAL:HG23	2.13	0.47
1:C:324:GLN:NE2	1:C:335:LYS:H	2.12	0.47
1:C:128:VAL:HG13	1:C:128:VAL:O	2.14	0.47
1:C:287:LYS:N	1:C:287:LYS:HD2	2.29	0.47
1:E:320:ASN:O	1:E:346:GLY:HA2	2.14	0.47
1:G:289:PHE:N	1:G:289:PHE:HD2	2.11	0.47
1:H:94:LEU:HD23	1:H:94:LEU:O	2.14	0.47
1:H:322:GLY:O	1:H:323:ASN:HB3	2.13	0.47
1:A:235:ILE:HG21	1:B:134:ILE:HD13	1.97	0.47
1:G:185:GLN:OE1	1:H:114:ARG:CB	2.62	0.47
1:B:72:ILE:HG12	1:B:277:MET:HE2	1.96	0.47
1:F:295:VAL:O	1:F:299:VAL:HG23	2.15	0.47
1:H:349:THR:O	1:H:352:ASP:HB3	2.14	0.47
1:H:111:GLU:O	1:H:111:GLU:HG3	2.15	0.47
1:F:167:TYR:C	1:F:168:LEU:HG	2.33	0.47
2:G:1002:PHE:OXT	1:H:169:ALA:HB1	2.14	0.47
1:B:111:GLU:HB3	1:B:121:GLY:HA3	1.95	0.47
1:B:78:ILE:HG23	1:B:84:ALA:HB2	1.95	0.47
1:F:257:TYR:CG	1:F:295:VAL:HG13	2.50	0.47
1:D:78:ILE:HG23	1:D:84:ALA:HB2	1.97	0.47
1:A:167:TYR:C	1:A:168:LEU:HG	2.34	0.47
1:E:286:ASN:HD22	1:E:286:ASN:HA	1.56	0.47
1:D:362:ARG:O	1:D:365:ARG:HB3	2.14	0.47
1:A:235:ILE:HB	1:B:29:ASP:HB2	1.97	0.47
1:F:81:LEU:HG	1:F:144:LEU:HD13	1.95	0.47
1:B:290:ARG:O	1:B:293:PRO:HD2	2.15	0.47
1:C:146:VAL:O	1:C:150:ASN:HB2	2.15	0.47
1:E:73:VAL:O	1:E:106:MET:HA	2.15	0.47
1:A:85:GLN:O	1:A:89:LEU:HD23	2.15	0.47
1:H:258:ASP:O	1:H:262:VAL:HG23	2.15	0.47
1:G:324:GLN:OE1	1:G:334:LEU:HD22	2.14	0.47
1:E:304:ALA:HA	1:E:363:GLN:HB3	1.97	0.47
1:E:281:SER:HA	1:E:285:SER:CB	2.45	0.47
1:B:317:SER:HB2	1:B:345:ILE:HG12	1.96	0.47
1:E:355:ARG:HG2	1:E:355:ARG:HH11	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:GLU:O	1:B:355:ARG:HG3	2.15	0.47
1:C:74:GLY:CA	1:C:107:ARG:HB2	2.45	0.47
1:A:327:PRO:HD2	1:A:334:LEU:CD2	2.45	0.47
1:D:144:LEU:HA	1:D:147:ASN:HD22	1.79	0.47
1:H:196:PHE:HB2	1:H:197:PRO:CD	2.45	0.47
1:D:317:SER:HB3	1:D:345:ILE:HG13	1.95	0.47
1:D:277:MET:HA	1:D:312:GLY:O	2.15	0.47
1:C:144:LEU:HA	1:C:147:ASN:HD22	1.80	0.47
1:A:232:VAL:CG2	1:D:232:VAL:HG21	2.45	0.47
1:C:85:GLN:O	1:C:89:LEU:HD23	2.15	0.47
1:F:196:PHE:HB2	1:F:197:PRO:CD	2.45	0.47
1:F:129:ASN:HD22	1:F:129:ASN:N	2.04	0.46
1:D:330:GLY:C	1:D:332:ALA:N	2.68	0.46
1:B:34:PRO:O	1:B:38:GLN:HG3	2.15	0.46
1:C:94:LEU:HD11	1:C:98:LEU:HD11	1.97	0.46
1:E:71:VAL:HG22	1:E:313:VAL:HG22	1.97	0.46
1:A:352:ASP:HB3	1:A:356:LYS:NZ	2.30	0.46
1:E:129:ASN:ND2	1:E:129:ASN:N	2.62	0.46
1:H:131:THR:HG22	1:H:132:PHE:N	2.30	0.46
1:B:87:TYR:OH	1:B:317:SER:OG	2.30	0.46
1:F:174:PHE:HE1	1:F:245:PHE:CZ	2.33	0.46
1:G:24:ARG:HD3	1:H:240:GLY:O	2.15	0.46
1:F:316:GLU:O	1:F:344:CYS:HB2	2.14	0.46
1:G:289:PHE:HD2	1:G:289:PHE:H	1.64	0.46
1:G:321:GLU:HB3	1:G:346:GLY:H	1.79	0.46
1:C:235:ILE:HG13	1:D:31:LEU:HB2	1.98	0.46
1:E:61:ILE:HG22	1:E:311:THR:HB	1.97	0.46
1:D:252:LYS:C	1:D:254:GLY:H	2.18	0.46
1:E:266:LYS:HB3	1:E:266:LYS:NZ	2.31	0.46
1:H:85:GLN:O	1:H:89:LEU:HD23	2.14	0.46
1:B:97:GLU:HG2	1:B:98:LEU:HD23	1.97	0.46
1:G:317:SER:CA	1:G:344:CYS:HB3	2.45	0.46
1:G:324:GLN:HE22	1:G:334:LEU:CB	2.24	0.46
