



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 01:30 PM EDT

PDB ID : 1NKQ  
Title : Crystal structure of yeast ynf8, a fumarylacetoacetate hydrolase family protein  
Authors : Eswaramoorthy, S.; Kumaran, D.; Daniels, B.; Studier, F.W.; Swaminathan, S.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2003-01-03  
Resolution : 2.20 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

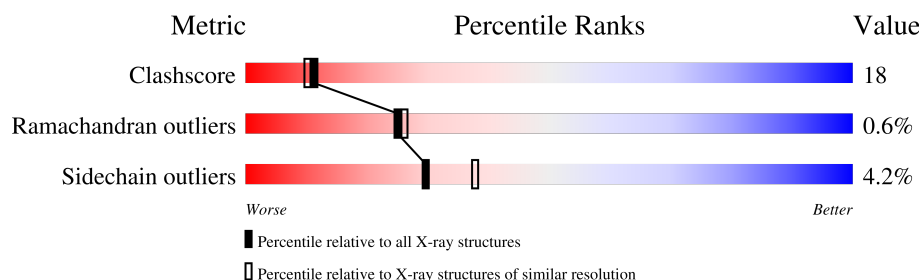
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	259	68% 25% • 5%
1	B	259	69% 23% • 6%
1	C	259	62% 30% • 5%
1	D	259	64% 27% • 6%
1	E	259	64% 29% • 5%
1	F	259	60% 29% • 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ACY	B	703	-	-	X	-
4	ACY	C	705	-	-	X	-
4	ACY	E	709	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12088 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 Hypothetical 28.8 kDa protein in PSD1-SKO1 intergenic region.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	Se	0	0	0
			1911	1214	328	360	4	5			
1	B	244	Total	C	N	O	S	Se	0	0	0
			1894	1204	326	355	4	5			
1	C	245	Total	C	N	O	S	Se	0	0	0
			1894	1204	324	357	4	5			
1	D	244	Total	C	N	O	S	Se	0	0	0
			1888	1201	323	355	4	5			
1	E	246	Total	C	N	O	S	Se	0	0	0
			1908	1212	330	357	4	5			
1	F	240	Total	C	N	O	S	Se	0	0	0
			1870	1187	325	349	4	5			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP P53889
A	104	MSE	MET	modified residue	UNP P53889
A	148	MSE	MET	modified residue	UNP P53889
A	189	MSE	MET	modified residue	UNP P53889
A	203	MSE	MET	modified residue	UNP P53889
A	243	MSE	MET	modified residue	UNP P53889
B	301	MSE	MET	modified residue	UNP P53889
B	404	MSE	MET	modified residue	UNP P53889
B	448	MSE	MET	modified residue	UNP P53889
B	489	MSE	MET	modified residue	UNP P53889
B	503	MSE	MET	modified residue	UNP P53889
B	543	MSE	MET	modified residue	UNP P53889
C	1	MSE	MET	modified residue	UNP P53889
C	104	MSE	MET	modified residue	UNP P53889
C	148	MSE	MET	modified residue	UNP P53889
C	189	MSE	MET	modified residue	UNP P53889
C	203	MSE	MET	modified residue	UNP P53889

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Chain	Residue	Modelled	Actual	Comment	Reference
C	243	MSE	MET	modified residue	UNP P53889
D	301	MSE	MET	modified residue	UNP P53889
D	404	MSE	MET	modified residue	UNP P53889
D	448	MSE	MET	modified residue	UNP P53889
D	489	MSE	MET	modified residue	UNP P53889
D	503	MSE	MET	modified residue	UNP P53889
D	543	MSE	MET	modified residue	UNP P53889
E	1	MSE	MET	modified residue	UNP P53889
E	104	MSE	MET	modified residue	UNP P53889
E	148	MSE	MET	modified residue	UNP P53889
E	189	MSE	MET	modified residue	UNP P53889
E	203	MSE	MET	modified residue	UNP P53889
E	243	MSE	MET	modified residue	UNP P53889
F	301	MSE	MET	modified residue	UNP P53889
F	404	MSE	MET	modified residue	UNP P53889
F	448	MSE	MET	modified residue	UNP P53889
F	489	MSE	MET	modified residue	UNP P53889
F	503	MSE	MET	modified residue	UNP P53889
F	543	MSE	MET	modified residue	UNP P53889

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0
2	F	1	Total Ca 1 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	112	Total 112	O 112	0	0
5	B	106	Total 106	O 106	0	0
5	C	99	Total 99	O 99	0	0
5	D	122	Total 122	O 122	0	0
5	E	107	Total 107	O 107	0	0
5	F	88	Total 88	O 88	0	0

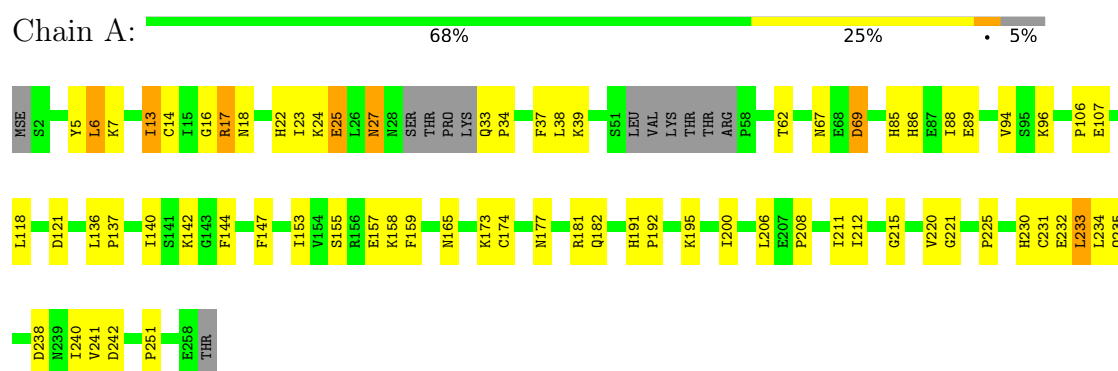


### 3 Residue-property plots [i](#)

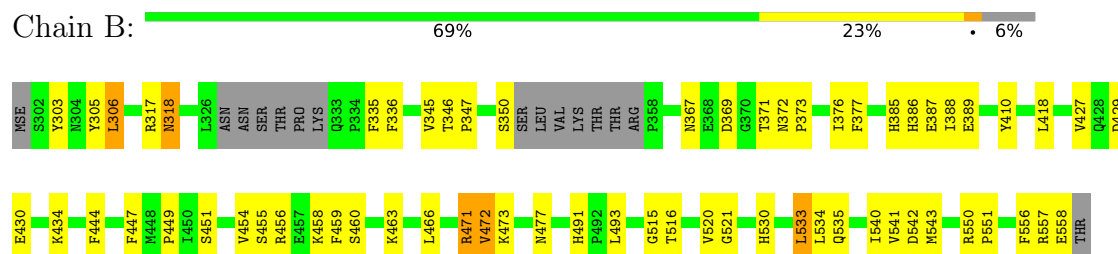
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

