



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:16 am GMT

PDB ID : 3WCH  
Title : The complex structure of HsSQS wtih ligand BPH1237  
Authors : Shang, N.; Li, Q.; Ko, T.P.; Chan, H.C.; Huang, C.H.; Ren, F.; Zheng, Y.;  
Zhu, Z.; Chen, C.C.; Guo, R.T.  
Deposited on : 2013-05-27  
Resolution : 2.50 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

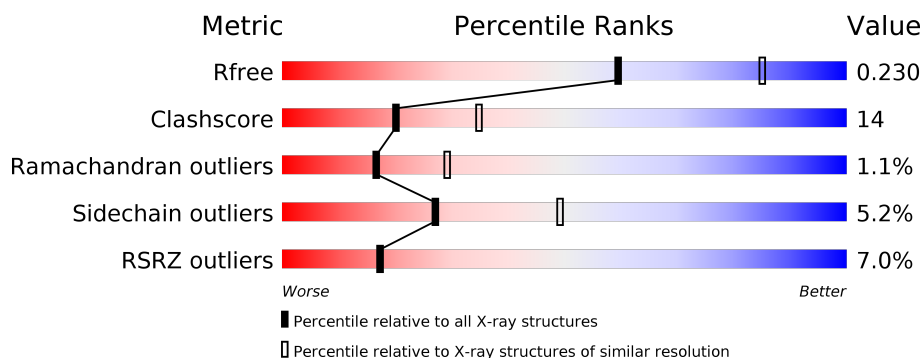
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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.

Mol	Chain	Length	Quality of chain
1	A	360	<div> <div>4%</div> <div>68% 23% 7%</div> </div>
1	B	360	<div> <div>7%</div> <div>65% 26% 7%</div> </div>
1	C	360	<div> <div>4%</div> <div>68% 23% 7%</div> </div>
1	D	360	<div> <div>8%</div> <div>61% 28% 7%</div> </div>
1	E	360	<div> <div>6%</div> <div>69% 21% 7%</div> </div>
1	F	360	<div> <div>9%</div> <div>60% 29% 7%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	8PH	A	401	-	-	-	X
2	8PH	A	402	-	-	-	X
2	8PH	C	401	-	-	-	X
2	8PH	D	401	-	-	-	X
2	8PH	E	401	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16820 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 Squalene synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2696	1717	458	503	18			
1	B	334	Total	C	N	O	S	0	0	0
			2696	1717	458	503	18			
1	C	334	Total	C	N	O	S	0	0	0
			2696	1717	458	503	18			
1	D	334	Total	C	N	O	S	0	0	0
			2696	1717	458	503	18			
1	E	334	Total	C	N	O	S	0	0	0
			2696	1717	458	503	18			
1	F	334	Total	C	N	O	S	0	0	0
			2696	1717	458	503	18			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	MET	-	EXPRESSION TAG	UNP P37268
A	12	GLY	-	EXPRESSION TAG	UNP P37268
A	13	SER	-	EXPRESSION TAG	UNP P37268
A	14	SER	-	EXPRESSION TAG	UNP P37268
A	15	HIS	-	EXPRESSION TAG	UNP P37268
A	16	HIS	-	EXPRESSION TAG	UNP P37268
A	17	HIS	-	EXPRESSION TAG	UNP P37268
A	18	HIS	-	EXPRESSION TAG	UNP P37268
A	19	HIS	-	EXPRESSION TAG	UNP P37268
A	20	HIS	-	EXPRESSION TAG	UNP P37268
A	21	SER	-	EXPRESSION TAG	UNP P37268
A	22	SER	-	EXPRESSION TAG	UNP P37268
A	23	GLY	-	EXPRESSION TAG	UNP P37268
A	24	LEU	-	EXPRESSION TAG	UNP P37268
A	25	VAL	-	EXPRESSION TAG	UNP P37268
A	26	PRO	-	EXPRESSION TAG	UNP P37268
A	27	ARG	-	EXPRESSION TAG	UNP P37268

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Chain	Residue	Modelled	Actual	Comment	Reference
A	28	GLY	-	EXPRESSION TAG	UNP P37268
A	29	SER	-	EXPRESSION TAG	UNP P37268
A	30	HIS	-	EXPRESSION TAG	UNP P37268
A	248	LEU	LYS	ENGINEERED MUTATION	UNP P37268
A	315	LEU	LYS	ENGINEERED MUTATION	UNP P37268
A	318	LEU	LYS	ENGINEERED MUTATION	UNP P37268
A	353	ASN	ASP	SEE REMARK 999	UNP P37268
B	11	MET	-	EXPRESSION TAG	UNP P37268
B	12	GLY	-	EXPRESSION TAG	UNP P37268
B	13	SER	-	EXPRESSION TAG	UNP P37268
B	14	SER	-	EXPRESSION TAG	UNP P37268
B	15	HIS	-	EXPRESSION TAG	UNP P37268
B	16	HIS	-	EXPRESSION TAG	UNP P37268
B	17	HIS	-	EXPRESSION TAG	UNP P37268
B	18	HIS	-	EXPRESSION TAG	UNP P37268
B	19	HIS	-	EXPRESSION TAG	UNP P37268
B	20	HIS	-	EXPRESSION TAG	UNP P37268
B	21	SER	-	EXPRESSION TAG	UNP P37268
B	22	SER	-	EXPRESSION TAG	UNP P37268
B	23	GLY	-	EXPRESSION TAG	UNP P37268
B	24	LEU	-	EXPRESSION TAG	UNP P37268
B	25	VAL	-	EXPRESSION TAG	UNP P37268
B	26	PRO	-	EXPRESSION TAG	UNP P37268
B	27	ARG	-	EXPRESSION TAG	UNP P37268
B	28	GLY	-	EXPRESSION TAG	UNP P37268
B	29	SER	-	EXPRESSION TAG	UNP P37268
B	30	HIS	-	EXPRESSION TAG	UNP P37268
B	248	LEU	LYS	ENGINEERED MUTATION	UNP P37268
B	315	LEU	LYS	ENGINEERED MUTATION	UNP P37268
B	318	LEU	LYS	ENGINEERED MUTATION	UNP P37268
B	353	ASN	ASP	SEE REMARK 999	UNP P37268
C	11	MET	-	EXPRESSION TAG	UNP P37268
C	12	GLY	-	EXPRESSION TAG	UNP P37268
C	13	SER	-	EXPRESSION TAG	UNP P37268
C	14	SER	-	EXPRESSION TAG	UNP P37268
C	15	HIS	-	EXPRESSION TAG	UNP P37268
C	16	HIS	-	EXPRESSION TAG	UNP P37268
C	17	HIS	-	EXPRESSION TAG	UNP P37268
C	18	HIS	-	EXPRESSION TAG	UNP P37268
C	19	HIS	-	EXPRESSION TAG	UNP P37268
C	20	HIS	-	EXPRESSION TAG	UNP P37268
C	21	SER	-	EXPRESSION TAG	UNP P37268