1:D:85:GLN:O	1:D:89:LEU:HD23	2.15	0.46
1:A:34:PRO:O	1:A:38:GLN:HG3	2.16	0.46
1:D:208:LEU:CD2	1:D:265:ALA:HA	2.46	0.46
1:A:117:VAL:CG1	1:A:118:GLY:H	2.29	0.46
1:G:294:LYS:HZ3	1:G:294:LYS:HB2	1.79	0.46
1:C:20:GLU:OE1	1:D:55:ARG:HD2	2.15	0.46
1:F:134:ILE:HD12	1:F:134:ILE:N	2.31	0.46
1:B:90:ARG:NH1	1:B:319:ILE:HG23	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:193:GLY:HA3	1:E:238:THR:CG2	2.46	0.46
1:D:110:LEU:N	1:D:110:LEU:HD13	2.31	0.46
1:E:128:VAL:O	1:E:129:ASN:HB3	2.15	0.46
1:B:74:GLY:CA	1:B:107:ARG:HB2	2.44	0.46
1:B:248:LEU:HB2	1:B:278:ILE:CD1	2.45	0.46
1:B:21:GLU:O	1:B:23:VAL:N	2.48	0.46
1:A:109:TYR:CD2	1:A:158:GLU:HB2	2.51	0.46
1:C:180:ARG:NH1	1:D:183:GLU:O	2.49	0.46
1:A:117:VAL:CG1	1:A:118:GLY:N	2.75	0.46
1:D:72:ILE:HB	1:D:314:MET:HG3	1.98	0.46
1:E:315:ILE:CD1	1:E:354:LEU:HD21	2.46	0.46
1:H:34:PRO:O	1:H:38:GLN:HG3	2.16	0.46
1:H:308:ASN:ND2	1:H:364:ARG:HD2	2.30	0.46
1:B:303:ILE:HG22	1:B:360:ALA:O	2.15	0.46
1:E:368:ASN:O	1:E:369:LYS:HG3	2.15	0.46
1:H:174:PHE:HE1	1:H:245:PHE:CZ	2.33	0.46
1:A:349:THR:O	1:A:353:VAL:HG23	2.16	0.46
1:H:82:GLU:OE2	1:H:82:GLU:N	2.48	0.46
1:A:129:ASN:HD22	1:A:131:THR:H	1.64	0.46
1:H:146:VAL:O	1:H:150:ASN:HB2	2.16	0.46
1:C:196:PHE:HB2	1:C:197:PRO:CD	2.46	0.46
1:B:196:PHE:HB2	1:B:197:PRO:CD	2.46	0.46
1:C:62:ILE:HD12	1:C:274:ASN:ND2	2.31	0.46
1:D:348:GLU:CD	1:D:348:GLU:N	2.55	0.45
1:F:93:LYS:HB2	1:F:93:LYS:HZ2	1.79	0.45
1:C:72:ILE:HG12	1:C:277:MET:CE	2.46	0.45
1:A:266:LYS:NZ	1:A:307:GLU:OE2	2.42	0.45
1:F:277:MET:HG3	1:F:312:GLY:C	2.37	0.45
1:D:266:LYS:HE2	1:D:309:ALA:CB	2.46	0.45
1:C:174:PHE:CE1	1:C:245:PHE:HZ	2.34	0.45
1:H:98:LEU:HD13	1:H:102:LEU:CD2	2.44	0.45
1:H:110:LEU:HD22	1:H:110:LEU:H	1.80	0.45
1:C:257:TYR:CG	1:C:295:VAL:HG13	2.51	0.45
1:C:111:GLU:HB3	1:C:121:GLY:HA3	1.97	0.45
1:A:174:PHE:HE1	1:A:245:PHE:CZ	2.34	0.45
1:H:167:TYR:C	1:H:168:LEU:HG	2.35	0.45
1:D:174:PHE:HE1	1:D:245:PHE:CZ	2.35	0.45
1:G:257:TYR:H	1:G:257:TYR:HD1	1.64	0.45
1:H:102:LEU:HD23	1:H:354:LEU:HD22	1.99	0.45
1:B:323:ASN:O	1:B:324:GLN:HB3	2.16	0.45
1:C:369:LYS:HB3	1:C:369:LYS:NZ	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LYS:HG2	1:A:113:PRO:HD2	1.97	0.45
1:C:247:ILE:HG12	1:C:277:MET:HB3	1.99	0.45
1:G:142:ARG:O	1:G:146:VAL:HG23	2.17	0.45
1:H:323:ASN:HA	1:H:339:SER:O	2.17	0.45
1:B:362:ARG:HG3	1:B:362:ARG:HH11	1.82	0.45
1:F:78:ILE:HG23	1:F:84:ALA:HB2	1.98	0.45
1:H:76:CYS:SG	1:H:112:LYS:HG3	2.57	0.45
1:G:93:LYS:HB2	1:G:93:LYS:HZ2	1.82	0.45
1:F:91:LEU:HD11	1:F:104:ILE:HG21	1.97	0.45
1:B:279:ASP:HA	1:B:314:MET:HB2	1.99	0.45
1:C:270:PRO:O	1:C:273:SER:HB2	2.16	0.45
1:E:29:ASP:HB2	1:F:235:ILE:HB	1.98	0.45
1:H:362:ARG:NH1	1:H:362:ARG:HG3	2.31	0.45
1:C:235:ILE:HB	1:D:29:ASP:HB2	1.99	0.45
1:A:196:PHE:HB2	1:A:197:PRO:CD	2.47	0.45
1:D:352:ASP:O	1:D:354:LEU:N	2.49	0.45
1:H:94:LEU:CD2	1:H:98:LEU:HD11	2.47	0.45
