



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:31 PM GMT

PDB ID : 1FZB  
Title : CRYSTAL STRUCTURE OF CROSSLINKED FRAGMENT D  
Authors : Spraggon, G.; Everse, S.J.; Doolittle, R.F.  
Deposited on : 1997-08-05  
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (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

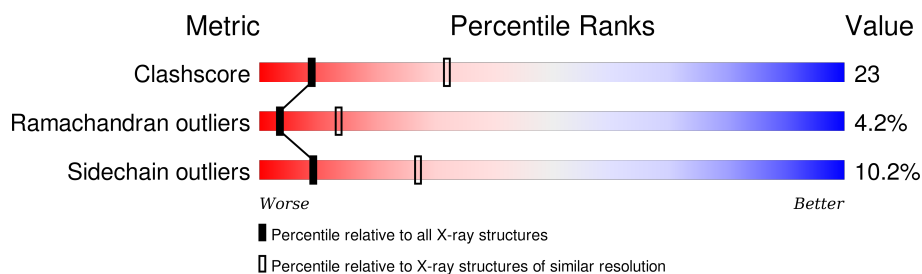
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)


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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	87	
1	D	87	
2	B	328	
2	E	328	
3	C	319	
3	F	319	
4	G	4	

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Mol	Chain	Length	Quality of chain
4	H	4	 A horizontal bar chart showing the quality of chain H. The bar is divided into three segments: green (25%), yellow (25%), and orange (50%). The segments are labeled with their respective percentages: 25%, 25%, and 50%.

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11417 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 FIBRINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	81	Total	C	N	O	S	0	0	0
			669	413	128	125	3			
1	D	81	Total	C	N	O	S	0	0	0
			669	413	128	125	3			

- Molecule 2 is a protein called FIBRINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	312	Total	C	N	O	S	0	0	0
			2508	1566	442	478	22			
2	E	312	Total	C	N	O	S	0	0	0
			2508	1566	442	478	22			

- Molecule 3 is a protein called FIBRINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	309	Total	C	N	O	S	0	0	0
			2480	1574	415	478	13			
3	F	311	Total	C	N	O	S	0	0	0
			2493	1581	418	481	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	88	LYS	ILE	CONFLICT	UNP P02679
F	88	LYS	ILE	CONFLICT	UNP P02679

- Molecule 4 is a protein called PEPTIDE LIGAND GPRG.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	4	Total	C	N	O	0	0	0
			30	18	7	5			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	4	Total	C	N	O	0	0	0
			30	18	7	5			

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

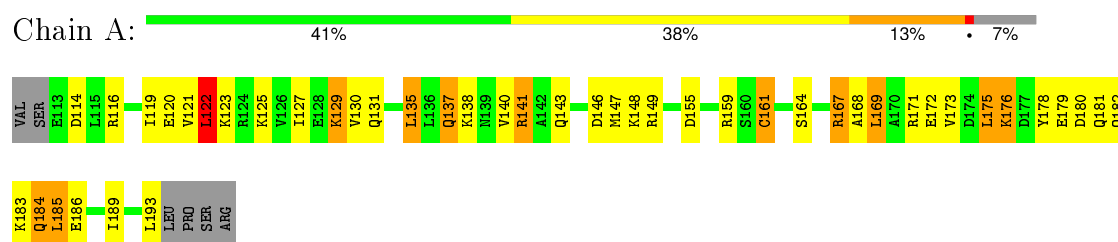
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Ca	0	0
			1	1		
6	F	1	Total	Ca	0	0
			1	1		

### 3 Residue-property plots [i](#)

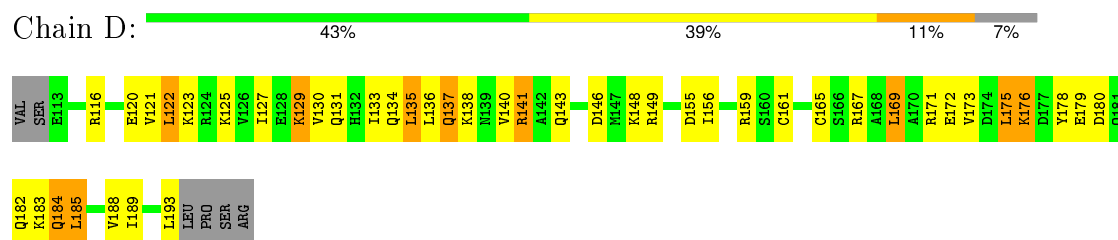
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