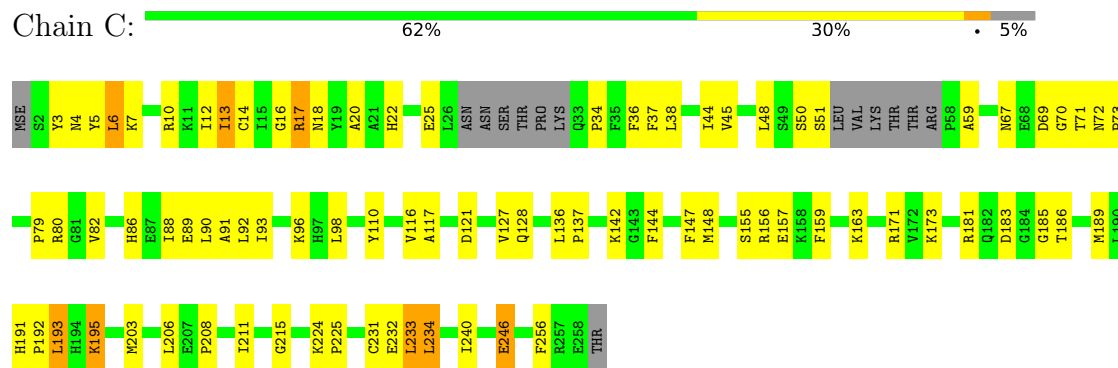
- Molecule 1: Hypothetical 28.8 kDa protein in PSD1-SKO1 intergenic region



- Molecule 1: Hypothetical 28.8 kDa protein in PSD1-SKO1 intergenic region

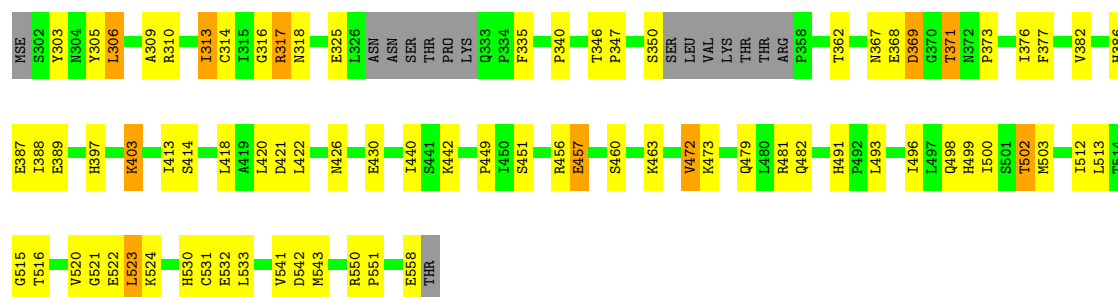


- Molecule 1: Hypothetical 28.8 kDa protein in PSD1-SKO1 intergenic region



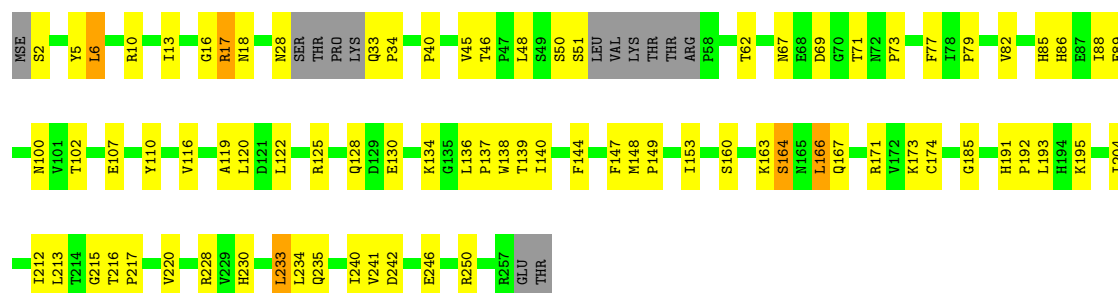
- Molecule 1: Hypothetical 28.8 kDa protein in PSD1-SKO1 intergenic region

Chain D:  64% 27% 6%



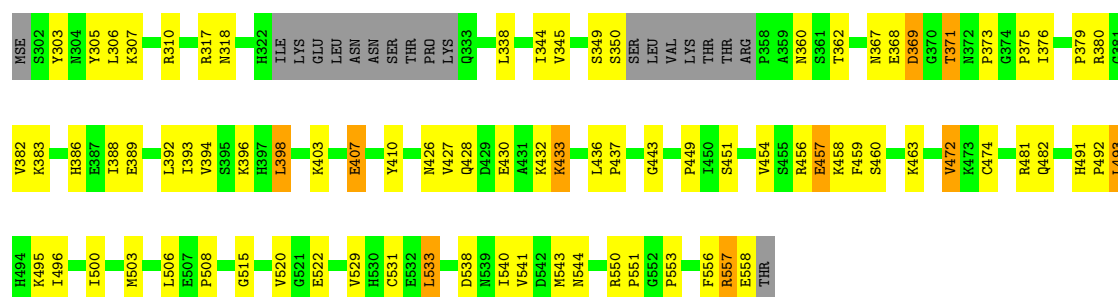
• Molecule 1: Hypothetical 28.8 kDa protein in PSD1-SKO1 intergenic region

Chain E:  64% 29% 5%



• Molecule 1: Hypothetical 28.8 kDa protein in PSD1-SKO1 intergenic region

Chain F:  60% 29% 7%



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.70Å 85.99Å 316.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-2.20)	Depositor
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.216 , 0.262	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12088	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ACY, SO4

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	0.35	0/1946	0.65	0/2625
1	B	0.35	0/1929	0.65	0/2602
1	C	0.34	0/1929	0.64	0/2603
1	D	0.36	0/1923	0.66	0/2595
1	E	0.35	0/1943	0.64	0/2620
1	F	0.41	0/1905	0.67	0/2568
All	All	0.36	0/11575	0.65	0/15613

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1911	0	1905	68	0
1	B	1894	0	1892	52	0
1	C	1894	0	1886	79	0
1	D	1888	0	1881	64	0
1	E	1908	0	1910	80	0
1	F	1870	0	1873	90	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	10	0	0	1	0
3	B	15	0	0	0	0
3	C	5	0	0	0	0
3	E	5	0	0	1	0
4	A	8	0	6	1	0
4	B	8	0	6	2	0
4	C	8	0	6	3	0
4	D	8	0	6	1	0
4	E	8	0	6	3	0
4	F	8	0	6	1	0
5	A	112	0	0	4	0
5	B	106	0	0	2	0
5	C	99	0	0	5	0
5	D	122	0	0	3	0
5	E	107	0	0	4	0
5	F	88	0	0	6	0
All	All	12088	0	11383	407	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 18.