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Chain	Residue	Modelled	Actual	Comment	Reference
C	22	SER	-	EXPRESSION TAG	UNP P37268
C	23	GLY	-	EXPRESSION TAG	UNP P37268
C	24	LEU	-	EXPRESSION TAG	UNP P37268
C	25	VAL	-	EXPRESSION TAG	UNP P37268
C	26	PRO	-	EXPRESSION TAG	UNP P37268
C	27	ARG	-	EXPRESSION TAG	UNP P37268
C	28	GLY	-	EXPRESSION TAG	UNP P37268
C	29	SER	-	EXPRESSION TAG	UNP P37268
C	30	HIS	-	EXPRESSION TAG	UNP P37268
C	248	LEU	LYS	ENGINEERED MUTATION	UNP P37268
C	315	LEU	LYS	ENGINEERED MUTATION	UNP P37268
C	318	LEU	LYS	ENGINEERED MUTATION	UNP P37268
C	353	ASN	ASP	SEE REMARK 999	UNP P37268
D	11	MET	-	EXPRESSION TAG	UNP P37268
D	12	GLY	-	EXPRESSION TAG	UNP P37268
D	13	SER	-	EXPRESSION TAG	UNP P37268
D	14	SER	-	EXPRESSION TAG	UNP P37268
D	15	HIS	-	EXPRESSION TAG	UNP P37268
D	16	HIS	-	EXPRESSION TAG	UNP P37268
D	17	HIS	-	EXPRESSION TAG	UNP P37268
D	18	HIS	-	EXPRESSION TAG	UNP P37268
D	19	HIS	-	EXPRESSION TAG	UNP P37268
D	20	HIS	-	EXPRESSION TAG	UNP P37268
D	21	SER	-	EXPRESSION TAG	UNP P37268
D	22	SER	-	EXPRESSION TAG	UNP P37268
D	23	GLY	-	EXPRESSION TAG	UNP P37268
D	24	LEU	-	EXPRESSION TAG	UNP P37268
D	25	VAL	-	EXPRESSION TAG	UNP P37268
D	26	PRO	-	EXPRESSION TAG	UNP P37268
D	27	ARG	-	EXPRESSION TAG	UNP P37268
D	28	GLY	-	EXPRESSION TAG	UNP P37268
D	29	SER	-	EXPRESSION TAG	UNP P37268
D	30	HIS	-	EXPRESSION TAG	UNP P37268
D	248	LEU	LYS	ENGINEERED MUTATION	UNP P37268
D	315	LEU	LYS	ENGINEERED MUTATION	UNP P37268
D	318	LEU	LYS	ENGINEERED MUTATION	UNP P37268
D	353	ASN	ASP	SEE REMARK 999	UNP P37268
E	11	MET	-	EXPRESSION TAG	UNP P37268
E	12	GLY	-	EXPRESSION TAG	UNP P37268
E	13	SER	-	EXPRESSION TAG	UNP P37268
E	14	SER	-	EXPRESSION TAG	UNP P37268
E	15	HIS	-	EXPRESSION TAG	UNP P37268

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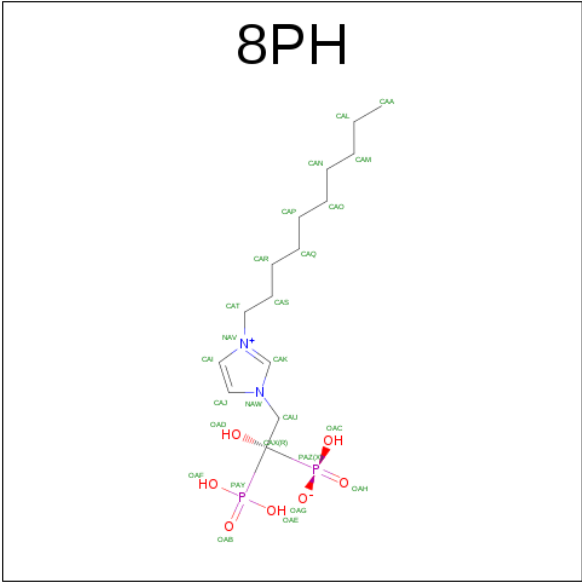
Chain	Residue	Modelled	Actual	Comment	Reference
E	16	HIS	-	EXPRESSION TAG	UNP P37268
E	17	HIS	-	EXPRESSION TAG	UNP P37268
E	18	HIS	-	EXPRESSION TAG	UNP P37268
E	19	HIS	-	EXPRESSION TAG	UNP P37268
E	20	HIS	-	EXPRESSION TAG	UNP P37268
E	21	SER	-	EXPRESSION TAG	UNP P37268
E	22	SER	-	EXPRESSION TAG	UNP P37268
E	23	GLY	-	EXPRESSION TAG	UNP P37268
E	24	LEU	-	EXPRESSION TAG	UNP P37268
E	25	VAL	-	EXPRESSION TAG	UNP P37268
E	26	PRO	-	EXPRESSION TAG	UNP P37268
E	27	ARG	-	EXPRESSION TAG	UNP P37268
E	28	GLY	-	EXPRESSION TAG	UNP P37268
E	29	SER	-	EXPRESSION TAG	UNP P37268
E	30	HIS	-	EXPRESSION TAG	UNP P37268
E	248	LEU	LYS	ENGINEERED MUTATION	UNP P37268
E	315	LEU	LYS	ENGINEERED MUTATION	UNP P37268
E	318	LEU	LYS	ENGINEERED MUTATION	UNP P37268
E	353	ASN	ASP	SEE REMARK 999	UNP P37268
F	11	MET	-	EXPRESSION TAG	UNP P37268
F	12	GLY	-	EXPRESSION TAG	UNP P37268
F	13	SER	-	EXPRESSION TAG	UNP P37268
F	14	SER	-	EXPRESSION TAG	UNP P37268
F	15	HIS	-	EXPRESSION TAG	UNP P37268
F	16	HIS	-	EXPRESSION TAG	UNP P37268
F	17	HIS	-	EXPRESSION TAG	UNP P37268
F	18	HIS	-	EXPRESSION TAG	UNP P37268
F	19	HIS	-	EXPRESSION TAG	UNP P37268
F	20	HIS	-	EXPRESSION TAG	UNP P37268
F	21	SER	-	EXPRESSION TAG	UNP P37268
F	22	SER	-	EXPRESSION TAG	UNP P37268
F	23	GLY	-	EXPRESSION TAG	UNP P37268
F	24	LEU	-	EXPRESSION TAG	UNP P37268
F	25	VAL	-	EXPRESSION TAG	UNP P37268
F	26	PRO	-	EXPRESSION TAG	UNP P37268
F	27	ARG	-	EXPRESSION TAG	UNP P37268
F	28	GLY	-	EXPRESSION TAG	UNP P37268
F	29	SER	-	EXPRESSION TAG	UNP P37268
F	30	HIS	-	EXPRESSION TAG	UNP P37268
F	248	LEU	LYS	ENGINEERED MUTATION	UNP P37268
F	315	LEU	LYS	ENGINEERED MUTATION	UNP P37268
F	318	LEU	LYS	ENGINEERED MUTATION	UNP P37268

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Chain	Residue	Modelled	Actual	Comment	Reference
F	353	ASN	ASP	SEE REMARK 999	UNP P37268

- Molecule 2 is HYDROGEN [(1R)-2-(3-DECYL-1H-IMIDAZOL-3-IUM-1-YL)-1-HYDROXY-1-PHOSPHONOETHYL]PHOSPHONATE (three-letter code: 8PH) (formula: C<sub>15</sub>H<sub>30</sub>N<sub>2</sub>O<sub>7</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 26	C 15	N 2	O 7	P 2	0	0
2	A	1	Total C 8 8					0	0
2	A	1	Total 18	C 7	N 2	O 7	P 2	0	0
2	B	1	Total 26	C 15	N 2	O 7	P 2	0	0
2	B	1	Total C 9 9					0	0
2	C	1	Total 26	C 15	N 2	O 7	P 2	0	0
2	D	1	Total 26	C 15	N 2	O 7	P 2	0	0
2	E	1	Total 26	C 15	N 2	O 7	P 2	0	0
2	F	1	Total 26	C 15	N 2	O 7	P 2	0	0
2	F	1	Total 26	C 15	N 2	O 7	P 2	0	0