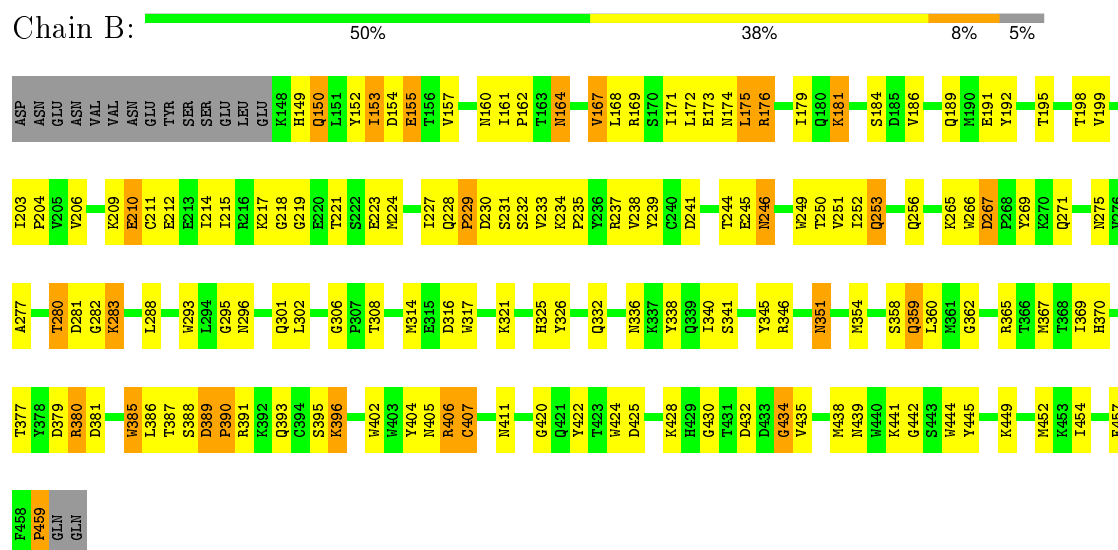
#### • Molecule 1: FIBRINOGEN



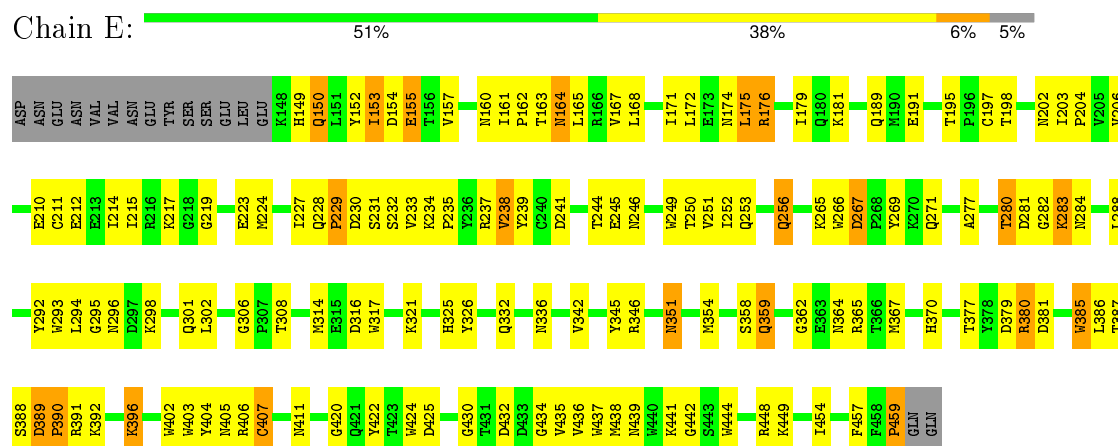
#### • Molecule 1: FIBRINOGEN



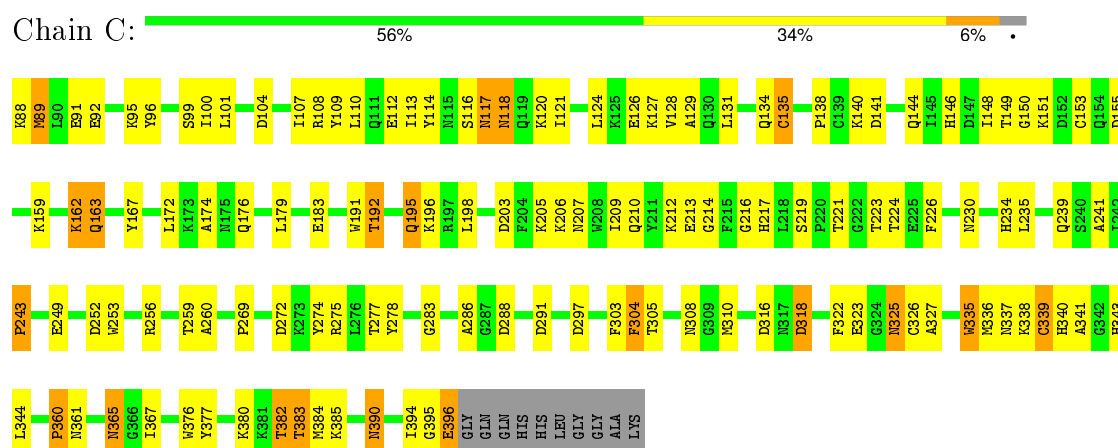
#### • Molecule 2: FIBRINOGEN



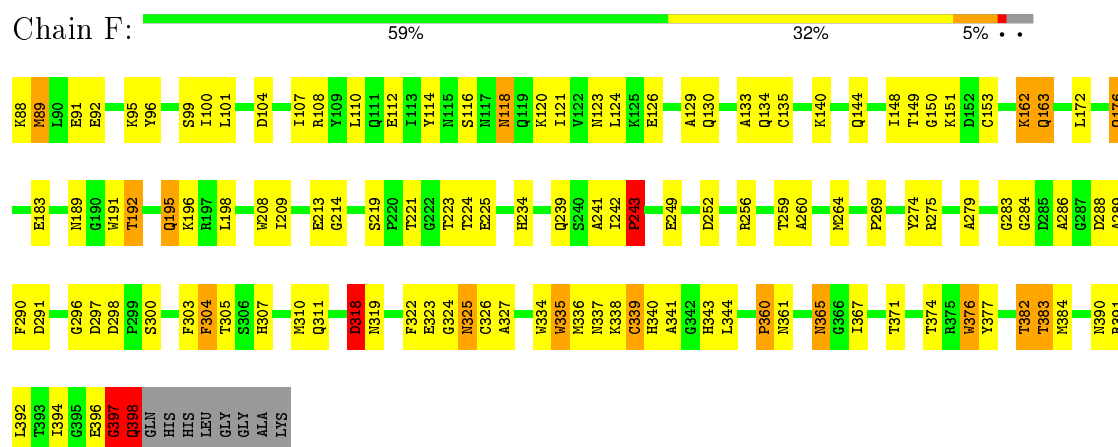
- Molecule 2: FIBRINOGEN



- Molecule 3: FIBRINOGEN



- Molecule 3: FIBRINOGEN



- Molecule 4: PEPTIDE LIGAND GPRG





● Molecule 4: PEPTIDE LIGAND GPRG

Chain H:  25% 25% 50%





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.82Å 95.50Å 113.76Å 90.00° 96.08° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90	Depositor
% Data completeness (in resolution range)	88.8 (30.00-2.90)	Depositor
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.241 , 0.318	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11417	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	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: CA, NAG

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	0.63	1/670 (0.1%)	0.70	1/892 (0.1%)
1	D	0.79	1/670 (0.1%)	0.73	1/892 (0.1%)
2	B	0.63	2/2572 (0.1%)	0.80	4/3475 (0.1%)
2	E	0.67	2/2572 (0.1%)	0.81	3/3475 (0.1%)
3	C	0.65	3/2546 (0.1%)	0.80	1/3440 (0.0%)
3	F	0.59	3/2559 (0.1%)	0.73	1/3457 (0.0%)
4	G	0.49	0/31	0.69	0/40
4	H	0.82	0/31	0.89	0/40
All	All	0.65	12/11651 (0.1%)	0.78	11/15711 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	459	PRO	C-O	17.70	1.58	1.23
1	D	193	LEU	C-O	16.14	1.54	1.23
2	B	459	PRO	C-O	15.17	1.53	1.23
3	C	396	GLU	C-O	-13.74	0.97	1.23
1	A	193	LEU	C-O	11.37	1.45	1.23
2	B	175	LEU	C-N	-9.65	1.11	1.34
3	C	396	GLU	CA-C	9.41	1.77	1.52
2	E	175	LEU	C-N	-9.12	1.13	1.34
3	F	398	GLN	CB-CG	-8.53	1.29	1.52
3	F	398	GLN	CA-CB	-7.59	1.37	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	397	GLY	C-N	-6.33	1.19	1.34
3	C	396	GLU	CD-OE2	5.10	1.31	1.25

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	396	GLU	CA-C-O	-20.43	77.20	120.10
2	E	459	PRO	CA-C-O	-11.70	92.13	120.20
2	B	459	PRO	CA-C-O	-9.82	96.64	120.20
1	D	193	LEU	CA-C-O	-8.89	101.43	120.10
3	F	398	GLN	N-CA-C	8.57	134.13	111.00
1	A	193	LEU	CA-C-O	-6.82	105.77	120.10
2	E	434	GLY	N-CA-C	5.90	127.84	113.10
2	E	175	LEU	O-C-N	5.71	131.83	122.70
2	B	434	GLY	N-CA-C	5.28	126.29	113.10
2	B	406	ARG	N-CA-C	-5.10	97.24	111.00
2	B	167	VAL	O-C-N	5.03	130.74	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	292	TYR	Sidechain