1:D:196:PHE:HB2	1:D:197:PRO:CD	2.47	0.45
1:F:177:ILE:HG13	1:F:200:PHE:CE1	2.52	0.45
1:H:70:LEU:HD11	1:H:105:ILE:CD1	2.47	0.45
1:D:278:ILE:HD12	1:D:310:ILE:HD13	1.97	0.45
1:E:81:LEU:HG	1:E:144:LEU:HD13	1.99	0.45
1:H:91:LEU:HA	1:H:347:TRP:CH2	2.50	0.45
1:C:324:GLN:HE22	1:C:335:LYS:N	2.15	0.45
1:A:193:GLY:HA3	1:A:238:THR:CG2	2.46	0.45
1:F:101:ASP:OD2	1:F:362:ARG:NH1	2.49	0.44
1:H:216:GLN:HE22	1:H:270:PRO:HG3	1.82	0.44
1:G:196:PHE:HB2	1:G:197:PRO:CD	2.47	0.44
1:C:61:ILE:HD11	1:C:103:SER:HB2	1.98	0.44
1:A:291:ASN:O	1:A:294:LYS:HB2	2.17	0.44
1:D:303:ILE:O	1:D:364:ARG:HB2	2.17	0.44
1:C:129:ASN:OD1	1:C:131:THR:HB	2.16	0.44
1:F:193:GLY:HA3	1:F:238:THR:CG2	2.47	0.44
1:G:307:GLU:CA	1:G:307:GLU:OE2	2.65	0.44
1:C:110:LEU:HD22	1:C:110:LEU:H	1.81	0.44
1:A:81:LEU:HG	1:A:144:LEU:HD13	2.00	0.44
1:E:270:PRO:HD2	1:E:273:SER:OG	2.18	0.44
1:D:146:VAL:O	1:D:150:ASN:HB2	2.17	0.44
1:H:193:GLY:HA3	1:H:238:THR:CG2	2.47	0.44
1:C:247:ILE:HD13	1:C:314:MET:HE1	1.99	0.44
1:G:294:LYS:HZ2	1:G:294:LYS:HB2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:TYR:HH	1:B:317:SER:HG	1.57	0.44
1:B:302:GLN:O	1:B:307:GLU:CB	2.66	0.44
1:D:111:GLU:O	1:D:112:LYS:HB2	2.17	0.44
1:B:193:GLY:HA3	1:B:238:THR:CG2	2.48	0.44
1:C:75:PRO:HA	1:C:317:SER:O	2.16	0.44
1:H:247:ILE:HG12	1:H:277:MET:HB3	1.99	0.44
1:F:301:GLU:HG3	1:F:305:ASN:ND2	2.33	0.44
1:G:81:LEU:HG	1:G:144:LEU:HD13	1.99	0.44
1:D:127:ASP:HB2	1:D:129:ASN:ND2	2.33	0.44
1:D:262:VAL:HG12	1:D:266:LYS:HD2	1.99	0.44
1:H:106:MET:CG	1:H:107:ARG:N	2.80	0.44
1:F:146:VAL:O	1:F:150:ASN:HB2	2.17	0.44
1:E:34:PRO:O	1:E:38:GLN:HG3	2.16	0.44
1:B:83:ALA:HB2	1:B:336:TYR:CE1	2.53	0.44
1:B:91:LEU:HD11	1:B:104:ILE:HG21	2.00	0.44
1:D:341:THR:HB	1:D:342:ASP:H	1.57	0.44
1:B:345:ILE:HG13	1:B:346:GLY:O	2.18	0.44
1:E:355:ARG:HG2	1:E:355:ARG:NH1	2.33	0.44
1:B:300:CYS:SG	1:B:357:LEU:HA	2.58	0.44
1:H:285:SER:HB2	1:H:288:ASP:O	2.18	0.44
1:A:112:LYS:HZ2	1:A:114:ARG:CB	2.28	0.44
1:H:104:ILE:CG2	1:H:105:ILE:N	2.81	0.44
1:G:359:ALA:O	1:G:361:VAL:N	2.51	0.43
1:A:29:ASP:HB2	1:B:235:ILE:HB	1.99	0.43
1:A:192:SER:O	1:A:238:THR:HB	2.18	0.43
1:C:126:PRO:HB3	1:C:137:GLY:HA2	2.00	0.43
1:B:174:PHE:HE1	1:B:245:PHE:CZ	2.36	0.43
1:G:127:ASP:OD2	1:G:136:LYS:NZ	2.35	0.43
1:A:259:ALA:HA	1:A:302:GLN:OE1	2.18	0.43
1:G:79:HIS:HB3	1:G:340:ILE:HD11	2.00	0.43
1:A:264:GLU:O	1:A:267:ALA:HB3	2.18	0.43
1:H:322:GLY:O	1:H:343:ALA:HA	2.18	0.43
1:E:193:GLY:HA3	1:E:238:THR:HG22	1.99	0.43
1:A:321:GLU:HA	1:A:344:CYS:O	2.18	0.43
1:E:324:GLN:HE22	1:E:335:LYS:HB2	1.82	0.43
1:E:134:ILE:HB	1:F:235:ILE:HD13	2.00	0.43
1:H:76:CYS:SG	1:H:342:ASP:HB2	2.57	0.43
1:H:318:ASN:ND2	1:H:339:SER:HB3	2.31	0.43
1:H:110:LEU:HD21	1:H:145:PHE:CZ	2.54	0.43
1:G:174:PHE:CE1	1:G:245:PHE:HZ	2.37	0.43
1:F:300:CYS:O	1:F:301:GLU:C	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:279:ASP:HA	1:H:314:MET:HB3	2.01	0.43