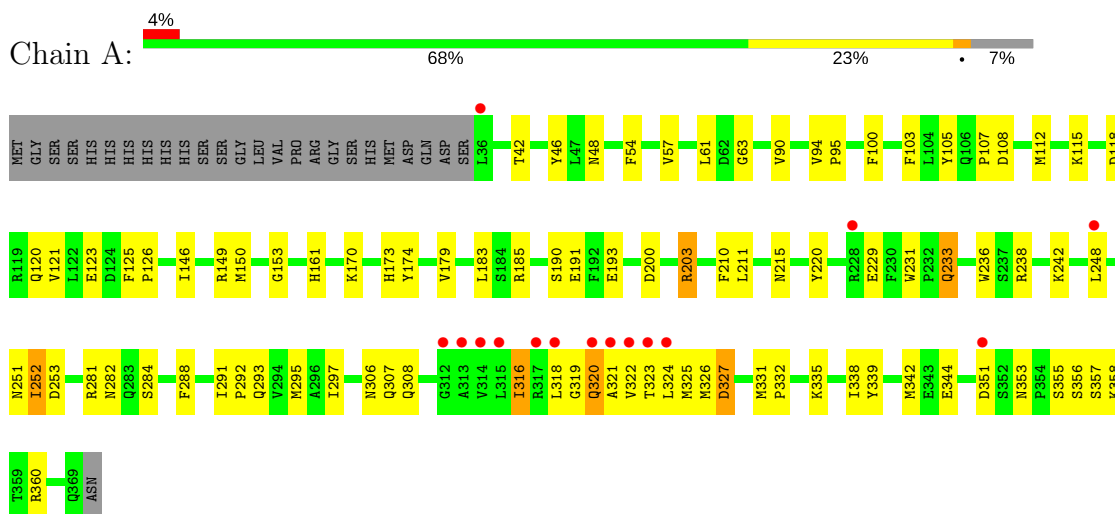
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	99	Total 99	O 99	0	0
3	B	89	Total 89	O 89	0	0
3	C	86	Total 86	O 86	0	0
3	D	62	Total 62	O 62	0	0
3	E	50	Total 50	O 50	0	0
3	F	41	Total 41	O 41	0	0