## 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	669	0	712	43	0
1	D	669	0	712	53	0
2	B	2508	0	2371	135	0
2	E	2508	0	2371	132	0
3	C	2480	0	2333	120	0
3	F	2493	0	2344	95	0
4	G	30	0	32	0	0
4	H	30	0	32	5	0
5	B	14	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	14	0	13	6	0
6	C	1	0	0	0	0
6	F	1	0	0	0	0
All	All	11417	0	10933	520	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 (520) 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)
3:C:396:GLU:CA	3:C:396:GLU:C	1.77	1.53
3:C:396:GLU:O	3:C:396:GLU:CA	1.82	1.22
2:E:389:ASP:HB3	2:E:390:PRO:HD2	1.38	1.05
2:B:389:ASP:HB3	2:B:390:PRO:HD2	1.37	1.02
3:C:209:ILE:H	3:C:209:ILE:HD12	1.25	0.98
2:E:380:ARG:HB2	2:E:380:ARG:HH11	1.28	0.98
2:B:380:ARG:HH11	2:B:380:ARG:HB2	1.31	0.96
3:F:209:ILE:HD12	3:F:209:ILE:H	1.29	0.96
2:E:351:ASN:HD21	2:E:354:MET:H	1.09	0.95
2:B:234:LYS:HD3	2:B:235:PRO:HD2	1.46	0.95
2:E:234:LYS:HD3	2:E:235:PRO:HD2	1.47	0.94
3:F:153:CYS:SG	3:F:192:THR:HB	2.07	0.94
1:D:176:LYS:H	1:D:176:LYS:HD2	1.32	0.94
2:E:351:ASN:ND2	2:E:354:MET:H	1.66	0.93
3:C:249:GLU:HB2	3:C:383:THR:HG23	1.53	0.91
1:A:176:LYS:HD2	1:A:176:LYS:H	1.33	0.91
3:F:310:MET:SD	3:F:337:ASN:HB2	2.11	0.90
3:F:322:PHE:HA	3:F:338:LYS:HD2	1.54	0.90
1:D:149:ARG:HH21	2:E:425:ASP:HA	1.35	0.89
3:F:397:GLY:O	3:F:398:GLN:HB2	1.71	0.89
3:C:322:PHE:HB2	3:C:338:LYS:HA	1.52	0.88
2:B:367:MET:HB3	2:B:406:ARG:HB3	1.54	0.88
3:F:322:PHE:HB2	3:F:338:LYS:HA	1.57	0.87
3:F:249:GLU:HB2	3:F:383:THR:HG23	1.55	0.87
2:B:351:ASN:ND2	2:B:354:MET:H	1.73	0.85
2:E:367:MET:HB3	2:E:406:ARG:HB3	1.56	0.85
3:C:322:PHE:HA	3:C:338:LYS:HD2	1.57	0.85
2:B:351:ASN:HD21	2:B:354:MET:H	1.22	0.84
5:E:1:NAG:H3	5:E:1:NAG:O7	1.77	0.83
2:E:359:GLN:H	2:E:359:GLN:HE21	1.26	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:LEU:H	2:E:189:GLN:HE22	1.26	0.83
3:C:310:MET:SD	3:C:337:ASN:HB2	2.19	0.82
2:B:198:THR:HG22	3:C:140:LYS:HB2	1.62	0.82
2:B:359:GLN:H	2:B:359:GLN:HE21	1.28	0.81
2:E:364:ASN:HD21	5:E:1:NAG:H5	1.46	0.79
3:F:151:LYS:HB3	3:F:239:GLN:HE22	1.47	0.79
1:A:169:LEU:H	2:B:189:GLN:HE22	1.29	0.79
3:C:151:LYS:HB3	3:C:239:GLN:HE22	1.46	0.78
3:C:209:ILE:H	3:C:209:ILE:CD1	1.96	0.78
3:F:397:GLY:O	3:F:398:GLN:CB	2.27	0.78
1:D:176:LYS:HD2	1:D:176:LYS:N	1.98	0.78
3:C:153:CYS:SG	3:C:192:THR:HB	2.24	0.78
1:A:176:LYS:N	1:A:176:LYS:HD2	1.99	0.77
2:B:359:GLN:H	2:B:359:GLN:NE2	1.82	0.77
1:D:125:LYS:HD3	3:F:100:ILE:HG12	1.64	0.77
1:D:140:VAL:HG12	2:E:172:LEU:HD13	1.66	0.77
1:D:127:ILE:O	1:D:131:GLN:HG2	1.84	0.77
1:D:123:LYS:NZ	2:E:154:ASP:HB2	2.00	0.77
3:F:100:ILE:HG13	3:F:101:LEU:HD22	1.68	0.76
1:D:141:ARG:HA	1:D:141:ARG:HH11	1.50	0.76
1:A:169:LEU:H	2:B:189:GLN:NE2	1.84	0.76
2:E:385:TRP:HE3	2:E:385:TRP:H	1.33	0.76
2:E:359:GLN:H	2:E:359:GLN:NE2	1.85	0.75
2:E:459:PRO:HG2	2:E:459:PRO:O	1.87	0.75
3:C:100:ILE:HG13	3:C:101:LEU:HD22	1.68	0.75
3:F:326:CYS:HB2	3:F:336:MET:HG3	1.69	0.74
3:C:326:CYS:HB2	3:C:336:MET:HG3	1.69	0.74
2:E:380:ARG:HH11	2:E:380:ARG:CB	2.00	0.74
1:A:141:ARG:HH11	1:A:141:ARG:HA	1.53	0.73
2:B:176:ARG:HG2	3:C:117:ASN:HD21	1.51	0.73
1:D:188:VAL:HG21	2:E:167:VAL:HG21	1.71	0.73
2:B:389:ASP:HB3	2:B:390:PRO:CD	2.17	0.73
1:D:133:ILE:HD12	2:E:165:LEU:HD11	1.70	0.72
2:B:396:LYS:HE3	2:B:396:LYS:HA	1.69	0.72
1:A:127:ILE:O	1:A:131:GLN:HG2	1.90	0.72
2:E:459:PRO:O	2:E:459:PRO:CG	2.38	0.72
1:D:140:VAL:HG23	1:D:185:LEU:HD11	1.73	0.71
1:D:135:LEU:HA	1:D:138:LYS:HE2	1.71	0.71
2:E:266:TRP:HA	2:E:377:THR:HG21	1.73	0.71
3:F:195:GLN:HG2	3:F:384:MET:SD	2.30	0.71
2:E:351:ASN:C	2:E:351:ASN:HD22	1.93	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:211:CYS:SG	2:E:250:THR:HA	2.30	0.70
2:B:212:GLU:O	2:B:215:ILE:HG22	1.91	0.70
2:B:385:TRP:HE3	2:B:385:TRP:H	1.39	0.70
2:B:176:ARG:CG	3:C:117:ASN:HD21	2.04	0.70
1:A:135:LEU:HA	1:A:138:LYS:HE2	1.72	0.70
2:B:380:ARG:HH11	2:B:380:ARG:CB	2.03	0.70
2:E:389:ASP:HB3	2:E:390:PRO:CD	2.19	0.69
2:B:266:TRP:HA	2:B:377:THR:HG21	1.74	0.69
2:E:396:LYS:HE3	2:E:396:LYS:HA	1.73	0.69
1:A:140:VAL:HG23	1:A:185:LEU:HD11	1.75	0.69
1:A:168:ALA:HA	2:B:189:GLN:HE22	1.56	0.69
2:B:269:TYR:O	2:B:295:GLY:HA2	1.93	0.69
3:F:209:ILE:H	3:F:209:ILE:CD1	2.02	0.69
2:B:157:VAL:HA	2:B:160:ASN:HB3	1.74	0.69
2:B:171:ILE:HG13	2:B:172:LEU:N	2.08	0.69
3:C:195:GLN:HG2	3:C:384:MET:SD	2.33	0.69
3:F:183:GLU:HB3	3:F:191:TRP:HB2	1.74	0.69
2:E:212:GLU:O	2:E:215:ILE:HG22	1.92	0.68
3:C:396:GLU:N	3:C:396:GLU:O	2.26	0.68
1:A:180:ASP:O	1:A:184:GLN:HG2	1.94	0.68
3:C:162:LYS:H	3:C:162:LYS:HD3	1.58	0.68
1:A:149:ARG:HH21	2:B:425:ASP:HA	1.58	0.68
1:D:135:LEU:O	1:D:138:LYS:HG2	1.94	0.68
2:E:210:GLU:OE1	2:E:212:GLU:HB3	1.93	0.68
1:D:149:ARG:NH2	2:E:425:ASP:HA	2.08	0.67
2:E:346:ARG:HG3	2:E:346:ARG:HH11	1.59	0.67
1:D:123:LYS:HZ2	2:E:154:ASP:HB2	1.60	0.67
2:E:386:LEU:H	2:E:386:LEU:HD23	1.58	0.66
3:C:221:THR:O	3:C:223:THR:HG23	1.95	0.66
3:F:305:THR:HB	3:F:341:ALA:HB2	1.77	0.66
2:B:210:GLU:OE1	2:B:212:GLU:HB3	1.95	0.66
2:B:351:ASN:C	2:B:351:ASN:HD22	1.98	0.66
1:A:135:LEU:O	1:A:138:LYS:HG2	1.96	0.66
2:E:405:ASN:C	2:E:407:CYS:H	1.99	0.66
3:C:395:GLY:O	3:C:396:GLU:HG3	1.96	0.66
2:B:211:CYS:SG	2:B:250:THR:HA	2.36	0.65
1:D:169:LEU:H	2:E:189:GLN:NE2	1.94	0.65
2:B:405:ASN:C	2:B:407:CYS:H	1.98	0.65
3:C:305:THR:HB	3:C:341:ALA:HB2	1.78	0.64
1:D:143:GLN:HG2	2:E:175:LEU:CD1	2.27	0.64
3:C:326:CYS:SG	3:C:339:CYS:N	2.71	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:385:TRP:N	2:E:385:TRP:HE3	1.96	0.64
2:E:171:ILE:HG13	2:E:172:LEU:N	2.13	0.63
3:F:339:CYS:HB2	4:H:1:GLY:O	1.98	0.63
1:D:180:ASP:O	1:D:184:GLN:HG2	1.97	0.63
3:F:162:LYS:H	3:F:162:LYS:HD3	1.63	0.63
2:E:230:ASP:O	2:E:233:VAL:HG22	1.99	0.63
3:F:95:LYS:HZ2	3:F:96:TYR:HE1	1.47	0.62
2:E:176:ARG:HG3	2:E:176:ARG:HH11	1.64	0.62
2:B:172:LEU:HG	3:C:113:ILE:CG2	2.28	0.62
2:B:386:LEU:H	2:B:386:LEU:HD23	1.64	0.62
2:B:346:ARG:HH11	2:B:346:ARG:HG3	1.65	0.62
2:B:169:ARG:HG3	3:C:110:LEU:HD21	1.82	0.62