1:A:306:GLY:HA3	1:A:367:VAL:HG11	1.99	0.43
1:C:313:VAL:HG21	1:C:357:LEU:HD21	2.01	0.43
1:C:174:PHE:HE1	1:C:245:PHE:HZ	1.66	0.43
1:B:34:PRO:HD2	1:B:229:LYS:O	2.18	0.43
1:H:62:ILE:O	1:H:274:ASN:HB3	2.18	0.43
1:C:208:LEU:HD11	1:C:246:VAL:CG1	2.37	0.43
1:E:123:ILE:O	1:E:134:ILE:HA	2.18	0.43
1:A:110:LEU:O	1:A:111:GLU:CB	2.66	0.43
1:F:275:GLY:HA3	1:F:311:THR:HG23	1.98	0.43
1:B:364:ARG:O	1:B:368:ASN:ND2	2.52	0.43
1:A:326:ILE:HA	1:A:327:PRO:HD2	1.84	0.43
1:B:330:GLY:C	1:B:332:ALA:H	2.21	0.43
1:G:202:ASN:HB2	1:G:207:THR:O	2.19	0.43
1:C:322:GLY:O	1:C:323:ASN:HB3	2.18	0.43
1:C:74:GLY:HA3	1:C:107:ARG:HB2	2.01	0.43
1:G:112:LYS:HE2	1:G:342:ASP:OD1	2.19	0.43
1:E:335:LYS:O	1:E:336:TYR:CB	2.66	0.43
1:A:261:SER:HA	1:A:264:GLU:OE2	2.18	0.43
1:E:202:ASN:HB2	1:E:207:THR:O	2.19	0.43
1:E:73:VAL:HG23	1:E:315:ILE:HB	2.00	0.43
1:E:196:PHE:HB2	1:E:197:PRO:CD	2.48	0.43
1:G:345:ILE:HG13	1:G:345:ILE:O	2.17	0.43
1:G:124:ASN:O	1:G:132:PHE:HA	2.18	0.43
1:A:118:GLY:O	1:A:120:LYS:NZ	2.51	0.43
1:B:306:GLY:HA2	1:B:364:ARG:HG3	2.01	0.43
1:E:90:ARG:HD3	1:E:347:TRP:CD1	2.53	0.43
1:B:331:LYS:HZ2	1:B:331:LYS:CB	2.32	0.43
1:H:174:PHE:CE1	1:H:245:PHE:HZ	2.37	0.43
1:A:193:GLY:HA3	1:A:238:THR:HG22	2.01	0.43
1:D:247:ILE:HD13	1:D:314:MET:HE3	1.99	0.43
1:E:281:SER:C	1:E:285:SER:HB2	2.39	0.43
1:G:93:LYS:CB	1:G:93:LYS:NZ	2.82	0.43
1:A:129:ASN:ND2	1:A:131:THR:OG1	2.52	0.43
1:H:78:ILE:O	1:H:119:TRP:HH2	2.02	0.43
1:C:62:ILE:O	1:C:274:ASN:HB3	2.19	0.43
1:D:275:GLY:HA3	1:D:311:THR:OG1	2.18	0.43
1:E:336:TYR:CD1	1:E:336:TYR:C	2.93	0.43
1:E:290:ARG:O	1:E:293:PRO:HD2	2.19	0.43
1:G:258:ASP:OD2	1:G:260:LYS:HB3	2.19	0.43
1:G:265:ALA:O	1:G:267:ALA:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:257:TYR:HD1	1:C:258:ASP:N	2.16	0.42
1:G:235:ILE:HB	1:H:29:ASP:HB2	2.01	0.42
1:D:262:VAL:O	1:D:262:VAL:HG12	2.19	0.42
1:B:142:ARG:O	1:B:146:VAL:HG23	2.19	0.42
1:B:192:SER:O	1:B:238:THR:HB	2.19	0.42
1:B:109:TYR:CE2	1:B:158:GLU:HB2	2.54	0.42
1:F:123:ILE:O	1:F:137:GLY:HA3	2.19	0.42
1:B:92:LYS:O	1:B:95:SER:HB3	2.19	0.42
1:A:102:LEU:CD2	1:A:357:LEU:HD13	2.48	0.42
1:G:193:GLY:HA3	1:G:238:THR:CG2	2.49	0.42
1:A:355:ARG:HG2	1:A:355:ARG:HH11	1.84	0.42
1:C:355:ARG:NH1	1:C:355:ARG:CG	2.80	0.42
1:E:363:GLN:O	1:E:367:VAL:HG23	2.19	0.42
1:D:193:GLY:HA3	1:D:238:THR:CG2	2.48	0.42
1:F:85:GLN:O	1:F:89:LEU:HD23	2.18	0.42
1:C:257:TYR:CD1	1:C:257:TYR:C	2.93	0.42
1:C:279:ASP:HA	1:C:314:MET:HB3	2.00	0.42
1:C:247:ILE:HD13	1:C:314:MET:HE3	2.02	0.42
1:B:335:LYS:HE2	1:B:338:VAL:HG21	2.01	0.42
1:F:355:ARG:HG2	1:F:355:ARG:NH1	2.33	0.42
1:G:41:ILE:HB	1:G:142:ARG:HD3	2.00	0.42
1:C:119:TRP:CD1	1:C:128:VAL:HG23	2.54	0.42
1:C:240:GLY:O	1:D:24:ARG:HD3	2.19	0.42
1:G:327:PRO:HD3	1:G:334:LEU:CD2	2.50	0.42
1:B:362:ARG:HG3	1:B:362:ARG:NH1	2.35	0.42
1:D:288:ASP:OD1	1:D:290:ARG:HG3	2.19	0.42
1:H:79:HIS:HB3	1:H:119:TRP:CH2	2.54	0.42