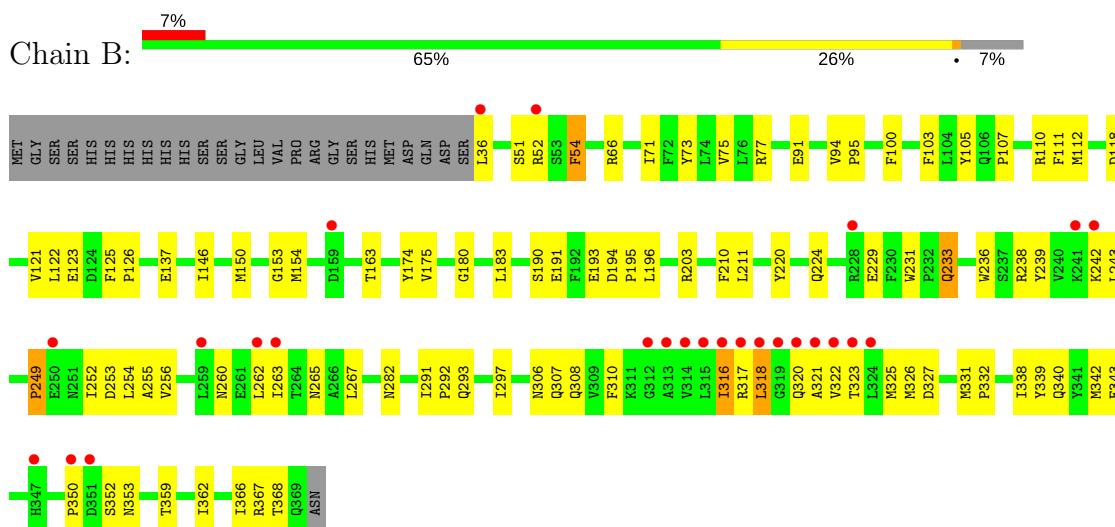
### 3 Residue-property plots

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

#### • Molecule 1: Squalene synthase

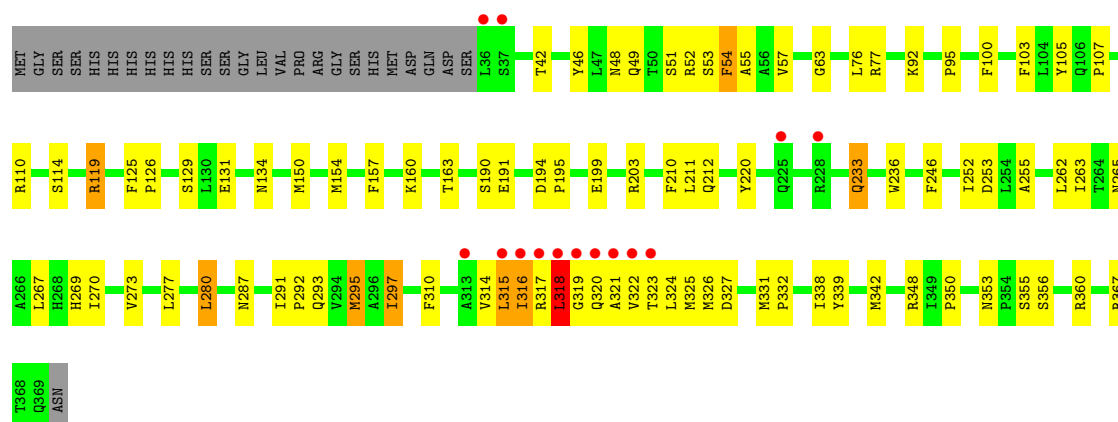


#### • Molecule 1: Squalene synthase

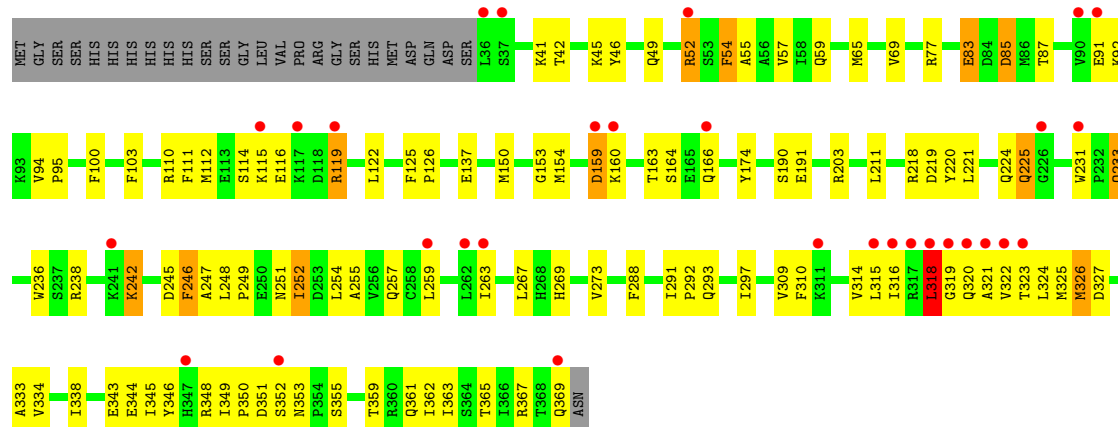


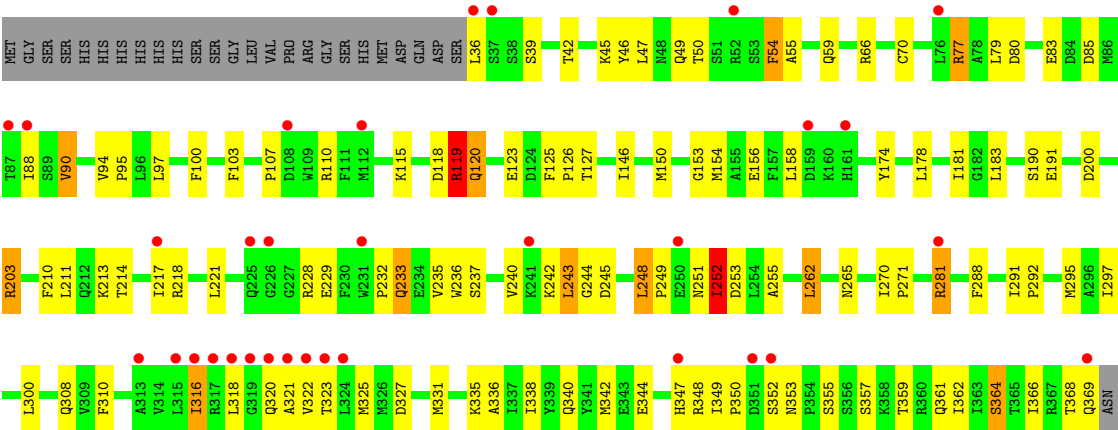
#### • Molecule 1: Squalene synthase





• Molecule 1: Squalene synthase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.63Å 153.55Å 90.40Å 90.00° 91.18° 90.00°	Depositor
Resolution (Å)	25.00 – 2.50 24.92 – 2.49	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.50) 96.7 (24.92-2.49)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.60 (at 2.50Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.192 , 0.250 0.202 , 0.230	Depositor DCC
$R_{free}$ test set	3966 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.6	Xtriage
Anisotropy	0.498	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 49.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	16820	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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: 8PH

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	0.38	0/2751	0.59	0/3724
1	B	0.35	0/2751	0.58	1/3724 (0.0%)
1	C	0.36	0/2751	0.60	0/3724
1	D	0.34	0/2751	0.57	1/3724 (0.0%)
1	E	0.35	0/2751	0.58	0/3724
1	F	0.33	0/2751	0.57	0/3724
All	All	0.35	0/16506	0.58	2/22344 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	54	PHE	N-CA-C	5.06	124.67	111.00
1	B	54	PHE	N-CA-C	5.04	124.62	111.00

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	2696	0	2676	68	0
1	B	2696	0	2676	85	0
1	C	2696	0	2676	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2696	0	2676	87	0
1	E	2696	0	2676	66	0
1	F	2696	0	2676	93	0
2	A	52	0	56	3	0
2	B	35	0	47	7	0
2	C	26	0	30	4	0
2	D	26	0	30	2	0
2	E	26	0	30	4	0
2	F	52	0	60	5	0
3	A	99	0	0	5	0
3	B	89	0	0	2	0
3	C	86	0	0	2	0
3	D	62	0	0	3	0
3	E	50	0	0	3	0
3	F	41	0	0	3	0
All	All	16820	0	16309	460	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 14.