2:E:176:ARG:HG3	2:E:176:ARG:NH1	2.16	0.61
5:E:1:NAG:C3	5:E:1:NAG:O7	2.47	0.61
1:D:123:LYS:HE3	2:E:152:TYR:HB3	1.82	0.61
3:C:344:LEU:HA	3:C:367:ILE:HG23	1.82	0.61
2:B:229:PRO:HD2	2:B:233:VAL:HG21	1.82	0.61
2:E:214:ILE:HD11	2:E:227:ILE:HG22	1.83	0.61
2:E:364:ASN:ND2	5:E:1:NAG:H5	2.13	0.61
2:B:164:ASN:HD22	2:B:164:ASN:C	2.04	0.61
3:C:104:ASP:HA	3:C:107:ILE:HD13	1.82	0.61
2:E:351:ASN:HD21	2:E:354:MET:N	1.92	0.61
2:B:172:LEU:O	3:C:113:ILE:HG21	2.00	0.60
3:F:172:LEU:HG	3:F:239:GLN:HE21	1.66	0.60
1:D:148:LYS:HE3	1:D:175:LEU:HB3	1.83	0.60
1:A:137:GLN:O	1:A:141:ARG:HB2	2.02	0.60
2:B:459:PRO:HG2	2:B:459:PRO:O	2.01	0.60
2:E:157:VAL:HA	2:E:160:ASN:HB3	1.82	0.60
2:E:326:TYR:CE2	2:E:345:TYR:HB2	2.37	0.60
3:C:252:ASP:HB2	3:C:377:TYR:OH	2.02	0.60
3:C:95:LYS:HZ2	3:C:96:TYR:HE1	1.50	0.59
1:A:148:LYS:HE3	1:A:175:LEU:HB3	1.84	0.59
3:C:209:ILE:N	3:C:209:ILE:HD12	2.07	0.59
1:D:169:LEU:HD12	1:D:171:ARG:CG	2.32	0.59
2:E:164:ASN:C	2:E:164:ASN:HD22	2.06	0.59
2:B:230:ASP:HB3	2:B:233:VAL:HG13	1.84	0.59
2:B:167:VAL:HG23	2:B:168:LEU:N	2.18	0.59
3:C:365:ASN:H	3:C:365:ASN:HD22	1.49	0.59
3:F:195:GLN:HG2	3:F:384:MET:CG	2.33	0.59
3:F:88:LYS:HB3	3:F:92:GLU:HB2	1.85	0.58
3:C:196:LYS:HE3	3:C:383:THR:HB	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:LEU:N	2:B:189:GLN:HE22	2.01	0.58
1:D:116:ARG:CZ	3:F:89:MET:HA	2.33	0.58
3:C:191:TRP:CE3	3:C:385:LYS:HG3	2.38	0.58
2:E:438:MET:HA	2:E:442:GLY:HA2	1.86	0.58
2:B:385:TRP:HE3	2:B:385:TRP:N	2.00	0.58
1:D:130:VAL:HG13	1:D:131:GLN:OE1	2.04	0.57
1:D:143:GLN:HG2	2:E:175:LEU:HD12	1.86	0.57
1:D:184:GLN:N	1:D:184:GLN:HE21	2.02	0.57
1:A:184:GLN:N	1:A:184:GLN:HE21	2.03	0.57
3:F:252:ASP:HB2	3:F:377:TYR:OH	2.04	0.57
3:C:151:LYS:HB3	3:C:239:GLN:NE2	2.18	0.57
2:B:267:ASP:O	2:B:271:GLN:HG2	2.03	0.57
3:C:395:GLY:O	3:C:396:GLU:CG	2.53	0.57
2:B:459:PRO:CG	2:B:459:PRO:O	2.53	0.57
2:E:385:TRP:N	2:E:385:TRP:CE3	2.73	0.56
2:B:161:ILE:HA	2:B:164:ASN:OD1	2.06	0.56
2:B:230:ASP:O	2:B:233:VAL:HG22	2.05	0.56
3:C:277:THR:HG21	3:F:303:PHE:CD2	2.41	0.56
2:E:167:VAL:HG23	2:E:168:LEU:N	2.20	0.56
1:A:179:GLU:HA	1:A:182:GLN:NE2	2.21	0.56
1:D:169:LEU:HD12	1:D:171:ARG:HG3	1.86	0.56
2:B:175:LEU:O	2:B:179:ILE:HG13	2.06	0.56
2:B:206:VAL:HG22	3:C:214:GLY:O	2.06	0.56
2:E:302:LEU:HD13	2:E:454:ILE:HD11	1.87	0.56
2:B:405:ASN:C	2:B:407:CYS:N	2.59	0.56
3:F:151:LYS:HB3	3:F:239:GLN:NE2	2.20	0.55
1:A:178:TYR:O	1:A:182:GLN:HG3	2.05	0.55
3:F:264:MET:HB2	3:F:279:ALA:HB2	1.88	0.55
2:B:154:ASP:O	2:B:157:VAL:HB	2.06	0.55
2:B:424:TRP:O	2:B:430:GLY:HA2	2.07	0.55
2:E:267:ASP:O	2:E:271:GLN:HG2	2.06	0.55
1:A:169:LEU:HD12	1:A:171:ARG:CG	2.36	0.55
3:F:149:THR:HG22	3:F:150:GLY:N	2.21	0.55
1:D:179:GLU:HA	1:D:182:GLN:HE21	1.72	0.55
3:C:274:TYR:O	3:C:335:TRP:HZ3	1.89	0.55
2:E:154:ASP:O	2:E:157:VAL:HB	2.07	0.55
2:B:179:ILE:HD13	3:C:120:LYS:HB2	1.89	0.55
1:A:169:LEU:HD12	1:A:171:ARG:HG3	1.89	0.55
2:B:199:VAL:O	3:C:141:ASP:HA	2.06	0.55
3:F:288:ASP:OD2	3:F:291:ASP:HB2	2.07	0.55
3:F:221:THR:O	3:F:223:THR:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:326:TYR:CE2	2:B:345:TYR:HB2	2.42	0.54
2:B:186:VAL:HG11	3:C:127:LYS:HG2	1.90	0.54
2:E:229:PRO:HD2	2:E:233:VAL:HG21	1.89	0.54
3:C:149:THR:HG22	3:C:150:GLY:N	2.23	0.54
3:C:390:ASN:O	3:C:394:ILE:HG23	2.08	0.54
2:B:157:VAL:HG13	2:B:161:ILE:HG12	1.89	0.54
1:D:178:TYR:O	1:D:182:GLN:HG3	2.08	0.54
1:A:122:LEU:HA	1:A:125:LYS:HD2	1.89	0.54
3:F:365:ASN:HD22	3:F:365:ASN:H	1.54	0.54
1:A:149:ARG:NH2	2:B:425:ASP:HA	2.21	0.54
1:D:123:LYS:HZ3	2:E:154:ASP:HB2	1.73	0.54
2:E:228:GLN:HB2	2:E:235:PRO:HB3	1.89	0.54
3:F:344:LEU:HA	3:F:367:ILE:HG23	1.90	0.53
2:E:230:ASP:HB3	2:E:233:VAL:HG13	1.89	0.53
3:C:344:LEU:HB3	3:C:382:THR:HG21	1.89	0.53
2:E:411:ASN:O	2:E:435:VAL:HA	2.08	0.53
1:D:137:GLN:O	1:D:141:ARG:HB2	2.09	0.53
1:D:165:CYS:O	2:E:197:CYS:HB3	2.08	0.53
3:C:196:LYS:CE	3:C:383:THR:HB	2.39	0.53
2:B:189:GLN:HG3	3:C:131:LEU:HD11	1.91	0.53
1:A:125:LYS:O	1:A:129:LYS:HG2	2.09	0.53
3:F:275:ARG:HA	3:F:311:GLN:HA	1.89	0.53
2:B:223:GLU:HA	2:B:239:TYR:CE1	2.44	0.53
1:D:125:LYS:O	1:D:129:LYS:HG2	2.09	0.53
2:E:405:ASN:C	2:E:407:CYS:N	2.62	0.53
3:C:365:ASN:N	3:C:365:ASN:HD22	2.05	0.53
2:E:239:TYR:HD2	2:E:251:VAL:HG21	1.74	0.53
2:E:294:LEU:O	2:E:298:LYS:HD2	2.08	0.53
3:C:195:GLN:HG2	3:C:384:MET:CG	2.39	0.53
1:D:179:GLU:HA	1:D:182:GLN:NE2	2.23	0.53
1:D:159:ARG:NH1	1:D:159:ARG:HB3	2.24	0.53
1:A:155:ASP:HB2	1:A:171:ARG:HH12	1.73	0.52
2:E:438:MET:HA	2:E:442:GLY:CA	2.39	0.52
3:F:288:ASP:CG	3:F:291:ASP:HB2	2.30	0.52
2:E:153:ILE:C	2:E:155:GLU:H	2.12	0.52
1:A:123:LYS:HE3	2:B:152:TYR:CD2	2.43	0.52
3:F:307:HIS:HD2	3:F:335:TRP:O	1.91	0.52
1:A:179:GLU:HA	1:A:182:GLN:HE21	1.74	0.52
3:F:123:ASN:O	3:F:126:GLU:HB2	2.09	0.52
2:B:153:ILE:C	2:B:155:GLU:H	2.13	0.52
2:B:234:LYS:HD3	2:B:235:PRO:CD	2.31	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:167:VAL:HG23	2:E:168:LEU:H	1.73	0.52
2:B:385:TRP:N	2:B:385:TRP:CE3	2.78	0.52
3:C:108:ARG:HD3	3:C:108:ARG:H	1.74	0.52
2:E:380:ARG:HB2	2:E:380:ARG:NH1	2.11	0.51
3:C:183:GLU:HB3	3:C:191:TRP:HB2	1.93	0.51
1:A:149:ARG:NH2	2:B:424:TRP:O	2.41	0.51
1:A:181:GLN:HE21	2:B:171:ILE:HG22	1.74	0.51
2:B:167:VAL:HG23	2:B:168:LEU:H	1.74	0.51
3:F:116:SER:O	3:F:120:LYS:HG2	2.09	0.51
2:B:314:MET:HA	2:B:449:LYS:O	2.10	0.51
3:C:88:LYS:HB3	3:C:92:GLU:HB2	1.93	0.51
2:E:314:MET:O	2:E:321:LYS:HG3	2.10	0.51
3:F:219:SER:OG	3:F:224:THR:HG22	2.11	0.51
3:C:304:PHE:O	3:C:337:ASN:O	2.28	0.51
2:B:173:GLU:HG2	3:C:113:ILE:CD1	2.41	0.51
3:C:114:TYR:O	3:C:118:ASN:HB2	2.11	0.51
2:B:317:TRP:CD1	2:B:420:GLY:HA3	2.46	0.51
2:B:157:VAL:HA	2:B:160:ASN:CB	2.41	0.50
3:C:234:HIS:CD2	3:C:269:PRO:HA	2.45	0.50
3:F:322:PHE:CD1	3:F:323:GLU:N	2.79	0.50
3:F:264:MET:HB2	3:F:279:ALA:CB	2.41	0.50
3:F:104:ASP:HA	3:F:107:ILE:HD13	1.93	0.50
2:E:245:GLU:O	2:E:246:ASN:HB2	2.11	0.50
2:B:237:ARG:HH11	2:B:237:ARG:HG3	1.75	0.50