All (407) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:148:MSE:HE3	1:E:213:LEU:HD11	1.38	1.01
1:F:367:ASN:HD22	1:F:371:THR:HG22	1.23	0.99
1:C:224:LYS:HD3	1:C:225:PRO:HD2	1.45	0.98
1:F:318:ASN:HD21	1:F:491:HIS:H	1.12	0.96
1:E:67:ASN:HD22	1:E:71:THR:HG23	1.31	0.94
1:F:317:ARG:H	4:F:711:ACY:H3	1.34	0.93
1:B:317:ARG:H	4:B:703:ACY:H3	1.34	0.93
1:F:371:THR:HG23	1:F:373:PRO:HD3	1.52	0.92
1:B:367:ASN:HD22	1:B:371:THR:HG23	1.36	0.90
1:E:18:ASN:HD21	1:E:191:HIS:H	1.15	0.89
1:B:318:ASN:HD21	1:B:491:HIS:H	1.22	0.87
1:C:67:ASN:HD22	1:C:71:THR:HG23	1.40	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:69:ASP:HB3	1:E:71:THR:HG22	1.60	0.83
1:D:362:THR:HG21	1:D:550:ARG:HG3	1.59	0.82
1:C:18:ASN:HD21	1:C:191:HIS:H	1.26	0.80
1:A:18:ASN:HD21	1:A:191:HIS:H	1.30	0.80
1:E:51:SER:HB3	1:E:71:THR:HG21	1.62	0.80
1:C:69:ASP:OD1	1:C:71:THR:HG22	1.82	0.79
1:E:17:ARG:H	4:E:709:ACY:H2	1.45	0.79
1:D:533:LEU:HB3	1:D:541:VAL:HB	1.65	0.79
1:C:233:LEU:HD13	1:C:240:ILE:HD11	1.66	0.77
1:D:371:THR:HG23	1:D:373:PRO:HD3	1.65	0.76
1:E:18:ASN:ND2	1:E:191:HIS:H	1.82	0.76
1:F:367:ASN:HD22	1:F:371:THR:CG2	1.96	0.76
1:A:17:ARG:H	4:A:701:ACY:H2	1.50	0.76
1:F:460:SER:O	1:F:463:LYS:HG3	1.87	0.75
1:F:369:ASP:HB3	1:F:371:THR:HB	1.67	0.74
1:C:37:PHE:CZ	1:C:142:LYS:HE2	2.23	0.74
1:C:67:ASN:HD22	1:C:71:THR:CG2	2.00	0.73
1:F:454:VAL:HG13	1:F:458:LYS:HD2	1.70	0.73
1:F:318:ASN:ND2	1:F:491:HIS:H	1.86	0.73
1:F:383:LYS:HD2	1:F:522:GLU:HG2	1.70	0.73
1:D:430:GLU:OE2	1:D:558:GLU:HG2	1.89	0.72
1:B:346:THR:HG23	1:B:347:PRO:HD2	1.69	0.72
1:F:533:LEU:HD13	1:F:540:ILE:HD11	1.70	0.72
1:D:479:GLN:HE21	1:D:481:ARG:HE	1.38	0.72
1:C:96:LYS:HA	1:C:208:PRO:HG3	1.72	0.71
1:A:96:LYS:HA	1:A:208:PRO:HG3	1.73	0.70
1:B:367:ASN:HD22	1:B:371:THR:CG2	2.05	0.70
1:E:233:LEU:HD13	1:E:240:ILE:HD11	1.74	0.70
1:F:318:ASN:HD21	1:F:491:HIS:N	1.88	0.70
1:F:368:GLU:HG2	5:F:719:HOH:O	1.90	0.70
1:C:18:ASN:ND2	1:C:191:HIS:H	1.90	0.69
1:C:6:LEU:HG	1:C:44:ILE:HD13	1.74	0.69
1:A:159:PHE:HB3	1:A:235:GLN:NE2	2.07	0.69
1:B:318:ASN:ND2	1:B:491:HIS:H	1.91	0.68
1:D:318:ASN:HD21	1:D:491:HIS:H	1.40	0.68
1:F:380:ARG:HD2	5:F:736:HOH:O	1.93	0.68
1:B:477:ASN:HA	1:F:457:GLU:CG	2.24	0.68
1:B:369:ASP:OD2	1:B:371:THR:HG22	1.95	0.67
1:C:38:LEU:HD11	1:D:340:PRO:HG3	1.76	0.67
1:F:388:ILE:HG13	1:F:472:VAL:HG22	1.77	0.67
1:C:17:ARG:H	4:C:705:ACY:H2	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:496:ILE:O	1:D:500:ILE:HG13	1.93	0.67
1:A:88:ILE:HD11	1:A:118:LEU:HD11	1.75	0.67
1:C:18:ASN:HD21	1:C:191:HIS:N	1.92	0.67
1:E:18:ASN:HD21	1:E:191:HIS:N	1.91	0.66
1:C:22:HIS:O	1:C:25:GLU:HG2	1.96	0.66
1:D:313:ILE:HD12	1:D:313:ILE:H	1.60	0.66
1:E:28:ASN:HA	5:E:825:HOH:O	1.96	0.66
1:F:379:PRO:HG2	1:F:382:VAL:HB	1.77	0.66
1:D:367:ASN:HD22	1:D:371:THR:CG2	2.08	0.65
1:E:140:ILE:HG21	1:F:503:MSE:CE	2.27	0.65
1:E:148:MSE:CE	1:E:213:LEU:HD21	2.26	0.65
1:E:102:THR:HG22	1:F:553:PRO:HG3	1.77	0.64
1:C:90:LEU:HD23	1:C:91:ALA:N	2.12	0.64
1:C:51:SER:HB2	1:C:71:THR:HG21	1.80	0.64
1:B:460:SER:O	1:B:463:LYS:HB2	1.97	0.64
1:C:48:LEU:HD12	1:C:246:GLU:OE2	1.98	0.64
1:A:18:ASN:ND2	1:A:191:HIS:H	1.96	0.63
1:A:233:LEU:HB3	1:A:241:VAL:CG1	2.29	0.63
1:D:479:GLN:NE2	1:D:481:ARG:HE	1.97	0.63
1:E:107:GLU:OE2	1:E:164:SER:HA	1.97	0.63
1:C:90:LEU:HD12	1:C:186:THR:HG21	1.80	0.62
1:E:140:ILE:HG21	1:F:503:MSE:HE3	1.82	0.61
1:B:477:ASN:HA	1:F:457:GLU:HG3	1.82	0.61
1:A:158:LYS:HB2	5:A:869:HOH:O	1.99	0.61
1:B:533:LEU:HD13	1:B:540:ILE:HD11	1.81	0.61
1:F:557:ARG:O	1:F:558:GLU:HB2	2.00	0.60
1:D:522:GLU:HB3	5:D:780:HOH:O	2.00	0.60
1:E:235:GLN:HB2	1:E:240:ILE:HD13	1.84	0.60
1:F:388:ILE:H	1:F:482:GLN:HE22	1.47	0.60
1:B:367:ASN:HB2	1:B:371:THR:HG22	1.84	0.60
1:C:233:LEU:C	1:C:234:LEU:HD23	2.22	0.60
1:F:492:PRO:HD2	1:F:495:LYS:HD2	1.85	0.59
1:D:310:ARG:HD2	5:D:765:HOH:O	2.03	0.59
1:B:533:LEU:HB3	1:B:541:VAL:HB	1.84	0.59
1:C:90:LEU:HD23	1:C:90:LEU:C	2.23	0.58
1:A:13:ILE:HD11	1:A:206:LEU:CD2	2.33	0.58
1:A:230:HIS:HE1	1:A:242:ASP:OD2	1.86	0.58
1:C:89:GLU:HG2	1:C:215:GLY:O	2.03	0.58
1:E:10:ARG:NH2	1:F:307:LYS:HA	2.18	0.58
1:C:93:ILE:N	1:C:93:ILE:HD12	2.19	0.58
1:E:228:ARG:HH11	1:E:246:GLU:HB3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:SER:HB3	1:C:73:PRO:HG2	1.86	0.57
1:F:456:ARG:HA	1:F:459:PHE:CZ	2.39	0.57
1:B:346:THR:CG2	1:B:347:PRO:HD2	2.34	0.57
1:E:148:MSE:HE3	1:E:213:LEU:CD1	2.25	0.57
1:A:192:PRO:HD2	1:A:195:LYS:HD2	1.85	0.57
1:C:110:TYR:CG	1:C:163:LYS:HG3	2.39	0.57
1:B:305:TYR:CE1	1:B:306:LEU:HD13	2.40	0.57
1:F:550:ARG:HD2	5:F:730:HOH:O	2.03	0.57