All (460) 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:164:SER:HA	1:E:234:GLU:HG3	1.22	1.08
1:E:316:ILE:H	1:E:316:ILE:HD12	1.19	1.03
1:D:320:GLN:HG2	1:D:321:ALA:H	1.28	0.98
1:B:316:ILE:H	1:B:316:ILE:HD12	1.29	0.96
1:A:316:ILE:H	1:A:316:ILE:HD12	1.29	0.94
1:B:233:GLN:HA	1:B:236:TRP:NE1	1.82	0.94
1:F:320:GLN:HG2	1:F:321:ALA:H	1.33	0.93
1:A:183:LEU:HD21	2:A:402:8PH:H30	1.48	0.92
1:B:320:GLN:HG2	1:B:321:ALA:H	1.34	0.92
1:F:235:VAL:HG11	1:F:262:LEU:HD21	1.51	0.91
1:A:320:GLN:HG2	1:A:321:ALA:H	1.34	0.90
1:F:249:PRO:HA	1:F:252:ILE:HD13	1.55	0.88
1:F:316:ILE:HD12	1:F:316:ILE:H	1.36	0.87
1:E:321:ALA:HA	1:E:324:LEU:HB2	1.54	0.87
1:E:320:GLN:HG2	1:E:321:ALA:H	1.40	0.86
1:E:325:MET:O	1:F:327:ASP:HB2	1.74	0.86
1:B:322:VAL:HG21	1:C:53:SER:HB2	1.56	0.86
1:A:327:ASP:HB2	1:C:325:MET:O	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:PRO:HA	1:D:252:ILE:HD13	1.59	0.85
1:E:316:ILE:H	1:E:316:ILE:CD1	1.88	0.84
1:C:211:LEU:HD23	2:C:401:8PH:H19	1.60	0.83
1:B:316:ILE:N	1:B:316:ILE:HD12	1.96	0.81
1:A:320:GLN:HG2	1:A:321:ALA:N	1.95	0.80
1:E:260:ASN:HD22	1:E:353:ASN:ND2	1.80	0.79
1:B:211:LEU:HD22	2:B:401:8PH:H20	1.63	0.78
1:F:320:GLN:O	1:F:323:THR:HG22	1.84	0.77
1:C:320:GLN:HG2	1:C:321:ALA:H	1.50	0.77
1:F:150:MET:HG3	1:F:174:TYR:O	1.83	0.77
1:D:116:GLU:O	1:D:119:ARG:HD3	1.86	0.76
1:B:118:ASP:O	1:B:121:VAL:HG22	1.85	0.76
1:B:320:GLN:HG2	1:B:321:ALA:N	2.00	0.76
1:B:320:GLN:O	1:B:323:THR:HG22	1.86	0.75
1:B:325:MET:HG3	1:C:291:ILE:HG23	1.69	0.75
1:D:211:LEU:HD23	2:D:401:8PH:H18	1.68	0.74
1:B:325:MET:O	1:C:327:ASP:HB2	1.88	0.74
1:D:321:ALA:HA	1:D:324:LEU:HG	1.71	0.73
1:A:325:MET:O	1:B:327:ASP:HB2	1.89	0.73
1:D:353:ASN:ND2	1:D:355:SER:H	1.86	0.73
1:C:316:ILE:HD12	1:C:316:ILE:H	1.54	0.73
1:C:321:ALA:O	1:C:325:MET:HG2	1.88	0.72
1:E:164:SER:CA	1:E:234:GLU:HG3	2.10	0.72
1:E:320:GLN:HG2	1:E:321:ALA:N	2.05	0.72
1:A:211:LEU:HD13	1:A:293:GLN:NE2	2.04	0.71
1:E:115:LYS:HE2	1:E:115:LYS:HA	1.72	0.71
1:A:320:GLN:CG	1:A:321:ALA:H	2.02	0.71
1:D:320:GLN:HG2	1:D:321:ALA:N	2.04	0.71
1:D:319:GLY:HA3	1:D:323:THR:HG21	1.72	0.71
1:C:210:PHE:CE2	1:C:297:ILE:HD13	2.26	0.70
1:F:320:GLN:HG2	1:F:321:ALA:N	2.06	0.70
1:E:228:ARG:HG3	1:E:228:ARG:HH11	1.56	0.70
1:C:320:GLN:O	1:C:324:LEU:HG	1.91	0.70
1:D:150:MET:O	1:D:154:MET:HG3	1.92	0.70
1:A:353:ASN:HD22	1:A:355:SER:H	1.37	0.70
2:E:401:8PH:H6	3:E:522:HOH:O	1.92	0.70
1:A:353:ASN:ND2	1:A:355:SER:H	1.89	0.69
1:B:316:ILE:CD1	1:B:316:ILE:H	2.00	0.69
1:E:297:ILE:HD13	1:E:338:ILE:HG12	1.73	0.68
1:B:183:LEU:HD12	2:B:401:8PH:H26	1.75	0.68
1:B:343:GLU:OE1	1:C:48:ASN:HB3	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:586:HOH:O	1:C:325:MET:HE1	1.93	0.68
1:B:260:ASN:HD22	1:B:353:ASN:ND2	1.92	0.67
1:F:297:ILE:HD12	1:F:338:ILE:HG12	1.75	0.67
1:E:150:MET:O	1:E:154:MET:HG3	1.95	0.67
1:D:325:MET:O	1:E:327:ASP:HB2	1.95	0.66
1:F:255:ALA:HB1	1:F:310:PHE:CE2	2.30	0.66
1:A:306:ASN:OD1	1:A:308:GLN:HB3	1.96	0.66
1:F:100:PHE:HA	1:F:103:PHE:CD2	2.30	0.66
1:F:233:GLN:HA	1:F:236:TRP:NE1	2.11	0.66
1:F:350:PRO:HG2	1:F:353:ASN:HB2	1.77	0.66
1:F:94:VAL:HB	1:F:95:PRO:HD3	1.79	0.66
1:F:235:VAL:HG11	1:F:262:LEU:CD2	2.24	0.65
1:A:190:SER:O	1:A:191:GLU:HB2	1.95	0.65
1:C:316:ILE:HD12	1:C:316:ILE:N	2.12	0.65
1:B:73:TYR:HD2	2:B:402:8PH:H28	1.60	0.64
1:E:297:ILE:CD1	1:E:338:ILE:HG12	2.27	0.64
3:D:518:HOH:O	1:F:325:MET:HE1	1.97	0.64
1:E:51:SER:OG	1:E:54:PHE:HB2	1.97	0.64
1:F:353:ASN:ND2	1:F:355:SER:H	1.95	0.64
1:B:233:GLN:HA	1:B:236:TRP:CD1	2.32	0.63
1:D:87:THR:HG22	1:D:87:THR:O	1.97	0.63
1:F:150:MET:O	1:F:154:MET:HG3	1.99	0.63
1:A:316:ILE:N	1:A:316:ILE:HD12	2.09	0.62
1:B:297:ILE:HD12	1:B:338:ILE:HG12	1.81	0.62
1:C:320:GLN:HG2	1:C:321:ALA:N	2.15	0.62
1:D:320:GLN:O	1:D:323:THR:HG22	2.00	0.62
1:E:83:GLU:HG3	1:E:154:MET:HB3	1.82	0.62
1:F:54:PHE:CD2	2:F:402:8PH:H17	2.34	0.62
1:D:233:GLN:HA	1:D:236:TRP:NE1	2.15	0.62
1:C:131:GLU:HA	1:C:134:ASN:ND2	2.14	0.61
1:D:85:ASP:OD2	1:D:87:THR:HB	2.00	0.61
1:C:317:ARG:HD2	1:C:318:LEU:HD12	1.82	0.61
1:D:263:ILE:O	1:D:267:LEU:HG	2.01	0.61
1:D:211:LEU:HD13	1:D:293:GLN:NE2	2.15	0.61
1:B:331:MET:HB3	1:B:332:PRO:HD3	1.82	0.61
1:D:52:ARG:HG3	3:D:559:HOH:O	2.00	0.61
1:A:200:ASP:OD2	1:A:203:ARG:HB2	2.00	0.60
1:B:368:THR:HG22	1:B:368:THR:O	2.01	0.60
1:C:211:LEU:CD2	2:C:401:8PH:H19	2.29	0.60
1:B:350:PRO:HG2	1:B:353:ASN:HB2	1.84	0.60
1:E:50:THR:HG1	1:E:73:TYR:HE1	1.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:365:THR:O	1:D:369:GLN:HG3	2.02	0.60