3:C:340:HIS:ND1	3:C:343:HIS:HB2	2.26	0.50
3:C:395:GLY:C	3:C:396:GLU:HG3	2.31	0.50
2:E:234:LYS:HD3	2:E:235:PRO:CD	2.32	0.50
2:E:157:VAL:HG13	2:E:161:ILE:HG12	1.94	0.50
3:F:365:ASN:N	3:F:365:ASN:HD22	2.08	0.50
3:C:172:LEU:HG	3:C:239:GLN:HE21	1.76	0.50
2:E:175:LEU:O	2:E:179:ILE:HG13	2.12	0.50
2:E:314:MET:HA	2:E:449:LYS:O	2.12	0.50
2:B:169:ARG:HE	3:C:109:TYR:HE2	1.59	0.50
3:F:360:PRO:HG2	3:F:361:ASN:H	1.76	0.50
3:F:196:LYS:CE	3:F:383:THR:HB	2.42	0.50
3:C:259:THR:O	3:C:286:ALA:HB3	2.12	0.50
2:E:161:ILE:HA	2:E:164:ASN:OD1	2.12	0.50
1:D:143:GLN:HG2	2:E:175:LEU:HD13	1.92	0.50
2:E:245:GLU:C	2:E:246:ASN:HD22	2.15	0.50
2:B:438:MET:HA	2:B:442:GLY:HA2	1.94	0.49
2:E:237:ARG:HG3	2:E:237:ARG:HH11	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:241:ASP:HB3	2:B:249:TRP:HB2	1.94	0.49
1:D:122:LEU:HA	1:D:125:LYS:HD2	1.94	0.49
1:A:161:CYS:HA	3:C:135:CYS:CB	2.42	0.49
3:F:196:LYS:HE3	3:F:383:THR:HB	1.94	0.49
1:A:130:VAL:HG13	1:A:131:GLN:OE1	2.12	0.49
2:B:438:MET:HA	2:B:442:GLY:CA	2.42	0.49
3:C:167:TYR:O	3:C:179:LEU:HD12	2.12	0.49
2:B:314:MET:O	2:B:321:LYS:HG3	2.13	0.49
3:F:326:CYS:SG	3:F:339:CYS:N	2.86	0.49
2:B:402:TRP:HB3	2:B:404:TYR:CE2	2.48	0.49
2:E:277:ALA:HA	2:E:288:LEU:O	2.12	0.49
3:F:304:PHE:O	3:F:337:ASN:O	2.31	0.49
3:C:343:HIS:O	3:C:367:ILE:HA	2.12	0.48
3:C:116:SER:O	3:C:120:LYS:HG2	2.13	0.48
3:C:325:ASN:HD21	3:C:327:ALA:HB3	1.77	0.48
2:E:198:THR:HG22	3:F:140:LYS:HB2	1.95	0.48
3:F:374:THR:HG23	3:F:376:TRP:H	1.77	0.48
1:D:135:LEU:HD22	1:D:138:LYS:NZ	2.28	0.48
2:B:358:SER:HA	2:B:365:ARG:CZ	2.43	0.48
3:C:275:ARG:NH1	3:F:300:SER:HB3	2.28	0.48
2:E:358:SER:HA	2:E:365:ARG:CZ	2.43	0.48
1:D:155:ASP:HB2	1:D:171:ARG:HH12	1.78	0.48
3:F:274:TYR:O	3:F:335:TRP:HZ3	1.97	0.48
3:C:108:ARG:O	3:C:112:GLU:HG3	2.13	0.48
3:C:219:SER:OG	3:C:224:THR:HG22	2.13	0.48
2:B:275:ASN:OD1	3:C:138:PRO:HB2	2.13	0.48
2:E:351:ASN:C	2:E:351:ASN:ND2	2.65	0.48
2:B:346:ARG:NH1	2:B:346:ARG:HG3	2.28	0.48
3:C:335:TRP:N	3:C:335:TRP:CD1	2.78	0.48
3:C:146:HIS:HB2	3:C:167:TYR:CD2	2.49	0.48
2:E:370:HIS:CE1	2:E:402:TRP:HE1	2.31	0.48
3:F:307:HIS:CE1	3:F:341:ALA:H	2.31	0.48
3:C:322:PHE:CD1	3:C:323:GLU:N	2.81	0.48
3:C:322:PHE:CB	3:C:338:LYS:HA	2.35	0.48
2:E:325:HIS:O	2:E:345:TYR:HA	2.14	0.48
2:E:223:GLU:HA	2:E:239:TYR:CE1	2.49	0.48
2:B:209:LYS:HA	2:B:228:GLN:O	2.14	0.47
3:F:114:TYR:O	3:F:118:ASN:HB2	2.14	0.47
2:E:269:TYR:O	2:E:295:GLY:HA2	2.14	0.47
1:A:180:ASP:HA	1:A:183:LYS:HD2	1.97	0.47
2:B:325:HIS:O	2:B:345:TYR:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:252:ASP:OD2	3:C:256:ARG:HB2	2.14	0.47
2:E:172:LEU:HD23	3:F:110:LEU:HD22	1.95	0.47
2:B:161:ILE:HB	2:B:162:PRO:HD3	1.96	0.47
3:F:89:MET:C	3:F:91:GLU:H	2.16	0.47
2:B:179:ILE:HG21	3:C:120:LYS:HB3	1.96	0.47
2:E:206:VAL:HG22	3:F:214:GLY:O	2.15	0.47
2:E:306:GLY:O	2:E:308:THR:HG23	2.13	0.47
2:B:245:GLU:O	2:B:246:ASN:HB2	2.15	0.47
1:A:135:LEU:HD22	1:A:138:LYS:NZ	2.30	0.47
2:E:424:TRP:O	2:E:430:GLY:HA2	2.14	0.47
2:E:439:ASN:H	2:E:439:ASN:HD22	1.63	0.47
3:F:195:GLN:HG2	3:F:384:MET:HG3	1.96	0.47
3:C:288:ASP:CG	3:C:291:ASP:HB2	2.35	0.47
3:F:108:ARG:H	3:F:108:ARG:HD3	1.79	0.47
4:H:2:PRO:O	4:H:3:ARG:HB2	2.15	0.47
2:E:150:GLN:HB3	2:E:152:TYR:CE1	2.50	0.47
1:D:135:LEU:HD13	1:D:138:LYS:HE2	1.97	0.46
3:C:212:LYS:HG3	3:C:274:TYR:OH	2.15	0.46
2:E:317:TRP:CD1	2:E:420:GLY:HA3	2.50	0.46
1:D:180:ASP:HA	1:D:183:LYS:HD2	1.97	0.46
3:C:140:LYS:HE2	3:C:140:LYS:HB3	1.84	0.46
2:B:172:LEU:HG	3:C:113:ILE:HG21	1.96	0.46
2:B:150:GLN:HB3	2:B:152:TYR:CE1	2.50	0.46
2:E:436:VAL:CG1	2:E:437:TRP:N	2.79	0.46
3:C:155:ASP:O	3:C:159:LYS:HG2	2.15	0.46
1:A:159:ARG:NH1	1:A:159:ARG:HB3	2.31	0.46
2:E:316:ASP:HB3	2:E:441:LYS:HE3	1.97	0.46
3:C:195:GLN:OE1	3:C:382:THR:HG22	2.16	0.46
2:B:214:ILE:HD11	2:B:227:ILE:HG22	1.96	0.46
1:D:137:GLN:HB2	1:D:189:ILE:HG12	1.98	0.46
1:A:135:LEU:HD13	1:A:138:LYS:HE2	1.97	0.46
3:F:126:GLU:O	3:F:129:ALA:HB3	2.15	0.46
3:F:325:ASN:HD21	3:F:327:ALA:HB3	1.81	0.46
1:A:167:ARG:HB3	2:B:192:TYR:CG	2.50	0.46
2:B:215:ILE:HA	2:B:219:GLY:O	2.16	0.46
2:E:215:ILE:HA	2:E:219:GLY:O	2.16	0.46
3:C:325:ASN:HD22	3:C:325:ASN:C	2.20	0.46
1:D:120:GLU:C	1:D:122:LEU:H	2.19	0.46
2:B:168:LEU:HD23	3:C:110:LEU:HD13	1.98	0.46
1:A:120:GLU:C	1:A:122:LEU:H	2.20	0.46
1:A:147:MET:SD	3:C:121:ILE:HD11	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:124:LEU:O	3:C:128:VAL:HG13	2.16	0.45
2:B:316:ASP:HB3	2:B:441:LYS:HE3	1.98	0.45
2:E:293:TRP:HZ2	2:E:296:ASN:ND2	2.14	0.45
3:C:89:MET:C	3:C:91:GLU:H	2.19	0.45
2:B:245:GLU:C	2:B:246:ASN:HD22	2.19	0.45
2:B:246:ASN:HD22	2:B:246:ASN:N	2.14	0.45
3:C:259:THR:O	3:C:286:ALA:CB	2.64	0.45
2:B:277:ALA:HA	2:B:288:LEU:O	2.16	0.45
2:B:351:ASN:C	2:B:351:ASN:ND2	2.68	0.45
2:B:176:ARG:HG3	2:B:176:ARG:NH1	2.31	0.45
2:E:157:VAL:HA	2:E:160:ASN:CB	2.46	0.45
3:F:195:GLN:HE21	3:F:195:GLN:HB2	1.63	0.45
2:E:402:TRP:HB3	2:E:404:TYR:CE2	2.51	0.45
2:B:369:ILE:O	2:B:405:ASN:HB2	2.16	0.45
3:C:88:LYS:HA	3:C:91:GLU:OE1	2.16	0.45
2:B:332:GLN:HB3	2:B:336:ASN:HB2	1.99	0.45
2:E:161:ILE:O	2:E:165:LEU:HB2	2.17	0.45
1:D:156:ILE:O	1:D:159:ARG:HG2	2.16	0.45
2:B:395:SER:HB2	2:B:404:TYR:CE2	2.52	0.45
2:E:293:TRP:HZ2	2:E:296:ASN:HD21	1.63	0.45
3:F:343:HIS:O	3:F:367:ILE:HA	2.17	0.45
3:F:252:ASP:OD2	3:F:256:ARG:HB2	2.17	0.45
2:B:411:ASN:O	2:B:435:VAL:HA	2.16	0.45
5:B:1:NAG:O7	5:B:1:NAG:H3	2.17	0.45
2:B:228:GLN:HB2	2:B:235:PRO:HB3	1.98	0.45
2:E:346:ARG:HG3	2:E:346:ARG:NH1	2.26	0.44
3:F:344:LEU:HB3	3:F:382:THR:HG21	1.99	0.44
1:D:136:LEU:HB3	2:E:168:LEU:HD11	1.98	0.44
2:B:230:ASP:C	2:B:232:SER:H	2.21	0.44
3:F:208:TRP:HB3	3:F:209:ILE:HD12	2.00	0.44
1:A:149:ARG:HD3	2:B:428:LYS:O	2.18	0.44
3:F:234:HIS:CD2	3:F:269:PRO:HA	2.52	0.44
3:C:206:LYS:HA	3:C:206:LYS:HD3	1.84	0.44
2:E:280:THR:OG1	2:E:281:ASP:N	2.49	0.44
1:A:182:GLN:O	1:A:186:GLU:HG2	2.17	0.44
3:F:121:ILE:HA	3:F:124:LEU:HB3	1.99	0.44
2:B:293:TRP:HZ2	2:B:296:ASN:HD21	1.65	0.44