1:A:173:LYS:HG3	1:A:232:GLU:HG3	1.86	0.57
1:F:383:LYS:NZ	1:F:522:GLU:HB3	2.20	0.57
1:C:80:ARG:HG2	5:C:812:HOH:O	2.04	0.56
1:E:228:ARG:NH1	1:E:246:GLU:HB3	2.19	0.56
1:A:136:LEU:HB3	1:A:137:PRO:HD2	1.86	0.56
1:D:318:ASN:ND2	1:D:491:HIS:H	2.02	0.56
1:E:233:LEU:HB3	1:E:241:VAL:HB	1.88	0.56
1:C:3:TYR:O	1:C:6:LEU:HB2	2.05	0.56
1:A:140:ILE:HD11	1:B:336:PHE:HB2	1.86	0.56
1:A:177:ASN:HA	1:D:457:GLU:HB2	1.88	0.56
1:A:225:PRO:O	1:D:414:SER:HB2	2.05	0.56
1:E:130:GLU:CG	1:E:134:LYS:HE2	2.36	0.56
1:D:367:ASN:HD22	1:D:371:THR:HG22	1.69	0.56
1:B:346:THR:O	1:B:373:PRO:HA	2.05	0.56
1:A:27:ASN:HA	5:A:817:HOH:O	2.05	0.56
1:E:33:GLN:N	1:E:34:PRO:HD2	2.21	0.56
1:E:130:GLU:HG3	1:E:134:LYS:HE2	1.89	0.55
1:A:235:GLN:HB2	1:A:240:ILE:HD13	1.87	0.55
1:E:17:ARG:H	4:E:709:ACY:CH3	2.16	0.55
1:F:456:ARG:HA	1:F:459:PHE:CE2	2.41	0.55
1:D:388:ILE:CG1	1:D:472:VAL:HG22	2.36	0.55
1:B:317:ARG:N	4:B:703:ACY:H3	2.14	0.55
1:C:67:ASN:ND2	1:C:71:THR:HG23	2.18	0.55
1:A:27:ASN:C	1:A:27:ASN:HD22	2.08	0.55
1:E:233:LEU:HD13	1:E:240:ILE:CD1	2.37	0.55
3:A:801:SO4:O1	1:D:397:HIS:HE1	1.89	0.55
1:B:346:THR:HG22	1:B:350:SER:OG	2.07	0.55
1:C:171:ARG:HA	1:C:185:GLY:HA2	1.89	0.55
1:C:5:TYR:CZ	1:C:6:LEU:HD13	2.42	0.54
1:D:313:ILE:HD12	1:D:313:ILE:N	2.22	0.54
1:E:119:ALA:CB	1:E:148:MSE:HE2	2.38	0.54
1:A:39:LYS:NZ	1:A:121:ASP:HA	2.23	0.54
5:C:832:HOH:O	1:D:397:HIS:HD2	1.91	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:THR:O	1:E:73:PRO:HA	2.06	0.54
1:C:67:ASN:HB2	1:C:71:THR:HG22	1.89	0.54
1:D:316:GLY:HA3	1:D:335:PHE:CZ	2.43	0.54
1:E:140:ILE:HD12	1:F:503:MSE:HE2	1.90	0.54
1:A:27:ASN:HB3	5:A:832:HOH:O	2.08	0.54
1:F:383:LYS:HZ3	1:F:522:GLU:HB3	1.73	0.54
1:C:136:LEU:HB3	1:C:137:PRO:HD2	1.89	0.53
1:F:383:LYS:HG2	5:F:787:HOH:O	2.08	0.53
1:F:433:LYS:HB2	1:F:433:LYS:NZ	2.23	0.53
1:A:13:ILE:HD11	1:A:206:LEU:HD21	1.90	0.53
1:D:317:ARG:H	4:D:707:ACY:H3	1.74	0.53
1:C:10:ARG:NH2	1:D:309:ALA:O	2.42	0.53
1:E:50:SER:HB3	1:E:71:THR:OG1	2.09	0.53
1:C:110:TYR:CB	1:C:163:LYS:HG3	2.39	0.53
1:A:16:GLY:O	1:A:17:ARG:C	2.46	0.52
1:F:388:ILE:CG1	1:F:472:VAL:HG22	2.38	0.52
1:C:116:VAL:HG12	1:C:117:ALA:N	2.24	0.52
1:B:471:ARG:HB3	1:B:534:LEU:HB2	1.92	0.52
1:A:5:TYR:CZ	1:A:6:LEU:HD13	2.45	0.52
1:D:403:LYS:HA	1:D:498:GLN:HG3	1.91	0.52
1:D:318:ASN:HD21	1:D:491:HIS:N	2.05	0.52
1:E:119:ALA:HB1	1:E:148:MSE:HE2	1.90	0.52
1:E:171:ARG:HA	1:E:185:GLY:HA2	1.90	0.52
1:A:155:SER:HB3	1:A:157:GLU:OE2	2.09	0.52
1:D:313:ILE:HD13	1:D:512:ILE:CD1	2.39	0.52
1:A:220:VAL:HG21	5:A:868:HOH:O	2.09	0.52
1:B:463:LYS:HG2	5:B:847:HOH:O	2.10	0.52
1:C:50:SER:OG	1:C:73:PRO:HG3	2.09	0.52
1:C:144:PHE:O	1:C:147:PHE:HB2	2.09	0.52
1:F:369:ASP:C	1:F:371:THR:H	2.13	0.51
1:D:413:ILE:O	1:D:456:ARG:HD3	2.10	0.51
1:C:13:ILE:HD11	1:C:206:LEU:CD2	2.41	0.51
1:F:427:VAL:HG22	1:F:556:PHE:CD1	2.46	0.51
1:A:88:ILE:HB	1:A:174:CYS:HB2	1.92	0.51
1:F:533:LEU:HD13	1:F:540:ILE:CD1	2.40	0.51
1:D:386:HIS:HD2	1:D:523:LEU:HD13	1.76	0.51
1:C:203:MSE:SE	1:D:440:ILE:HD13	2.61	0.51
1:D:388:ILE:H	1:D:482:GLN:HE22	1.57	0.51
1:D:524:LYS:HE3	5:D:780:HOH:O	2.10	0.51
1:E:48:LEU:HD23	5:E:852:HOH:O	2.09	0.51
1:F:398:LEU:HB2	1:F:506:LEU:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2:SER:N	5:E:908:HOH:O	2.44	0.51
1:A:88:ILE:HD11	1:A:118:LEU:CD1	2.41	0.50
1:C:156:ARG:HA	1:C:159:PHE:CZ	2.46	0.50
1:E:110:TYR:CD2	1:E:163:LYS:HD3	2.46	0.50
1:D:362:THR:HG22	1:D:377:PHE:CD1	2.46	0.50
1:A:39:LYS:HZ1	1:A:121:ASP:HA	1.76	0.50
1:E:144:PHE:CE2	1:F:503:MSE:HG2	2.45	0.50
1:C:10:ARG:HD3	5:C:897:HOH:O	2.12	0.50
1:C:86:HIS:HE2	1:C:181:ARG:HD2	1.77	0.50
1:C:234:LEU:HD23	1:C:234:LEU:N	2.26	0.50
1:D:305:TYR:CZ	1:D:306:LEU:HD13	2.47	0.50
1:C:16:GLY:O	1:C:17:ARG:C	2.50	0.50
1:A:89:GLU:HG2	1:A:215:GLY:O	2.12	0.50
1:B:385:HIS:HA	1:B:521:GLY:O	2.12	0.50
1:B:389:GLU:HG2	1:B:515:GLY:O	2.11	0.50
1:D:499:HIS:O	1:D:502:THR:HG22	2.12	0.50
1:A:18:ASN:HD21	1:A:191:HIS:N	2.03	0.49
1:B:346:THR:HG23	1:B:347:PRO:CD	2.40	0.49
1:A:5:TYR:CE1	1:A:6:LEU:HD13	2.47	0.49
1:F:379:PRO:HG2	1:F:382:VAL:CB	2.42	0.49
1:F:386:HIS:HD2	1:F:482:GLN:NE2	2.11	0.49
1:D:376:ILE:HD13	1:D:422:LEU:HD11	1.94	0.49
1:F:388:ILE:HG13	1:F:472:VAL:CG2	2.42	0.49
1:F:367:ASN:C	1:F:369:ASP:N	2.64	0.49
1:E:77:PHE:HB3	1:E:250:ARG:HB2	1.94	0.49
1:B:387:GLU:HG2	1:B:516:THR:HG21	1.94	0.49
1:D:313:ILE:HD13	1:D:512:ILE:HD13	1.94	0.49
1:E:10:ARG:HG3	1:E:10:ARG:HH11	1.78	0.49
1:E:140:ILE:CG2	1:F:503:MSE:CE	2.90	0.49
1:F:383:LYS:HD2	1:F:522:GLU:CG	2.40	0.49
1:A:39:LYS:HE2	1:A:142:LYS:O	2.11	0.49
1:B:317:ARG:HD2	1:B:335:PHE:HE2	1.77	0.49