1:E:119:ARG:O	1:E:123:GLU:HG3	2.02	0.60
1:F:200:ASP:OD2	1:F:203:ARG:HB2	2.02	0.60
1:A:293:GLN:O	1:A:297:ILE:HG12	2.02	0.59
1:E:260:ASN:HD22	1:E:353:ASN:HD21	1.46	0.59
1:C:211:LEU:HD13	1:C:293:GLN:NE2	2.16	0.59
1:F:245:ASP:O	1:F:248:LEU:HG	2.02	0.59
1:E:94:VAL:HB	1:E:95:PRO:HD3	1.84	0.59
1:A:211:LEU:HD13	1:A:293:GLN:HE22	1.67	0.59
1:A:233:GLN:HA	1:A:236:TRP:NE1	2.18	0.58
1:D:159:ASP:OD1	1:D:160:LYS:N	2.37	0.58
1:C:353:ASN:ND2	1:C:355:SER:H	2.01	0.58
1:D:163:THR:OG1	1:D:164:SER:N	2.36	0.58
1:A:319:GLY:O	1:A:320:GLN:O	2.20	0.58
1:F:119:ARG:O	1:F:123:GLU:HG3	2.02	0.58
1:C:100:PHE:HA	1:C:103:PHE:CD2	2.38	0.58
1:C:212:GLN:OE1	2:C:401:8PH:H12	2.04	0.58
1:D:291:ILE:HB	1:D:292:PRO:HD3	1.85	0.58
1:D:322:VAL:HG12	1:D:322:VAL:O	2.04	0.58
1:F:183:LEU:CD1	2:F:401:8PH:H26	2.33	0.58
1:A:220:TYR:HB2	1:A:231:TRP:CZ2	2.38	0.57
1:B:343:GLU:OE1	1:B:367:ARG:NH2	2.37	0.57
1:D:94:VAL:HB	1:D:95:PRO:HD3	1.86	0.57
1:E:180:GLY:HA2	2:E:401:8PH:H27	1.86	0.57
1:A:215:ASN:HD21	2:A:403:8PH:CAS	2.16	0.57
1:C:348:ARG:O	1:C:350:PRO:HD3	2.05	0.57
1:D:242:LYS:HB2	1:D:242:LYS:NZ	2.19	0.57
1:B:66:ARG:HD2	3:B:565:HOH:O	2.03	0.57
1:D:255:ALA:HB1	1:D:310:PHE:CE1	2.38	0.57
1:F:297:ILE:CD1	1:F:338:ILE:HG12	2.34	0.57
1:B:342:MET:CE	1:B:342:MET:HA	2.35	0.57
1:D:211:LEU:HD13	1:D:293:GLN:HE22	1.70	0.57
1:A:291:ILE:HB	1:A:292:PRO:HD3	1.87	0.56
1:D:346:TYR:HA	1:D:349:ILE:CD1	2.35	0.56
1:F:79:LEU:O	1:F:79:LEU:HD12	2.05	0.56
1:B:112:MET:SD	1:B:123:GLU:HG2	2.45	0.56
1:A:291:ILE:HD11	1:C:326:MET:CE	2.35	0.56
1:E:238:ARG:HH22	1:E:261:GLU:CD	2.07	0.56
1:B:326:MET:HE3	1:C:291:ILE:HD11	1.88	0.56
1:B:190:SER:O	1:B:191:GLU:HB2	2.05	0.56
1:B:320:GLN:CG	1:B:321:ALA:H	2.15	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:120:GLN:HE21	1:F:120:GLN:HA	1.70	0.56
1:E:325:MET:C	1:F:327:ASP:HB2	2.26	0.56
1:E:97:LEU:HD12	1:E:158:LEU:HD11	1.88	0.56
1:D:220:TYR:HB2	1:D:231:TRP:CZ2	2.42	0.55
1:E:316:ILE:HD12	1:E:316:ILE:N	2.04	0.55
1:A:331:MET:HB3	1:A:332:PRO:HD3	1.87	0.55
1:E:263:ILE:HG12	1:E:300:LEU:HD22	1.87	0.55
1:A:61:LEU:HA	1:A:284:SER:HB2	1.88	0.55
1:B:94:VAL:HB	1:B:95:PRO:HD3	1.87	0.55
1:F:291:ILE:HB	1:F:292:PRO:HD3	1.87	0.55
1:C:211:LEU:HD13	1:C:293:GLN:HE22	1.72	0.55
1:C:277:LEU:HA	1:C:280:LEU:HD22	1.87	0.55
1:C:338:ILE:O	1:C:342:MET:HG2	2.07	0.55
1:B:211:LEU:CD1	1:B:293:GLN:NE2	2.70	0.55
1:A:291:ILE:HD11	1:C:326:MET:HE1	1.88	0.55
1:A:316:ILE:H	1:A:316:ILE:CD1	2.09	0.55
1:E:77:ARG:HD3	1:E:77:ARG:O	2.07	0.55
1:F:255:ALA:HB1	1:F:310:PHE:CZ	2.41	0.54
1:A:112:MET:SD	1:A:123:GLU:HG2	2.47	0.54
1:A:210:PHE:CZ	1:A:297:ILE:HD13	2.43	0.54
1:A:94:VAL:HB	1:A:95:PRO:HD3	1.89	0.54
1:B:362:ILE:O	1:B:366:ILE:HG13	2.07	0.54
1:E:320:GLN:CG	1:E:321:ALA:H	2.18	0.54
1:B:297:ILE:HD13	1:B:338:ILE:HG23	1.88	0.54
1:E:209:LEU:HD23	1:E:269:HIS:CE1	2.43	0.54
1:F:233:GLN:HA	1:F:236:TRP:CD1	2.43	0.54
1:C:321:ALA:HA	1:C:324:LEU:HG	1.90	0.54
1:B:338:ILE:O	1:B:342:MET:HG2	2.08	0.54
1:C:263:ILE:O	1:C:267:LEU:HG	2.08	0.54
1:B:36:LEU:HB2	1:D:137:GLU:OE1	2.08	0.54
1:E:85:ASP:HB3	1:E:88:ILE:HD12	1.89	0.54
1:A:48:ASN:ND2	1:C:367:ARG:HD3	2.24	0.53
1:F:281:ARG:HH21	1:F:281:ARG:CG	2.21	0.53
1:F:320:GLN:CG	1:F:321:ALA:H	2.14	0.53
1:B:229:GLU:HG2	1:B:243:LEU:HD23	1.91	0.53
1:A:108:ASP:HB2	3:A:551:HOH:O	2.08	0.53
1:E:331:MET:HB3	1:E:332:PRO:HD3	1.90	0.53
1:B:252:ILE:CG2	1:B:253:ASP:N	2.71	0.53
1:F:336:ALA:O	1:F:340:GLN:HG2	2.09	0.53
1:F:349:ILE:HD13	1:F:359:THR:HB	1.92	0.52
1:B:239:TYR:O	1:B:254:LEU:HD13	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:ARG:HG3	1:B:318:LEU:N	2.22	0.52
1:C:105:TYR:O	1:C:107:PRO:HD3	2.09	0.52
1:D:245:ASP:O	1:D:247:ALA:N	2.43	0.52
1:E:211:LEU:HD13	1:E:293:GLN:NE2	2.25	0.52
1:F:211:LEU:HD23	2:F:401:8PH:H18	1.90	0.52
1:F:353:ASN:HD22	1:F:355:SER:H	1.57	0.52
1:C:220:TYR:CZ	1:C:246:PHE:HB2	2.43	0.52
1:F:362:ILE:O	1:F:366:ILE:HG13	2.10	0.52
1:F:45:LYS:HG2	1:F:49:GLN:HE21	1.73	0.52
1:A:57:VAL:HG11	1:A:288:PHE:HA	1.91	0.51
1:B:175:VAL:O	2:B:401:8PH:H10	2.11	0.51
1:F:344:GLU:O	1:F:348:ARG:HD3	2.10	0.51
1:A:150:MET:HG3	1:A:174:TYR:O	2.10	0.51
1:D:65:MET:O	1:D:69:VAL:HG23	2.10	0.51
1:E:321:ALA:CA	1:E:324:LEU:HB2	2.34	0.51
1:C:350:PRO:HG2	1:C:353:ASN:HB2	1.92	0.51
1:D:159:ASP:CG	1:D:160:LYS:N	2.64	0.51
1:D:55:ALA:O	1:D:59:GLN:HG3	2.10	0.51
1:E:261:GLU:HG3	3:E:543:HOH:O	2.10	0.51
1:F:39:SER:HB2	1:F:127:THR:HG23	1.93	0.51
1:F:55:ALA:O	1:F:59:GLN:HG3	2.10	0.51