1:E:194:LEU:HD13	1:E:196:PHE:CE1	2.54	0.42
1:A:351:GLU:O	1:A:355:ARG:HG3	2.19	0.42
1:G:289:PHE:CD2	1:G:290:ARG:N	2.88	0.42
1:D:110:LEU:HB3	1:D:122:LEU:HB3	2.01	0.42
1:B:72:ILE:HG22	1:B:107:ARG:HG3	2.01	0.42
1:D:266:LYS:CB	1:D:266:LYS:NZ	2.82	0.42
1:A:194:LEU:HD13	1:A:196:PHE:CE1	2.55	0.42
1:F:193:GLY:HA3	1:F:238:THR:HG22	2.02	0.42
1:B:327:PRO:C	1:B:329:GLU:N	2.73	0.42
1:A:52:LYS:HD3	1:B:20:GLU:HB2	2.02	0.42
1:A:111:GLU:HB3	1:A:121:GLY:HA3	2.01	0.42
1:E:59:ILE:HD13	1:E:243:HIS:CE1	2.55	0.42
1:H:104:ILE:HG22	1:H:105:ILE:N	2.35	0.42
1:C:162:THR:HG21	1:C:186:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:THR:OG1	1:B:152:GLY:HA2	2.20	0.42
1:C:351:GLU:HG2	1:C:355:ARG:NH1	2.35	0.42
1:D:357:LEU:O	1:D:361:VAL:HG23	2.20	0.42
1:D:310:ILE:O	1:D:310:ILE:HG22	2.20	0.42
1:A:129:ASN:ND2	1:A:131:THR:H	2.17	0.42
1:F:194:LEU:HD13	1:F:196:PHE:CE1	2.55	0.42
1:H:41:ILE:HB	1:H:142:ARG:HD3	2.01	0.42
1:F:50:THR:OG1	1:F:152:GLY:HA2	2.19	0.42
1:A:114:ARG:HB2	1:A:116:THR:O	2.20	0.42
1:C:323:ASN:HA	1:C:339:SER:O	2.20	0.42
1:D:363:GLN:NE2	1:D:367:VAL:HG23	2.34	0.42
1:E:41:ILE:HB	1:E:142:ARG:HD3	2.01	0.42
1:E:142:ARG:O	1:E:146:VAL:HG23	2.20	0.42
1:F:34:PRO:O	1:F:38:GLN:HG3	2.19	0.42
1:D:208:LEU:HD11	1:D:246:VAL:CG1	2.35	0.41
1:D:317:SER:HB3	1:D:345:ILE:CG1	2.50	0.41
1:B:366:GLU:O	1:B:368:ASN:N	2.53	0.41
1:C:366:GLU:OE2	1:C:369:LYS:HD2	2.20	0.41
1:E:133:ASN:ND2	1:E:136:LYS:CB	2.82	0.41
1:B:72:ILE:CG1	1:B:277:MET:HE1	2.51	0.41
1:B:59:ILE:HD13	1:B:243:HIS:CE1	2.55	0.41
1:E:235:ILE:HD13	1:F:134:ILE:HB	2.02	0.41
1:A:41:ILE:HB	1:A:142:ARG:HD3	2.02	0.41
1:D:366:GLU:C	1:D:368:ASN:N	2.73	0.41
1:C:132:PHE:CD2	1:D:223:HIS:HB2	2.54	0.41
1:C:41:ILE:HB	1:C:142:ARG:HD3	2.02	0.41
1:E:174:PHE:HE1	1:E:245:PHE:CZ	2.39	0.41
1:G:298:VAL:O	1:G:298:VAL:HG12	2.20	0.41
1:D:119:TRP:CZ2	1:D:122:LEU:N	2.88	0.41
1:E:269:LEU:HA	1:E:270:PRO:HD3	1.79	0.41
1:G:164:SER:HB2	1:G:165:PRO:HD3	2.01	0.41
1:C:223:HIS:HB2	1:D:132:PHE:CD1	2.55	0.41
1:F:109:TYR:CE2	1:F:158:GLU:HB2	2.55	0.41
1:C:29:ASP:HB2	1:D:235:ILE:HB	2.02	0.41
1:H:122:LEU:O	1:H:126:PRO:HB3	2.21	0.41
1:G:281:SER:O	1:G:282:HIS:HB2	2.20	0.41
1:A:202:ASN:HB2	1:A:207:THR:O	2.20	0.41
1:B:369:LYS:HB2	1:B:369:LYS:HE3	1.81	0.41
1:E:347:TRP:HA	1:E:347:TRP:CE3	2.56	0.41
1:H:120:LYS:HE3	1:H:132:PHE:CE2	2.56	0.41
1:H:194:LEU:HD13	1:H:196:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:ILE:HB	1:D:142:ARG:HD3	2.01	0.41
1:D:132:PHE:CD2	1:D:132:PHE:N	2.88	0.41
1:H:366:GLU:O	1:H:368:ASN:O	2.38	0.41
1:H:281:SER:OG	1:H:282:HIS:N	2.51	0.41
1:C:290:ARG:HH11	1:C:290:ARG:HG2	1.85	0.41
1:G:235:ILE:HG13	1:H:31:LEU:HB2	2.03	0.41
1:B:303:ILE:HG23	1:B:364:ARG:HD3	2.03	0.41
1:F:59:ILE:HD13	1:F:243:HIS:CE1	2.56	0.41
1:E:86:GLU:OE2	1:E:319:ILE:HD13	2.21	0.41
1:C:111:GLU:CB	1:C:121:GLY:HA2	2.48	0.41
1:F:212:VAL:HG22	1:F:269:LEU:HD23	2.01	0.41