1:C:37:PHE:CE1	1:C:142:LYS:HE2	2.48	0.49
1:C:155:SER:HB3	1:C:157:GLU:OE1	2.12	0.49
1:E:230:HIS:HE1	1:E:242:ASP:OD1	1.95	0.49
1:E:88:ILE:HB	1:E:174:CYS:HB2	1.95	0.49
1:E:40:PRO:HD3	1:F:338:LEU:HD11	1.94	0.48
1:C:127:VAL:HG22	1:C:256:PHE:CD1	2.48	0.48
1:B:444:PHE:O	1:B:447:PHE:HB2	2.14	0.48
1:D:388:ILE:HG12	1:D:472:VAL:HG22	1.95	0.48
1:D:502:THR:CG2	1:D:503:MSE:HG3	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:SER:HB2	1:E:73:PRO:HB3	1.93	0.48
1:A:13:ILE:HG23	1:A:38:LEU:CD2	2.44	0.48
1:A:144:PHE:O	1:A:147:PHE:HB2	2.13	0.48
1:F:388:ILE:H	1:F:482:GLN:NE2	2.10	0.48
1:C:50:SER:HA	5:C:873:HOH:O	2.12	0.48
1:A:233:LEU:HD13	1:A:240:ILE:HD11	1.96	0.48
1:B:303:TYR:CE2	1:B:346:THR:HG23	2.48	0.48
1:C:17:ARG:H	4:C:705:ACY:CH3	2.26	0.48
1:F:392:LEU:HD11	1:F:493:LEU:HG	1.96	0.48
1:D:388:ILE:HG13	1:D:472:VAL:HG22	1.95	0.47
1:F:386:HIS:O	1:F:520:VAL:HG13	2.14	0.47
1:A:140:ILE:N	1:A:140:ILE:HD12	2.29	0.47
1:A:88:ILE:HD13	1:A:231:CYS:HB3	1.96	0.47
1:E:140:ILE:CG1	1:F:503:MSE:HE2	2.44	0.47
1:F:533:LEU:HB3	1:F:541:VAL:HB	1.96	0.47
1:C:34:PRO:HA	5:C:902:HOH:O	2.13	0.47
1:D:430:GLU:OE2	1:D:558:GLU:CG	2.62	0.47
1:E:140:ILE:CG2	1:F:503:MSE:HE2	2.45	0.47
1:B:540:ILE:HG13	1:B:541:VAL:HG23	1.97	0.47
1:D:346:THR:O	1:D:373:PRO:HA	2.15	0.47
1:F:495:LYS:HE2	5:F:759:HOH:O	2.14	0.47
1:B:386:HIS:O	1:B:520:VAL:HG13	2.15	0.47
1:F:436:LEU:HB3	1:F:437:PRO:CD	2.45	0.47
1:C:88:ILE:CD1	1:C:231:CYS:HB3	2.45	0.47
1:F:386:HIS:HD2	1:F:482:GLN:HE21	1.60	0.47
1:B:346:THR:CG2	1:B:347:PRO:CD	2.93	0.47
1:D:388:ILE:HD13	1:D:531:CYS:HB3	1.96	0.47
1:C:79:PRO:HB2	1:C:82:VAL:HG21	1.96	0.46
1:C:110:TYR:HB3	1:C:163:LYS:HG3	1.96	0.46
1:D:389:GLU:HG2	1:D:515:GLY:O	2.15	0.46
1:A:23:ILE:HG23	1:A:24:LYS:N	2.30	0.46
1:D:473:LYS:CG	1:D:532:GLU:HB2	2.45	0.46
1:F:349:SER:O	1:F:350:SER:HB2	2.15	0.46
1:F:376:ILE:CD1	1:F:449:PRO:HG3	2.45	0.46
1:C:12:ILE:HG12	1:C:211:ILE:HB	1.97	0.46
1:C:14:CYS:O	1:C:36:PHE:HA	2.15	0.46
1:C:89:GLU:OE2	1:C:121:ASP:HB3	2.15	0.46
1:E:235:GLN:HE21	1:E:240:ILE:HG21	1.80	0.46
1:C:98:LEU:HB2	1:C:206:LEU:HB2	1.98	0.46
1:E:140:ILE:CD1	1:F:503:MSE:HE2	2.45	0.46
1:F:451:SER:HB3	1:F:543:MSE:SE	2.65	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:33:GLN:N	1:E:34:PRO:CD	2.78	0.46
1:A:67:ASN:C	1:A:69:ASP:N	2.69	0.46
1:E:10:ARG:HH21	1:F:307:LYS:HA	1.78	0.46
1:D:369:ASP:HB3	1:D:371:THR:HB	1.98	0.46
1:D:314:CYS:SG	1:D:513:LEU:HD12	2.56	0.45
1:F:396:LYS:HA	1:F:508:PRO:HG3	1.98	0.45
1:F:430:GLU:HA	1:F:433:LYS:HG2	1.97	0.45
1:B:427:VAL:HG22	1:B:556:PHE:CD1	2.51	0.45
1:A:85:HIS:HA	1:A:221:GLY:O	2.17	0.45
1:C:192:PRO:CG	1:C:195:LYS:HE2	2.47	0.45
1:D:387:GLU:HG2	1:D:516:THR:HG21	1.97	0.45
1:E:69:ASP:HB2	5:E:884:HOH:O	2.17	0.45
1:E:86:HIS:O	1:E:220:VAL:HG23	2.17	0.45
1:E:122:LEU:HD12	1:E:147:PHE:HA	1.99	0.45
1:F:386:HIS:HE1	1:F:481:ARG:HH11	1.65	0.45
1:A:13:ILE:CD1	1:A:206:LEU:HD21	2.47	0.45
1:F:367:ASN:C	1:F:369:ASP:H	2.19	0.45
1:A:106:PRO:HD2	1:A:107:GLU:OE1	2.16	0.45
1:C:90:LEU:CD1	1:C:186:THR:HG21	2.46	0.45
1:F:345:VAL:HG13	1:F:449:PRO:HA	1.98	0.45
1:B:305:TYR:CZ	1:B:306:LEU:HD13	2.51	0.45
1:D:316:GLY:O	1:D:317:ARG:C	2.55	0.45
1:D:386:HIS:CE1	1:D:521:GLY:H	2.34	0.45
1:F:383:LYS:HE3	1:F:522:GLU:OE2	2.17	0.45
1:C:79:PRO:HB2	1:C:82:VAL:CG2	2.46	0.45
1:C:192:PRO:HG2	1:C:195:LYS:HB2	1.99	0.45
1:B:376:ILE:CD1	1:B:449:PRO:HG3	2.47	0.45
1:D:420:LEU:HB2	1:D:449:PRO:HD2	1.97	0.45
1:E:5:TYR:CE1	1:E:6:LEU:HD13	2.52	0.45
1:E:89:GLU:HG2	1:E:215:GLY:O	2.16	0.45
1:E:100:ASN:HD21	1:F:362:THR:HG23	1.82	0.45
1:E:120:LEU:HB2	1:E:149:PRO:HD2	1.99	0.45
1:F:398:LEU:HD23	1:F:506:LEU:HD12	1.98	0.45
1:C:18:ASN:HD21	1:C:191:HIS:HB2	1.83	0.44
1:E:140:ILE:HG13	1:F:503:MSE:HE2	1.99	0.44
1:F:529:VAL:O	1:F:544:ASN:HA	2.17	0.44
1:F:375:PRO:HA	5:F:792:HOH:O	2.17	0.44
1:B:318:ASN:HD21	1:B:491:HIS:N	2.02	0.44
1:C:90:LEU:C	1:C:90:LEU:CD2	2.85	0.44
1:C:92:LEU:HD11	1:C:193:LEU:HG	1.98	0.44
1:E:138:TRP:CE3	1:F:437:PRO:HG3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:LYS:CG	1:A:232:GLU:HG3	2.48	0.44
1:A:212:ILE:N	1:A:212:ILE:HD12	2.33	0.44
1:D:460:SER:O	1:D:463:LYS:HD2	2.17	0.44
1:B:410:TYR:CD2	1:B:463:LYS:HG3	2.51	0.44
1:F:496:ILE:O	1:F:500:ILE:HG13	2.18	0.44
1:F:306:LEU:HD12	1:F:344:ILE:HD13	1.99	0.44
1:E:5:TYR:CD2	1:E:153:ILE:HB	2.52	0.44
1:E:192:PRO:HG2	1:E:195:LYS:HB2	2.00	0.44
1:F:433:LYS:HB2	1:F:433:LYS:HZ2	1.83	0.44
1:A:13:ILE:HG23	1:A:38:LEU:HD23	2.00	0.44
1:B:410:TYR:CE1	1:B:456:ARG:HB2	2.53	0.43
1:D:418:LEU:HD13	1:D:533:LEU:HB2	1.99	0.43