1:E:51:SER:HB2	1:E:73:TYR:CZ	2.45	0.51
1:F:271:PRO:HB3	1:F:369:GLN:HE22	1.76	0.51
1:A:321:ALA:HA	1:A:324:LEU:CD1	2.41	0.51
1:C:255:ALA:HB1	1:C:310:PHE:CZ	2.46	0.51
1:F:77:ARG:HE	1:F:77:ARG:HA	1.75	0.51
1:B:193:GLU:OE2	1:B:282:ASN:HB3	2.11	0.51
1:D:45:LYS:O	1:D:49:GLN:HG3	2.10	0.51
1:B:211:LEU:HD13	1:B:293:GLN:HE22	1.76	0.51
1:F:353:ASN:ND2	1:F:355:SER:HB2	2.26	0.51
1:D:225:GLN:H	1:D:225:GLN:HE21	1.57	0.51
1:D:91:GLU:HG3	1:D:92:LYS:N	2.25	0.51
1:A:321:ALA:HA	1:A:324:LEU:HG	1.93	0.50
1:C:131:GLU:HA	1:C:134:ASN:HD22	1.73	0.50
1:B:233:GLN:HA	1:B:236:TRP:HE1	1.72	0.50
1:C:291:ILE:HB	1:C:292:PRO:HD3	1.91	0.50
1:C:339:TYR:O	1:C:342:MET:HB2	2.11	0.50
1:D:163:THR:HA	1:D:233:GLN:HB3	1.93	0.50
1:F:357:SER:O	1:F:361:GLN:HG3	2.11	0.50
1:A:327:ASP:HB2	1:C:325:MET:C	2.31	0.50
1:D:85:ASP:OD1	1:D:114:SER:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:356:SER:O	1:E:360:ARG:HG3	2.12	0.50
1:B:322:VAL:O	1:B:322:VAL:HG12	2.11	0.50
1:B:71:ILE:O	1:B:75:VAL:HG13	2.11	0.50
1:C:293:GLN:O	1:C:297:ILE:HG12	2.11	0.50
1:E:193:GLU:HA	1:E:281:ARG:HD3	1.93	0.50
1:B:291:ILE:HB	1:B:292:PRO:HD3	1.94	0.50
1:D:259:LEU:HD21	1:D:309:VAL:HG21	1.92	0.50
1:E:183:LEU:HD12	2:E:401:8PH:H26	1.92	0.50
1:E:118:ASP:O	1:E:121:VAL:HG13	2.12	0.50
1:E:149:ARG:NH2	1:E:185:ARG:HH12	2.10	0.50
1:B:256:VAL:HG21	1:B:307:GLN:HG2	1.94	0.49
1:B:91:GLU:CD	1:B:91:GLU:H	2.15	0.49
1:B:322:VAL:CG2	1:C:53:SER:HB2	2.33	0.49
1:E:321:ALA:HA	1:E:324:LEU:HD12	1.94	0.49
1:F:281:ARG:HD2	3:F:523:HOH:O	2.12	0.49
1:F:348:ARG:O	1:F:350:PRO:HD3	2.12	0.49
1:D:125:PHE:N	1:D:126:PRO:CD	2.76	0.49
1:D:87:THR:CG2	1:D:87:THR:O	2.60	0.49
1:A:149:ARG:NH2	1:A:185:ARG:HH22	2.11	0.49
1:C:314:VAL:CG1	1:C:315:LEU:N	2.74	0.49
1:F:322:VAL:HG12	1:F:322:VAL:O	2.12	0.49
1:A:100:PHE:HA	1:A:103:PHE:CD2	2.47	0.49
1:D:343:GLU:CD	1:D:367:ARG:HH21	2.15	0.49
1:F:190:SER:O	1:F:191:GLU:HB2	2.13	0.49
1:C:157:PHE:CE2	1:C:160:LYS:HE3	2.48	0.49
1:C:320:GLN:O	1:C:323:THR:HG22	2.13	0.49
1:D:254:LEU:HA	1:D:257:GLN:NE2	2.27	0.49
1:D:41:LYS:HD3	1:F:364:SER:OG	2.13	0.49
1:A:125:PHE:N	1:A:126:PRO:CD	2.76	0.49
1:A:210:PHE:CE2	1:A:297:ILE:HD13	2.48	0.49
1:C:195:PRO:O	1:C:199:GLU:HG3	2.12	0.49
1:C:317:ARG:HD2	1:C:318:LEU:CD1	2.42	0.49
1:D:110:ARG:HD2	1:D:112:MET:SD	2.53	0.49
1:F:240:VAL:HG21	1:F:245:ASP:HB2	1.95	0.49
1:F:331:MET:O	1:F:335:LYS:HG3	2.13	0.49
1:F:248:LEU:HD12	1:F:251:ASN:HD21	1.78	0.48
1:D:246:PHE:CD1	1:D:255:ALA:HA	2.48	0.48
1:F:232:PRO:HD2	1:F:262:LEU:HD11	1.95	0.48
1:D:153:GLY:HA3	1:D:174:TYR:CD1	2.48	0.48
1:D:345:ILE:O	1:D:349:ILE:HG13	2.12	0.48
1:A:118:ASP:O	1:A:121:VAL:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:322:VAL:HG22	1:E:295:MET:CE	2.44	0.48
1:A:63:GLY:HA3	3:A:510:HOH:O	2.12	0.48
1:A:327:ASP:OD2	1:B:327:ASP:OD2	2.32	0.48
1:B:150:MET:HG3	1:B:174:TYR:O	2.12	0.48
1:F:368:THR:HG22	1:F:368:THR:O	2.12	0.48
1:A:356:SER:O	1:A:360:ARG:HG3	2.13	0.48
1:A:90:VAL:O	1:A:94:VAL:HG23	2.14	0.48
1:D:211:LEU:CD2	2:D:401:8PH:H18	2.42	0.48
1:F:221:LEU:HD13	1:F:310:PHE:HA	1.96	0.48
1:C:114:SER:HB3	1:C:119:ARG:HB2	1.95	0.48
1:C:92:LYS:O	1:C:95:PRO:HG2	2.14	0.48
1:E:228:ARG:NH1	1:E:228:ARG:HG3	2.26	0.48
1:E:223:ASP:OD1	1:E:228:ARG:NH2	2.47	0.48
1:C:150:MET:O	1:C:154:MET:HG3	2.14	0.47
1:D:114:SER:O	1:D:115:LYS:HD2	2.14	0.47
1:D:163:THR:HA	1:D:233:GLN:HE21	1.77	0.47
1:D:238:ARG:NH1	1:D:238:ARG:HB2	2.28	0.47
1:A:320:GLN:CG	1:A:321:ALA:N	2.63	0.47
1:A:248:LEU:HB2	1:A:251:ASN:ND2	2.29	0.47
1:B:297:ILE:CD1	1:B:338:ILE:HG23	2.43	0.47
1:C:125:PHE:N	1:C:126:PRO:CD	2.78	0.47
1:D:255:ALA:HB1	1:D:310:PHE:CZ	2.50	0.47
1:C:42:THR:HG22	1:C:46:TYR:CE2	2.50	0.47
1:D:322:VAL:HG22	1:E:295:MET:HE1	1.97	0.47
1:D:353:ASN:HD22	1:D:355:SER:H	1.61	0.47
1:E:194:ASP:OD1	1:E:195:PRO:HD2	2.15	0.47
1:F:210:PHE:CZ	1:F:297:ILE:HG12	2.50	0.47
1:F:36:LEU:N	3:F:533:HOH:O	2.48	0.47
1:C:190:SER:O	1:C:191:GLU:HB2	2.14	0.47
1:F:146:ILE:HG22	1:F:150:MET:HE3	1.97	0.47
1:A:153:GLY:HA3	1:A:174:TYR:CG	2.50	0.46
1:C:210:PHE:HE2	1:C:297:ILE:HD13	1.78	0.46
1:C:270:ILE:HD13	1:C:342:MET:SD	2.55	0.46
1:F:146:ILE:HG22	1:F:150:MET:CE	2.44	0.46
1:B:326:MET:HE1	1:C:287:ASN:HB3	1.96	0.46
1:C:322:VAL:O	1:C:322:VAL:HG12	2.15	0.46
1:E:126:PRO:HA	1:E:129:SER:OG	2.15	0.46
1:F:47:LEU:HD22	1:F:70:CYS:SG	2.55	0.46
1:B:100:PHE:HA	1:B:103:PHE:CD2	2.50	0.46
1:E:324:LEU:HD13	3:E:517:HOH:O	2.14	0.46