1:F:247:ILE:HD13	1:F:314:MET:HE3	2.02	0.41
1:F:41:ILE:HB	1:F:142:ARG:HD3	2.01	0.41
1:B:330:GLY:O	1:B:332:ALA:N	2.49	0.41
1:D:193:GLY:HA3	1:D:238:THR:HG22	2.03	0.41
1:G:164:SER:N	1:G:165:PRO:CD	2.84	0.41
1:G:348:GLU:N	1:G:348:GLU:CD	2.74	0.41
1:H:94:LEU:HD11	1:H:351:GLU:HG3	2.03	0.41
1:G:299:VAL:O	1:G:302:GLN:N	2.49	0.41
1:E:89:LEU:HD13	1:E:89:LEU:HA	1.92	0.41
1:B:41:ILE:HB	1:B:142:ARG:HD3	2.03	0.41
1:F:142:ARG:O	1:F:146:VAL:HG23	2.20	0.41
1:G:193:GLY:HA3	1:G:238:THR:HG22	2.03	0.41
1:B:135:ASN:O	1:B:139:GLN:HG3	2.20	0.41
1:G:280:TYR:CD1	1:G:295:VAL:CG1	3.03	0.41
1:G:292:GLN:HB2	1:G:293:PRO:HD3	2.02	0.41
1:G:269:LEU:HD22	1:G:273:SER:OG	2.21	0.41
1:B:242:GLU:HG2	1:B:243:HIS:CD2	2.56	0.41
1:C:341:THR:O	1:C:342:ASP:C	2.57	0.41
1:D:174:PHE:CE1	1:D:245:PHE:HZ	2.38	0.41
1:F:281:SER:HA	1:F:285:SER:OG	2.20	0.41
1:H:193:GLY:HA3	1:H:238:THR:HG22	2.02	0.41
1:D:124:ASN:O	1:D:132:PHE:HA	2.20	0.41
1:G:34:PRO:O	1:G:38:GLN:HG3	2.20	0.41
1:G:69:VAL:HG13	1:G:312:GLY:HA2	2.02	0.41
1:H:73:VAL:HG23	1:H:315:ILE:HB	2.02	0.41
1:A:112:LYS:HE3	1:A:112:LYS:HB3	1.91	0.41
1:C:323:ASN:O	1:C:323:ASN:CG	2.59	0.41
1:G:112:LYS:HG3	1:G:113:PRO:CD	2.47	0.41
1:B:248:LEU:HD12	1:B:278:ILE:CD1	2.51	0.41
1:A:303:ILE:HG23	1:A:364:ARG:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:TYR:CE2	1:C:158:GLU:HB2	2.56	0.41
1:G:279:ASP:HA	1:G:314:MET:HB3	2.03	0.41
1:F:174:PHE:CE1	1:F:245:PHE:HZ	2.38	0.41
1:A:174:PHE:CE1	1:A:245:PHE:HZ	2.39	0.41
1:D:352:ASP:O	1:D:353:VAL:C	2.57	0.41
1:G:127:ASP:O	1:G:128:VAL:HB	2.21	0.41
1:E:135:ASN:O	1:E:139:GLN:HG3	2.21	0.41
1:F:164:SER:N	1:F:165:PRO:CD	2.84	0.41
1:D:202:ASN:HB2	1:D:207:THR:O	2.21	0.41
1:G:183:GLU:HB3	1:H:180:ARG:HB3	2.03	0.41
1:H:61:ILE:HD11	1:H:103:SER:HB2	2.03	0.41
1:F:249:ARG:HA	1:F:284:ASN:ND2	2.35	0.41
1:A:142:ARG:O	1:A:146:VAL:HG23	2.21	0.41
1:C:193:GLY:HA3	1:C:238:THR:CG2	2.50	0.41
1:E:50:THR:OG1	1:E:152:GLY:HA2	2.21	0.41
1:D:134:ILE:HD12	1:D:134:ILE:H	1.86	0.41
1:H:128:VAL:O	1:H:129:ASN:HB3	2.21	0.41
1:H:262:VAL:O	1:H:265:ALA:HB3	2.21	0.40
1:A:111:GLU:HG3	1:A:112:LYS:N	2.36	0.40
1:G:319:ILE:CD1	1:G:336:TYR:HE1	2.34	0.40
1:G:174:PHE:HE1	1:G:245:PHE:HZ	1.68	0.40
1:B:194:LEU:HD13	1:B:196:PHE:CE1	2.56	0.40
1:F:192:SER:O	1:F:238:THR:HB	2.20	0.40
1:B:193:GLY:HA3	1:B:238:THR:HG22	2.02	0.40
1:B:275:GLY:HA3	1:B:311:THR:OG1	2.21	0.40
1:B:202:ASN:HB2	1:B:207:THR:O	2.21	0.40
1:C:277:MET:HA	1:C:312:GLY:O	2.20	0.40
1:H:94:LEU:HD11	1:H:351:GLU:HA	2.03	0.40
1:A:257:TYR:CG	1:A:295:VAL:HG13	2.56	0.40
1:C:202:ASN:HB2	1:C:207:THR:O	2.21	0.40
1:C:79:HIS:NE2	1:C:334:LEU:HD23	2.36	0.40
1:A:353:VAL:O	1:A:357:LEU:HB2	2.21	0.40
1:E:216:GLN:NE2	1:E:270:PRO:HG2	2.36	0.40
1:D:292:GLN:HB2	1:D:293:PRO:HD3	2.03	0.40
1:G:34:PRO:HD2	1:G:229:LYS:O	2.22	0.40
1:D:134:ILE:CD1	1:D:134:ILE:H	2.34	0.40
1:B:352:ASP:O	1:B:354:LEU:N	2.54	0.40