1:A:88:ILE:H	1:A:182:GLN:HE22	1.67	0.43
1:D:367:ASN:C	1:D:369:ASP:N	2.70	0.43
1:F:393:ILE:HD12	1:F:393:ILE:N	2.33	0.43
1:A:22:HIS:O	1:A:25:GLU:HG3	2.19	0.43
1:A:86:HIS:HE2	1:A:181:ARG:HH11	1.66	0.43
1:C:233:LEU:HD13	1:C:240:ILE:CD1	2.43	0.43
1:D:347:PRO:HG2	1:D:350:SER:HB3	2.00	0.43
1:A:62:THR:CG2	1:A:251:PRO:HD2	2.48	0.43
1:A:94:VAL:HG23	1:A:212:ILE:HD13	1.99	0.43
1:B:466:LEU:CD1	1:B:466:LEU:N	2.81	0.43
1:B:459:PHE:HB3	1:B:535:GLN:OE1	2.18	0.43
1:B:477:ASN:HB3	1:F:457:GLU:HA	2.01	0.43
1:E:110:TYR:CE2	1:E:163:LYS:HD3	2.54	0.43
1:E:140:ILE:HG13	1:F:503:MSE:CE	2.49	0.43
1:B:451:SER:HB3	1:B:543:MSE:SE	2.69	0.43
1:E:148:MSE:HE1	1:E:213:LEU:HD21	1.99	0.43
1:A:173:LYS:HA	1:A:182:GLN:O	2.19	0.43
1:C:7:LYS:HD3	1:C:70:GLY:HA2	2.01	0.43
1:D:502:THR:HG23	1:D:503:MSE:HG3	2.01	0.43
1:E:13:ILE:HG22	1:E:212:ILE:HD13	2.00	0.43
1:E:16:GLY:O	1:E:17:ARG:C	2.57	0.43
1:C:13:ILE:HD11	1:C:206:LEU:HD21	2.00	0.43
1:A:173:LYS:HG3	1:A:232:GLU:CG	2.48	0.42
1:D:382:VAL:HA	1:D:426:ASN:HD21	1.84	0.42
1:E:79:PRO:HB2	1:E:82:VAL:HG21	2.00	0.42
1:A:7:LYS:HE3	5:B:882:HOH:O	2.19	0.42
1:B:345:VAL:HA	1:B:372:ASN:HD22	1.84	0.42
1:D:318:ASN:HD21	1:D:491:HIS:HB2	1.83	0.42
1:D:530:HIS:HE1	1:D:542:ASP:OD1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:139:THR:N	3:E:807:SO4:O4	2.53	0.42
1:B:455:SER:O	1:B:458:LYS:HB2	2.19	0.42
1:A:33:GLN:N	1:A:34:PRO:CD	2.82	0.42
1:E:85:HIS:CE1	1:E:125:ARG:HD3	2.55	0.42
1:E:216:THR:HA	1:E:217:PRO:HD3	1.88	0.42
1:A:14:CYS:HB2	1:A:37:PHE:CE1	2.53	0.42
1:E:71:THR:OG1	1:E:73:PRO:HD3	2.19	0.42
1:C:232:GLU:HG3	1:C:234:LEU:HD21	2.02	0.42
1:C:4:ASN:H	1:C:4:ASN:ND2	2.18	0.42
1:A:234:LEU:HD12	1:A:234:LEU:N	2.34	0.42
1:B:466:LEU:N	1:B:466:LEU:HD12	2.35	0.42
1:C:224:LYS:CD	1:C:225:PRO:HD2	2.31	0.42
1:D:388:ILE:HG13	1:D:472:VAL:CG2	2.50	0.42
1:E:45:VAL:CG1	1:E:149:PRO:HA	2.49	0.42
1:D:386:HIS:HD1	1:D:482:GLN:NE2	2.18	0.42
1:F:388:ILE:HB	1:F:474:CYS:HB2	2.02	0.42
1:C:128:GLN:HE22	4:C:704:ACY:H1	1.84	0.41
1:E:62:THR:HG21	1:E:250:ARG:HG3	2.02	0.41
1:A:240:ILE:HG13	1:A:241:VAL:HG12	2.01	0.41
1:D:451:SER:HB3	1:D:543:MSE:SE	2.71	0.41
1:F:426:ASN:ND2	1:F:556:PHE:CD2	2.89	0.41
1:A:67:ASN:C	1:A:69:ASP:H	2.24	0.41
1:C:13:ILE:CD1	1:C:206:LEU:HD21	2.51	0.41
1:E:204:ILE:HG12	1:F:443:GLY:O	2.20	0.41
1:F:389:GLU:HG2	1:F:515:GLY:O	2.20	0.41
1:B:388:ILE:CG1	1:B:472:VAL:HG22	2.51	0.41
1:C:173:LYS:HD2	1:C:183:ASP:CG	2.41	0.41
1:D:421:ASP:OD1	1:D:442:LYS:HD2	2.20	0.41
1:F:388:ILE:HG23	1:F:472:VAL:HG13	2.03	0.41
1:F:394:VAL:HG12	1:F:396:LYS:H	1.85	0.41
1:B:388:ILE:HD11	1:B:418:LEU:HD11	2.01	0.41
1:E:166:LEU:HD13	1:E:166:LEU:O	2.21	0.41
1:A:211:ILE:C	1:A:212:ILE:HD12	2.41	0.41
1:C:45:VAL:HA	1:C:72:ASN:HD22	1.86	0.41
1:F:428:GLN:HG2	1:F:432:LYS:HE3	2.03	0.41
1:A:5:TYR:CD2	1:A:153:ILE:HB	2.56	0.41
1:A:23:ILE:CG2	1:A:24:LYS:N	2.84	0.41
1:B:530:HIS:HE1	1:B:542:ASP:OD1	2.04	0.41
1:C:89:GLU:HG2	1:C:215:GLY:C	2.41	0.41
1:C:173:LYS:NZ	1:C:232:GLU:CD	2.75	0.41
1:E:173:LYS:HE2	1:E:234:LEU:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:HIS:HE2	1:A:181:ARG:HD2	1.85	0.41
1:B:377:PHE:HB3	1:B:550:ARG:HB2	2.02	0.41
1:C:189:MSE:SE	1:C:193:LEU:HD13	2.71	0.41
1:E:128:GLN:HE22	4:E:708:ACY:H1	1.86	0.41
1:E:167:GLN:OE1	1:E:193:LEU:HG	2.21	0.41
1:C:12:ILE:HD13	1:C:148:MSE:SE	2.72	0.40
1:C:163:LYS:O	1:C:163:LYS:HG2	2.20	0.40
1:F:305:TYR:CE2	1:F:306:LEU:HD22	2.56	0.40
1:F:410:TYR:CE2	1:F:463:LYS:HG2	2.56	0.40
1:A:27:ASN:C	1:A:27:ASN:ND2	2.75	0.40
1:A:157:GLU:CD	1:A:157:GLU:H	2.25	0.40
1:C:20:ALA:HB1	1:C:25:GLU:HG3	2.04	0.40
1:E:136:LEU:HB3	1:E:137:PRO:CD	2.50	0.40
1:A:233:LEU:HB3	1:A:241:VAL:HG13	2.03	0.40
1:A:234:LEU:HA	1:A:238:ASP:O	2.22	0.40
1:B:430:GLU:HG3	1:B:434:LYS:HE2	2.04	0.40
1:D:303:TYR:CE1	1:D:350:SER:HB2	2.56	0.40
1:F:407:GLU:H	1:F:407:GLU:HG3	1.43	0.40
1:F:550:ARG:HG2	1:F:551:PRO:O	2.21	0.40
1:A:13:ILE:HD12	1:A:200:ILE:HD13	2.03	0.40
1:B:454:VAL:HG13	1:B:458:LYS:HD2	2.02	0.40
1:B:557:ARG:HD3	1:B:557:ARG:HA	1.90	0.40
1:E:160:SER:O	1:E:163:LYS:HG2	2.21	0.40
1:B:346:THR:CG2	1:B:350:SER:OG	2.68	0.40
1:E:10:ARG:HG3	1:E:10:ARG:NH1	2.37	0.40
1:F:303:TYR:HB3	1:F:306:LEU:HD23	2.03	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	241/259 (93%)	229 (95%)	10 (4%)	2 (1%)	19	19
1	B	238/259 (92%)	223 (94%)	14 (6%)	1 (0%)	34	37
1	C	239/259 (92%)	229 (96%)	8 (3%)	2 (1%)	19	19
1	D	238/259 (92%)	230 (97%)	6 (2%)	2 (1%)	19	19
1	E	240/259 (93%)	229 (95%)	9 (4%)	2 (1%)	19	19
1	F	234/259 (90%)	222 (95%)	12 (5%)	0	100	100
All	All	1430/1554 (92%)	1362 (95%)	59 (4%)	9 (1%)	25	26