2:B:203:ILE:HA	2:B:204:PRO:HD3	1.78	0.44
3:F:310:MET:SD	3:F:337:ASN:CB	2.97	0.44
1:D:155:ASP:HA	1:D:171:ARG:NH1	2.33	0.44
1:D:140:VAL:HG21	2:E:171:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:207:ASN:HB2	3:C:316:ASP:OD2	2.17	0.44
2:B:239:TYR:HD2	2:B:251:VAL:HG21	1.83	0.44
2:E:364:ASN:HD21	5:E:1:NAG:H3	1.82	0.44
2:E:161:ILE:HB	2:E:162:PRO:HD3	1.99	0.44
3:F:340:HIS:N	4:H:1:GLY:O	2.46	0.44
2:B:293:TRP:HZ2	2:B:296:ASN:ND2	2.16	0.44
2:B:265:LYS:HB3	2:B:379:ASP:OD2	2.18	0.44
2:B:164:ASN:ND2	2:B:164:ASN:C	2.71	0.43
1:D:159:ARG:CB	1:D:159:ARG:HH11	2.31	0.43
2:B:280:THR:OG1	2:B:283:LYS:HB2	2.18	0.43
2:E:230:ASP:C	2:E:232:SER:H	2.22	0.43
3:C:239:GLN:C	3:C:241:ALA:H	2.20	0.43
3:F:108:ARG:O	3:F:112:GLU:HG3	2.18	0.43
2:E:238:VAL:HG23	2:E:294:LEU:HD11	2.01	0.43
2:B:380:ARG:NH1	2:B:380:ARG:HB2	2.15	0.43
1:D:185:LEU:HG	2:E:171:ILE:HD13	2.00	0.43
1:A:116:ARG:O	1:A:119:ILE:HG13	2.18	0.43
3:F:296:GLY:O	3:F:298:ASP:N	2.52	0.43
2:E:164:ASN:C	2:E:164:ASN:ND2	2.71	0.43
3:C:162:LYS:NZ	3:C:163:GLN:HB2	2.34	0.43
3:F:162:LYS:NZ	3:F:163:GLN:HB2	2.33	0.43
2:B:186:VAL:HG21	3:C:128:VAL:HG12	2.00	0.43
2:E:280:THR:OG1	2:E:283:LYS:HB2	2.18	0.43
2:E:364:ASN:HD21	5:E:1:NAG:C5	2.23	0.43
3:C:167:TYR:O	3:C:179:LEU:HA	2.18	0.43
2:B:218:GLY:HA3	3:C:210:GLN:HG2	2.01	0.43
3:F:259:THR:O	3:F:286:ALA:HB3	2.19	0.43
2:E:392:LYS:HZ2	2:E:406:ARG:NH1	2.16	0.43
4:H:1:GLY:H2	4:H:3:ARG:NH2	2.16	0.43
3:C:195:GLN:HG2	3:C:384:MET:HG3	2.00	0.43
3:C:303:PHE:O	3:C:305:THR:N	2.52	0.43
2:B:386:LEU:O	2:B:388:SER:N	2.46	0.43
2:B:316:ASP:HB2	2:B:445:TYR:OH	2.18	0.43
2:E:358:SER:HA	2:E:365:ARG:NH2	2.34	0.43
3:C:217:HIS:O	3:C:224:THR:HG23	2.19	0.43
2:B:340:ILE:HG12	2:B:341:SER:N	2.33	0.43
3:C:360:PRO:HG2	3:C:361:ASN:H	1.84	0.43
3:F:196:LYS:O	3:F:225:GLU:HB2	2.18	0.42
2:B:370:HIS:CE1	2:B:402:TRP:HE1	2.37	0.42
2:B:306:GLY:O	2:B:308:THR:HG23	2.20	0.42
3:F:307:HIS:HE1	3:F:341:ALA:H	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:386:LEU:O	2:E:388:SER:N	2.47	0.42
1:D:159:ARG:NH1	1:D:159:ARG:CB	2.82	0.42
2:B:181:LYS:O	2:B:184:SER:HB3	2.19	0.42
1:D:136:LEU:HD13	2:E:168:LEU:HD21	2.01	0.42
2:E:217:LYS:HB3	3:F:213:GLU:HG3	2.00	0.42
3:C:174:ALA:HB2	3:C:235:LEU:HD13	2.01	0.42
3:F:334:TRP:CH2	3:F:344:LEU:HB2	2.54	0.42
1:A:164:SER:HB2	3:C:135:CYS:HB3	2.01	0.42
2:E:203:ILE:HA	2:E:204:PRO:HD3	1.77	0.42
2:B:217:LYS:HB3	3:C:213:GLU:HG3	2.02	0.42
2:B:199:VAL:HG23	3:C:141:ASP:HA	2.01	0.42
3:C:288:ASP:OD2	3:C:291:ASP:HB2	2.20	0.42
3:F:189:ASN:CG	3:F:391:ARG:HH21	2.23	0.42
2:E:332:GLN:HB3	2:E:336:ASN:HB2	2.01	0.42
1:D:130:VAL:O	1:D:134:GLN:HG3	2.19	0.42
1:A:137:GLN:HB2	1:A:189:ILE:HG12	2.01	0.42
3:F:339:CYS:CB	4:H:1:GLY:O	2.67	0.42
3:C:303:PHE:C	3:C:305:THR:H	2.22	0.42
2:B:253:GLN:HB3	2:B:452:MET:HB2	2.02	0.42
3:C:310:MET:CG	3:C:337:ASN:HB2	2.49	0.42
2:E:317:TRP:HA	2:E:448:ARG:NH1	2.34	0.42
3:F:242:ILE:HG23	3:F:243:PRO:HD2	2.02	0.42
2:E:402:TRP:CG	2:E:403:TRP:N	2.87	0.41
3:F:259:THR:OG1	3:F:284:GLY:HA2	2.19	0.41
2:E:202:ASN:ND2	2:E:284:ASN:O	2.52	0.41
2:E:294:LEU:HG	2:E:298:LYS:HD2	2.01	0.41
3:C:146:HIS:HB2	3:C:167:TYR:CE2	2.55	0.41
2:B:359:GLN:NE2	2:B:359:GLN:N	2.60	0.41
3:F:340:HIS:ND1	3:F:343:HIS:HB2	2.36	0.41
3:F:176:GLN:O	3:F:176:GLN:HG2	2.20	0.41
2:E:163:THR:C	2:E:165:LEU:H	2.23	0.41
3:C:95:LYS:O	3:C:99:SER:HB2	2.20	0.41
2:B:280:THR:OG1	2:B:281:ASP:N	2.52	0.41
3:F:149:THR:CG2	3:F:150:GLY:N	2.82	0.41
3:F:140:LYS:HB3	3:F:140:LYS:HE2	1.86	0.41
2:B:176:ARG:HG3	2:B:176:ARG:HH11	1.85	0.41
3:F:290:PHE:HA	3:F:290:PHE:HD1	1.76	0.41
3:F:307:HIS:HA	3:F:310:MET:HG3	2.02	0.41
3:F:325:ASN:HD22	3:F:325:ASN:C	2.24	0.41
2:B:302:LEU:HD13	2:B:454:ILE:HD11	2.02	0.41
3:F:172:LEU:H	3:F:239:GLN:NE2	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:325:HIS:HB3	2:B:346:ARG:O	2.21	0.41
3:C:230:ASN:HB3	3:C:274:TYR:CG	2.55	0.41
3:C:272:ASP:OD1	3:C:275:ARG:NH1	2.54	0.41
3:F:130:GLN:O	3:F:133:ALA:HB3	2.20	0.41
2:E:422:TYR:CE1	2:E:444:TRP:HA	2.56	0.41
3:C:278:TYR:CE2	3:C:308:ASN:HB2	2.56	0.41
1:D:123:LYS:HA	1:D:123:LYS:HD3	1.87	0.41
2:B:167:VAL:CG2	2:B:168:LEU:N	2.84	0.41
3:F:88:LYS:HA	3:F:91:GLU:OE1	2.21	0.41
2:E:246:ASN:HD22	2:E:246:ASN:N	2.19	0.41
2:B:393:GLN:HB3	2:B:393:GLN:HE21	1.69	0.41
3:F:318:ASP:HB3	3:F:319:ASN:H	1.71	0.41
3:C:195:GLN:OE1	3:C:382:THR:CG2	2.68	0.41
2:E:256:GLN:HA	2:E:449:LYS:HG2	2.03	0.41
2:B:360:LEU:HD23	2:B:360:LEU:HA	1.86	0.41
2:B:396:LYS:HA	2:B:396:LYS:CE	2.44	0.40
2:E:325:HIS:HB3	2:E:346:ARG:O	2.21	0.40
2:B:296:ASN:HB3	2:B:338:TYR:CD1	2.56	0.40
2:B:422:TYR:CE1	2:B:444:TRP:HA	2.56	0.40
2:B:439:ASN:H	2:B:439:ASN:HD22	1.69	0.40
3:C:216:GLY:HA3	3:C:226:PHE:HA	2.03	0.40
2:B:389:ASP:CB	2:B:390:PRO:HD2	2.28	0.40
2:E:342:VAL:HG23	2:E:354:MET:HG2	2.03	0.40
3:F:239:GLN:C	3:F:241:ALA:H	2.25	0.40
3:F:95:LYS:O	3:F:99:SER:HB2	2.22	0.40
3:F:289:ALA:HA	3:F:371:THR:HG23	2.02	0.40
3:C:253:TRP:HA	3:C:380:LYS:HD2	2.04	0.40
2:E:266:TRP:CE3	2:E:380:ARG:HD2	2.56	0.40
3:C:310:MET:SD	3:C:337:ASN:CB	3.02	0.40
3:C:239:GLN:O	3:C:241:ALA:N	2.54	0.40
2:B:176:ARG:HG2	3:C:117:ASN:ND2	2.29	0.40
3:C:149:THR:CG2	3:C:150:GLY:N	2.84	0.40
1:A:119:ILE:O	1:A:122:LEU:HB3	2.22	0.40
3:C:126:GLU:O	3:C:129:ALA:HB3	2.21	0.40
2:E:367:MET:HG3	2:E:406:ARG:HD2	2.03	0.40
2:E:386:LEU:CD2	2:E:386:LEU:H	2.32	0.40
2:E:265:LYS:HB3	2:E:379:ASP:OD2	2.22	0.40
2:E:241:ASP:HB3	2:E:249:TRP:HB2	2.04	0.40
3:C:203:ASP:OD2	3:C:205:LYS:HB3	2.22	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	79/87 (91%)	72 (91%)	5 (6%)	2 (2%)	7	27
1	D	79/87 (91%)	72 (91%)	5 (6%)	2 (2%)	7	27
2	B	310/328 (94%)	263 (85%)	33 (11%)	14 (4%)	3	12
2	E	310/328 (94%)	258 (83%)	39 (13%)	13 (4%)	3	13
3	C	307/319 (96%)	264 (86%)	33 (11%)	10 (3%)	5	20
3	F	309/319 (97%)	257 (83%)	38 (12%)	14 (4%)	3	12
4	G	2/4 (50%)	0	0	2 (100%)	0	0
4	H	2/4 (50%)	0	0	2 (100%)	0	0
All	All	1398/1476 (95%)	1186 (85%)	153 (11%)	59 (4%)	3	13