1:A:50:THR:OG1	1:A:152:GLY:HA2	2.21	0.40
1:B:287:LYS:O	1:B:288:ASP:HB2	2.20	0.40
1:G:73:VAL:HA	1:G:315:ILE:O	2.21	0.40
1:A:114:ARG:NE	1:A:120:LYS:HE3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:262:VAL:HG21	1:D:310:ILE:HD11	2.03	0.40
1:B:232:VAL:HG21	1:C:232:VAL:CG2	2.50	0.40
1:C:249:ARG:O	1:C:283:GLY:CA	2.69	0.40
1:H:34:PRO:HD2	1:H:229:LYS:O	2.21	0.40
1:C:164:SER:N	1:C:165:PRO:CD	2.85	0.40
1:B:160:LEU:CD2	1:B:160:LEU:H	2.29	0.40
1:H:323:ASN:HB3	1:H:343:ALA:HA	2.02	0.40
1:D:97:GLU:OE1	1:D:355:ARG:NH1	2.41	0.40
1:D:89:LEU:HD13	1:D:89:LEU:HA	1.93	0.40
1:D:142:ARG:O	1:D:146:VAL:HG23	2.22	0.40
1:G:301:GLU:HG2	1:G:301:GLU:O	2.21	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	346/370 (94%)	298 (86%)	41 (12%)	7 (2%)	9 24
1	B	340/370 (92%)	296 (87%)	35 (10%)	9 (3%)	7 16
1	C	345/370 (93%)	302 (88%)	35 (10%)	8 (2%)	8 20
1	D	347/370 (94%)	299 (86%)	38 (11%)	10 (3%)	6 14
1	E	333/370 (90%)	294 (88%)	35 (10%)	4 (1%)	16 39
1	F	341/370 (92%)	307 (90%)	32 (9%)	2 (1%)	30 59
1	G	336/370 (91%)	287 (85%)	38 (11%)	11 (3%)	5 11
1	H	343/370 (93%)	298 (87%)	34 (10%)	11 (3%)	5 12
All	All	2731/2960 (92%)	2381 (87%)	288 (10%)	62 (2%)	8 20

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	GLU
1	B	22	ASP
1	B	286	ASN
1	B	324	GLN
1	C	323	ASN
1	E	129	ASN
1	G	334	LEU
1	H	129	ASN
1	H	327	PRO
1	A	253	LYS
1	A	330	GLY
1	A	364	ARG
1	B	130	ASN
1	B	331	LYS
1	C	283	GLY
1	C	336	TYR
1	D	331	LYS
1	E	336	TYR
1	F	334	LEU
1	G	271	ALA
1	G	286	ASN
1	H	253	LYS
1	H	274	ASN
1	H	323	ASN
1	A	332	ALA
1	B	353	VAL
1	C	133	ASN
1	D	286	ASN
1	D	305	ASN
1	D	353	VAL
1	E	133	ASN
1	F	113	PRO
1	G	119	TRP
1	G	133	ASN
1	G	266	LYS
1	G	360	ALA
1	H	113	PRO
1	B	256	ASN
1	C	113	PRO
1	C	119	TRP
1	C	128	VAL
1	C	341	THR
1	D	133	ASN

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Mol	Chain	Res	Type
1	H	101	ASP
1	H	117	VAL
1	A	22	ASP
1	A	281	SER
1	D	352	ASP
1	D	367	VAL
1	G	287	LYS
1	B	367	VAL
1	E	128	VAL
1	G	126	PRO
1	G	128	VAL
1	G	134	ILE
1	D	112	LYS
1	H	118	GLY
1	B	113	PRO
1	D	113	PRO
1	H	128	VAL
1	H	275	GLY
1	D	275	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	280/298 (94%)	260 (93%)	20 (7%)	18	41
1	B	279/298 (94%)	267 (96%)	12 (4%)	35	66
1	C	280/298 (94%)	264 (94%)	16 (6%)	25	53
1	D	277/298 (93%)	266 (96%)	11 (4%)	38	69
1	E	275/298 (92%)	258 (94%)	17 (6%)	23	49
1	F	277/298 (93%)	258 (93%)	19 (7%)	19	43
1	G	274/298 (92%)	255 (93%)	19 (7%)	19	43
1	H	276/298 (93%)	266 (96%)	10 (4%)	42	73
All	All	2218/2384 (93%)	2094 (94%)	124 (6%)	26	54

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ASP
1	A	37	LEU
1	A	107	ARG
1	A	112	LYS
1	A	114	ARG
1	A	120	LYS
1	A	124	ASN
1	A	129	ASN
1	A	131	THR
1	A	160	LEU
1	A	168	LEU
1	A	180	ARG
1	A	242	GLU
1	A	249	ARG
1	A	294	LYS
1	A	300	CYS
1	A	344	CYS
1	A	348	GLU
1	A	349	THR
1	A	357	LEU
1	B	37	LEU
1	B	101	ASP
1	B	110	LEU