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	59	ALA
1	B	551	PRO
1	A	17	ARG
1	C	17	ARG
1	A	165	ASN
1	D	551	PRO
1	E	17	ARG
1	E	164	SER
1	D	317	ARG

### 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	214/224 (96%)	208 (97%)	6 (3%)	43	56
1	B	212/224 (95%)	203 (96%)	9 (4%)	30	38
1	C	212/224 (95%)	205 (97%)	7 (3%)	38	49
1	D	211/224 (94%)	198 (94%)	13 (6%)	18	21
1	E	214/224 (96%)	210 (98%)	4 (2%)	57	71
1	F	210/224 (94%)	195 (93%)	15 (7%)	14	16
All	All	1273/1344 (95%)	1219 (96%)	54 (4%)	30	38



All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	13	ILE
1	A	25	GLU
1	A	27	ASN
1	A	69	ASP
1	A	233	LEU
1	B	306	LEU
1	B	318	ASN
1	B	429	ASP
1	B	471	ARG
1	B	472	VAL
1	B	473	LYS
1	B	493	LEU
1	B	533	LEU
1	B	558	GLU
1	C	6	LEU
1	C	13	ILE
1	C	193	LEU
1	C	195	LYS
1	C	233	LEU
1	C	234	LEU
1	C	246	GLU
1	D	306	LEU
1	D	313	ILE
1	D	325	GLU
1	D	368	GLU
1	D	369	ASP
1	D	371	THR
1	D	403	LYS
1	D	457	GLU
1	D	472	VAL
1	D	493	LEU
1	D	502	THR
1	D	520	VAL
1	D	523	LEU
1	E	6	LEU
1	E	116	VAL
1	E	166	LEU
1	E	233	LEU
1	F	310	ARG
1	F	360	ASN
1	F	369	ASP