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	149	HIS
2	B	280	THR
2	B	391	ARG
2	B	407	CYS
3	C	89	MET
3	C	318	ASP
2	E	149	HIS
2	E	280	THR
2	E	391	ARG
2	E	407	CYS
3	F	89	MET
3	F	318	ASP
3	F	339	CYS
1	A	122	LEU
2	B	231	SER
2	B	389	ASP
3	C	283	GLY

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Mol	Chain	Res	Type
3	C	304	PHE
3	C	339	CYS
1	D	122	LEU
2	E	362	GLY
2	E	389	ASP
3	F	283	GLY
3	F	297	ASP
3	F	304	PHE
4	H	2	PRO
2	B	256	GLN
2	B	362	GLY
2	B	387	THR
3	C	198	LEU
3	C	243	PRO
2	E	231	SER
2	E	256	GLN
2	E	387	THR
3	F	243	PRO
3	F	394	ILE
3	F	396	GLU
4	G	2	PRO
3	C	260	ALA
3	C	297	ASP
3	F	198	LEU
3	F	360	PRO
4	G	3	ARG
2	B	434	GLY
3	C	360	PRO
2	E	229	PRO
3	F	397	GLY
2	B	229	PRO
2	B	390	PRO
3	F	260	ALA
2	B	282	GLY
2	E	282	GLY
2	E	390	PRO
1	A	121	VAL
1	D	121	VAL
4	H	3	ARG
2	B	153	ILE
3	F	324	GLY
2	E	153	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	76/82 (93%)	59 (78%)	17 (22%)	1	3
1	D	76/82 (93%)	62 (82%)	14 (18%)	2	6
2	B	270/286 (94%)	243 (90%)	27 (10%)	9	28
2	E	270/286 (94%)	246 (91%)	24 (9%)	12	35
3	C	261/267 (98%)	241 (92%)	20 (8%)	16	42
3	F	262/267 (98%)	241 (92%)	21 (8%)	15	40
4	G	3/3 (100%)	2 (67%)	1 (33%)	0	1
4	H	3/3 (100%)	3 (100%)	0	100	100
All	All	1221/1276 (96%)	1097 (90%)	124 (10%)	9	27