1	B	112	LYS
1	B	130	ASN
1	B	160	LEU
1	B	168	LEU
1	B	242	GLU
1	B	249	ARG
1	B	261	SER
1	B	301	GLU
1	B	341	THR
1	C	21	GLU
1	C	37	LEU
1	C	99	LYS
1	C	111	GLU
1	C	160	LEU
1	C	168	LEU
1	C	242	GLU
1	C	249	ARG
1	C	257	TYR
1	C	264	GLU

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Mol	Chain	Res	Type
1	C	277	MET
1	C	318	ASN
1	C	341	THR
1	C	348	GLU
1	C	350	THR
1	C	369	LYS
1	D	37	LEU
1	D	110	LEU
1	D	160	LEU
1	D	168	LEU
1	D	242	GLU
1	D	249	ARG
1	D	264	GLU
1	D	266	LYS
1	D	301	GLU
1	D	318	ASN
1	D	341	THR
1	E	37	LEU
1	E	111	GLU
1	E	127	ASP
1	E	129	ASN
1	E	160	LEU
1	E	168	LEU
1	E	223	HIS
1	E	242	GLU
1	E	249	ARG
1	E	252	LYS
1	E	285	SER
1	E	286	ASN
1	E	300	CYS
1	E	318	ASN
1	E	341	THR
1	E	349	THR
1	E	352	ASP
1	F	37	LEU
1	F	99	LYS
1	F	101	ASP
1	F	110	LEU
1	F	120	LYS
1	F	125	ASP
1	F	129	ASN
1	F	160	LEU

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Mol	Chain	Res	Type
1	F	168	LEU
1	F	223	HIS
1	F	242	GLU
1	F	249	ARG
1	F	261	SER
1	F	287	LYS
1	F	339	SER
1	F	344	CYS
1	F	350	THR
1	F	357	LEU
1	F	363	GLN
1	G	37	LEU
1	G	96	ASP
1	G	102	LEU
1	G	110	LEU
1	G	111	GLU
1	G	129	ASN
1	G	160	LEU
1	G	168	LEU
1	G	242	GLU
1	G	249	ARG
1	G	257	TYR
1	G	289	PHE
1	G	291	ASN
1	G	317	SER
1	G	318	ASN
1	G	324	GLN
1	G	347	TRP
1	G	353	VAL
1	G	355	ARG
1	H	37	LEU
1	H	113	PRO
1	H	114	ARG
1	H	116	THR
1	H	127	ASP
1	H	160	LEU
1	H	168	LEU
1	H	242	GLU
1	H	249	ARG
1	H	294	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	ASN
1	A	143	GLN
1	A	147	ASN
1	A	216	GLN
1	A	243	HIS
1	A	324	GLN
1	B	133	ASN
1	B	143	GLN
1	B	147	ASN
1	B	243	HIS
1	B	324	GLN
1	B	363	GLN
1	C	143	GLN
1	C	147	ASN
1	C	216	GLN
1	C	274	ASN
1	D	130	ASN
1	D	143	GLN
1	D	147	ASN
1	D	216	GLN
1	D	243	HIS
1	D	363	GLN
1	D	368	ASN
1	E	129	ASN
1	E	133	ASN
1	E	143	GLN
1	E	147	ASN
1	E	216	GLN
1	E	286	ASN
1	E	291	ASN
1	E	320	ASN
1	E	324	GLN
1	F	129	ASN
1	F	143	GLN
1	F	147	ASN
1	F	216	GLN
1	F	305	ASN
1	F	320	ASN
1	F	368	ASN
1	G	124	ASN
1	G	129	ASN
1	G	143	GLN
1	G	147	ASN

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Mol	Chain	Res	Type
1	G	216	GLN
1	G	243	HIS
1	G	268	GLN
1	G	286	ASN
1	G	291	ASN
1	G	292	GLN
1	G	320	ASN
1	G	324	GLN
1	H	143	GLN
1	H	147	ASN
1	H	216	GLN
1	H	243	HIS
1	H	305	ASN
1	H	308	ASN
1	H	318	ASN
1	H	363	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 8 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	$\#\|Z\|>2$
2	PHE	C	1002	-	9,12,12	0.43	0	9,15,15	0.27	0
2	PHE	D	1002	-	9,12,12	0.61	0	9,15,15	0.25	0
2	PHE	G	1002	-	9,12,12	0.44	0	9,15,15	0.29	0
2	PHE	H	1002	-	9,12,12	0.42	0	9,15,15	0.28	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PHE	C	1002	-	-	0/4/8/8	0/1/1/1
2	PHE	D	1002	-	-	0/4/8/8	0/1/1/1
2	PHE	G	1002	-	-	0/4/8/8	0/1/1/1
2	PHE	H	1002	-	-	0/4/8/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1002	PHE	1	0
2	H	1002	PHE	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.