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Mol	Chain	Res	Type
1	F	371	THR
1	F	398	LEU
1	F	403	LYS
1	F	407	GLU
1	F	433	LYS
1	F	457	GLU
1	F	472	VAL
1	F	493	LEU
1	F	531	CYS
1	F	533	LEU
1	F	538	ASP
1	F	557	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	27	ASN
1	A	64	ASN
1	A	179	GLN
1	A	182	GLN
1	A	230	HIS
1	A	235	GLN
1	B	318	ASN
1	B	367	ASN
1	B	397	HIS
1	B	479	GLN
1	B	482	GLN
1	B	499	HIS
1	C	4	ASN
1	C	18	ASN
1	C	64	ASN
1	C	67	ASN
1	C	97	HIS
1	C	128	GLN
1	C	165	ASN
1	C	182	GLN
1	C	230	HIS
1	C	235	GLN
1	D	318	ASN
1	D	364	ASN
1	D	367	ASN

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Mol	Chain	Res	Type
1	D	397	HIS
1	D	479	GLN
1	D	482	GLN
1	D	535	GLN
1	E	4	ASN
1	E	18	ASN
1	E	64	ASN
1	E	67	ASN
1	E	128	GLN
1	E	182	GLN
1	E	191	HIS
1	E	230	HIS
1	E	235	GLN
1	F	318	ASN
1	F	364	ASN
1	F	367	ASN
1	F	386	HIS
1	F	482	GLN
1	F	491	HIS
1	F	535	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 6 are monoatomic - leaving 19 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	$\# Z  > 2$
4	ACY	F	710	-	3,3,3	1.23	0	3,3,3	1.64	1 (33%)
4	ACY	F	711	2	3,3,3	1.22	0	3,3,3	1.70	1 (33%)
3	SO4	C	806	-	4,4,4	0.29	0	6,6,6	0.18	0
4	ACY	E	708	-	3,3,3	1.23	0	3,3,3	1.68	1 (33%)
3	SO4	A	801	-	4,4,4	0.26	0	6,6,6	0.14	0
4	ACY	E	709	2	3,3,3	1.24	0	3,3,3	1.69	1 (33%)
4	ACY	B	702	-	3,3,3	1.21	0	3,3,3	1.63	1 (33%)
3	SO4	A	803	-	4,4,4	0.25	0	6,6,6	0.13	0
4	ACY	C	705	2	3,3,3	1.28	1 (33%)	3,3,3	1.65	1 (33%)
4	ACY	A	701	2	3,3,3	1.31	1 (33%)	3,3,3	1.65	1 (33%)
3	SO4	B	805	-	4,4,4	0.27	0	6,6,6	0.17	0
4	ACY	B	703	2	3,3,3	1.23	0	3,3,3	1.70	1 (33%)
3	SO4	B	802	-	4,4,4	0.25	0	6,6,6	0.15	0
4	ACY	D	707	2	3,3,3	1.23	0	3,3,3	1.73	1 (33%)
4	ACY	C	704	-	3,3,3	1.20	0	3,3,3	1.67	1 (33%)
3	SO4	E	807	-	4,4,4	0.23	0	6,6,6	0.12	0
4	ACY	D	706	-	3,3,3	1.21	0	3,3,3	1.64	1 (33%)
4	ACY	A	700	-	3,3,3	1.19	0	3,3,3	1.66	1 (33%)
3	SO4	B	800	-	4,4,4	0.27	0	6,6,6	0.11	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	ACY	O-C	2.05	1.31	1.22
4	C	705	ACY	O-C	2.04	1.31	1.22

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	707	ACY	O-C-CH3	-2.38	113.07	122.33
4	B	703	ACY	O-C-CH3	-2.35	113.19	122.33
4	F	711	ACY	O-C-CH3	-2.35	113.20	122.33
4	E	709	ACY	O-C-CH3	-2.32	113.29	122.33
4	E	708	ACY	O-C-CH3	-2.32	113.30	122.33
4	C	704	ACY	O-C-CH3	-2.31	113.34	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	700	ACY	O-C-CH3	-2.29	113.40	122.33
4	F	710	ACY	O-C-CH3	-2.27	113.50	122.33
4	D	706	ACY	O-C-CH3	-2.26	113.53	122.33
4	A	701	ACY	O-C-CH3	-2.25	113.56	122.33
4	B	702	ACY	O-C-CH3	-2.25	113.58	122.33
4	C	705	ACY	O-C-CH3	-2.25	113.58	122.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	711	ACY	1	0
4	E	708	ACY	1	0
3	A	801	SO4	1	0
4	E	709	ACY	2	0
4	C	705	ACY	2	0
4	A	701	ACY	1	0
4	B	703	ACY	2	0
4	D	707	ACY	1	0
4	C	704	ACY	1	0
3	E	807	SO4	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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.