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

Mol	Chain	Res	Type
1	A	114	ASP
1	A	122	LEU
1	A	129	LYS
1	A	135	LEU
1	A	137	GLN
1	A	141	ARG
1	A	143	GLN
1	A	146	ASP
1	A	161	CYS
1	A	167	ARG
1	A	169	LEU
1	A	172	GLU
1	A	173	VAL
1	A	175	LEU
1	A	176	LYS
1	A	184	GLN
1	A	185	LEU
2	B	150	GLN
2	B	155	GLU

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Mol	Chain	Res	Type
2	B	164	ASN
2	B	174	ASN
2	B	176	ARG
2	B	181	LYS
2	B	191	GLU
2	B	195	THR
2	B	210	GLU
2	B	221	THR
2	B	224	MET
2	B	238	VAL
2	B	244	THR
2	B	246	ASN
2	B	252	ILE
2	B	253	GLN
2	B	267	ASP
2	B	283	LYS
2	B	301	GLN
2	B	351	ASN
2	B	359	GLN
2	B	380	ARG
2	B	381	ASP
2	B	385	TRP
2	B	396	LYS
2	B	432	ASP
2	B	457	PHE
3	C	117	ASN
3	C	118	ASN
3	C	134	GLN
3	C	135	CYS
3	C	144	GLN
3	C	148	ILE
3	C	162	LYS
3	C	163	GLN
3	C	176	GLN
3	C	192	THR
3	C	195	GLN
3	C	243	PRO
3	C	318	ASP
3	C	325	ASN
3	C	335	TRP
3	C	365	ASN
3	C	376	TRP

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Mol	Chain	Res	Type
3	C	382	THR
3	C	383	THR
3	C	390	ASN
1	D	129	LYS
1	D	135	LEU
1	D	137	GLN
1	D	141	ARG
1	D	146	ASP
1	D	161	CYS
1	D	167	ARG
1	D	169	LEU
1	D	172	GLU
1	D	173	VAL
1	D	175	LEU
1	D	176	LYS
1	D	184	GLN
1	D	185	LEU
2	E	150	GLN
2	E	155	GLU
2	E	164	ASN
2	E	174	ASN
2	E	176	ARG
2	E	181	LYS
2	E	191	GLU
2	E	195	THR
2	E	224	MET
2	E	238	VAL
2	E	244	THR
2	E	252	ILE
2	E	253	GLN
2	E	267	ASP
2	E	283	LYS
2	E	301	GLN
2	E	351	ASN
2	E	359	GLN
2	E	380	ARG
2	E	381	ASP
2	E	385	TRP
2	E	396	LYS
2	E	432	ASP
2	E	457	PHE
3	F	118	ASN

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Mol	Chain	Res	Type
3	F	134	GLN
3	F	135	CYS
3	F	144	GLN
3	F	148	ILE
3	F	162	LYS
3	F	163	GLN
3	F	176	GLN
3	F	192	THR
3	F	195	GLN
3	F	243	PRO
3	F	318	ASP
3	F	325	ASN
3	F	335	TRP
3	F	365	ASN
3	F	376	TRP
3	F	382	THR
3	F	383	THR
3	F	390	ASN
3	F	392	LEU
3	F	398	GLN
4	G	3	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	GLN
1	A	181	GLN
1	A	182	GLN
1	A	184	GLN
2	B	158	ASN
2	B	189	GLN
2	B	228	GLN
2	B	246	ASN
2	B	253	GLN
2	B	256	GLN
2	B	296	ASN
2	B	301	GLN
2	B	325	HIS
2	B	332	GLN
2	B	351	ASN
2	B	359	GLN
2	B	393	GLN

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Mol	Chain	Res	Type
2	B	408	HIS
2	B	439	ASN
3	C	117	ASN
3	C	118	ASN
3	C	130	GLN
3	C	177	GLN
3	C	189	ASN
3	C	230	ASN
3	C	239	GLN
3	C	319	ASN
3	C	325	ASN
3	C	361	ASN
3	C	365	ASN
3	C	390	ASN
1	D	181	GLN
1	D	182	GLN
1	D	184	GLN
2	E	158	ASN
2	E	189	GLN
2	E	228	GLN
2	E	246	ASN
2	E	253	GLN
2	E	256	GLN
2	E	296	ASN
2	E	301	GLN
2	E	325	HIS
2	E	332	GLN
2	E	351	ASN
2	E	359	GLN
2	E	364	ASN
2	E	393	GLN
2	E	408	HIS
2	E	439	ASN
3	F	117	ASN
3	F	118	ASN
3	F	130	GLN
3	F	136	GLN
3	F	177	GLN
3	F	189	ASN
3	F	230	ASN
3	F	239	GLN
3	F	307	HIS

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Mol	Chain	Res	Type
3	F	311	GLN
3	F	325	ASN
3	F	361	ASN
3	F	365	ASN
3	F	390	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z  > 2$
5	NAG	B	1	-	14,14,15	0.43	0	15,19,21	0.73	0
5	NAG	E	1	-	14,14,15	0.49	0	15,19,21	0.64	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
5	NAG	B	1	-	-	0/6/23/26	0/1/1/1
5	NAG	E	1	-	-	0/6/23/26	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 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1	NAG	1	0
5	E	1	NAG	6	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.