1:C:320:GLN:CG	1:C:321:ALA:H	2.25	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:HIS:HD2	1:A:229:GLU:HB2	1.80	0.46
1:B:262:LEU:O	1:B:265:ASN:HB3	2.15	0.46
1:B:339:TYR:O	1:B:342:MET:HB2	2.16	0.46
1:D:83:GLU:HG3	1:D:154:MET:HB3	1.98	0.46
1:B:252:ILE:HG21	1:B:307:GLN:NE2	2.31	0.46
1:A:316:ILE:N	1:A:316:ILE:CD1	2.76	0.46
1:E:321:ALA:HA	1:E:324:LEU:CB	2.37	0.46
1:F:178:LEU:HD23	1:F:181:ILE:HD12	1.98	0.46
1:B:125:PHE:N	1:B:126:PRO:CD	2.79	0.46
1:D:318:LEU:HG	1:D:318:LEU:H	1.51	0.46
1:D:359:THR:O	1:D:362:ILE:HG22	2.15	0.46
1:F:218:ARG:HG2	1:F:218:ARG:O	2.16	0.46
1:A:338:ILE:O	1:A:342:MET:HG2	2.16	0.46
1:B:105:TYR:O	1:B:107:PRO:HD3	2.16	0.46
1:C:317:ARG:NH1	1:C:348:ARG:NH2	2.64	0.46
1:D:297:ILE:CD1	1:D:338:ILE:HG12	2.46	0.46
1:A:146:ILE:HG22	1:A:150:MET:HE3	1.98	0.45
1:A:242:LYS:HB2	1:A:242:LYS:NZ	2.30	0.45
1:B:52:ARG:HG3	3:B:572:HOH:O	2.16	0.45
1:F:66:ARG:HB3	3:F:532:HOH:O	2.16	0.45
1:F:85:ASP:HB3	1:F:88:ILE:HD12	1.98	0.45
1:A:335:LYS:HB3	1:A:339:TYR:CE2	2.52	0.45
1:D:346:TYR:HA	1:D:349:ILE:HD11	1.97	0.45
1:B:153:GLY:HA3	1:B:174:TYR:CG	2.52	0.45
1:C:220:TYR:OH	1:C:246:PHE:HB2	2.16	0.45
1:D:348:ARG:O	1:D:350:PRO:HD3	2.17	0.45
1:F:243:LEU:HD12	1:F:243:LEU:O	2.16	0.45
1:A:358:LYS:NZ	3:A:565:HOH:O	2.49	0.45
1:C:316:ILE:CD1	1:C:316:ILE:H	2.13	0.45
1:F:153:GLY:HA3	1:F:174:TYR:CD1	2.51	0.45
1:F:214:THR:HG23	1:F:300:LEU:CD2	2.46	0.45
1:B:183:LEU:CD1	2:B:401:8PH:H26	2.46	0.45
1:D:248:LEU:HB2	1:D:251:ASN:HD22	1.82	0.45
1:D:362:ILE:HG23	1:D:363:ILE:N	2.32	0.45
1:E:45:LYS:HG2	1:E:49:GLN:NE2	2.32	0.45
1:F:42:THR:HG22	1:F:46:TYR:CE2	2.51	0.45
1:F:125:PHE:N	1:F:126:PRO:CD	2.79	0.45
1:A:252:ILE:HD11	1:A:307:GLN:HB3	1.99	0.44
1:B:51:SER:O	1:B:52:ARG:C	2.55	0.44
1:C:321:ALA:O	1:C:325:MET:CG	2.60	0.44
1:D:238:ARG:HB2	1:D:238:ARG:HH11	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:233:GLN:O	1:F:237:SER:HB3	2.18	0.44
1:F:248:LEU:HA	1:F:249:PRO:HD3	1.88	0.44
1:A:322:VAL:O	1:A:322:VAL:CG1	2.64	0.44
1:C:331:MET:HB3	1:C:332:PRO:HD3	2.00	0.44
1:D:100:PHE:HA	1:D:103:PHE:CD2	2.53	0.44
1:E:155:ALA:HA	1:E:158:LEU:CD1	2.48	0.44
1:C:54:PHE:O	1:C:57:VAL:HG22	2.18	0.44
1:D:321:ALA:O	1:D:325:MET:HG2	2.17	0.44
2:C:401:8PH:H27	3:C:543:HOH:O	2.18	0.44
1:D:42:THR:HG22	1:D:46:TYR:CE2	2.53	0.44
1:B:211:LEU:HD11	1:B:293:GLN:NE2	2.32	0.44
1:F:156:GLU:O	1:F:156:GLU:HG2	2.18	0.44
1:C:318:LEU:HB2	1:C:319:GLY:H	1.47	0.44
1:B:325:MET:HE2	1:C:295:MET:HG3	2.00	0.43
1:B:252:ILE:HG23	1:B:307:GLN:HE21	1.83	0.43
1:D:269:HIS:O	1:D:273:VAL:HG23	2.18	0.43
1:E:100:PHE:HA	1:E:103:PHE:CD2	2.53	0.43
1:F:50:THR:HG22	1:F:118:ASP:OD1	2.18	0.43
1:F:228:ARG:HG3	1:F:228:ARG:HH11	1.82	0.43
1:B:211:LEU:CD1	1:B:293:GLN:HE22	2.31	0.43
1:D:190:SER:O	1:D:191:GLU:HB2	2.19	0.43
1:E:92:LYS:O	1:E:95:PRO:HD2	2.18	0.43
1:A:193:GLU:OE2	1:A:282:ASN:HB3	2.18	0.43
1:D:150:MET:HG3	1:D:174:TYR:O	2.19	0.43
1:A:291:ILE:HG21	1:C:322:VAL:HG13	2.01	0.43
1:C:163:THR:HA	1:C:233:GLN:HB3	2.00	0.43
1:C:51:SER:HB3	1:C:55:ALA:HB2	2.00	0.43
1:E:125:PHE:N	1:E:126:PRO:CD	2.81	0.43
1:E:133:ARG:HA	1:E:140:GLN:NE2	2.33	0.43
1:C:324:LEU:HD12	3:C:535:HOH:O	2.18	0.43
1:D:334:VAL:O	1:D:338:ILE:HG13	2.19	0.43
1:F:213:LYS:O	1:F:217:ILE:HG13	2.19	0.43
1:B:150:MET:O	1:B:154:MET:HG3	2.18	0.43
1:B:359:THR:O	1:B:362:ILE:HG22	2.18	0.43
1:B:236:TRP:CZ3	1:B:242:LYS:HA	2.54	0.43
1:C:317:ARG:NH1	1:C:348:ARG:HH21	2.17	0.43
1:D:153:GLY:HA3	1:D:174:TYR:CG	2.53	0.43
1:B:111:PHE:HB3	1:B:122:LEU:HB3	2.01	0.43
1:B:194:ASP:OD1	1:B:195:PRO:HD2	2.18	0.43
1:B:306:ASN:OD1	1:B:306:ASN:C	2.57	0.43
1:F:262:LEU:O	1:F:265:ASN:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ARG:HB2	1:A:238:ARG:HH11	1.84	0.43
1:D:221:LEU:O	1:D:224:GLN:N	2.52	0.43
2:E:401:8PH:H17	2:E:401:8PH:H10	2.01	0.43
1:F:338:ILE:O	1:F:342:MET:HG2	2.19	0.43
1:A:252:ILE:HG23	1:A:253:ASP:N	2.33	0.42
1:E:150:MET:HG3	1:E:174:TYR:O	2.19	0.42
1:E:109:TRP:CH2	1:E:111:PHE:HB2	2.54	0.42
1:F:281:ARG:NH2	1:F:281:ARG:CG	2.81	0.42
1:F:79:LEU:HB2	1:F:100:PHE:CE2	2.55	0.42
1:A:238:ARG:NH1	1:A:238:ARG:HB2	2.35	0.42
1:B:263:ILE:O	1:B:267:LEU:HG	2.20	0.42
1:B:220:TYR:CZ	1:B:224:GLN:HG3	2.54	0.42
1:F:233:GLN:HB3	1:F:233:GLN:HE21	1.51	0.42
3:A:578:HOH:O	1:B:66:ARG:HD3	2.19	0.42
1:D:344:GLU:HG2	3:D:540:HOH:O	2.19	0.42
1:F:45:LYS:HG2	1:F:49:GLN:NE2	2.35	0.42
1:F:90:VAL:O	1:F:94:VAL:HG23	2.18	0.42
1:F:270:ILE:CD1	1:F:342:MET:HE3	2.50	0.42
1:A:170:LYS:O	1:A:173:HIS:HB3	2.20	0.42
1:A:353:ASN:ND2	1:A:355:SER:HB2	2.35	0.42
1:B:210:PHE:CZ	1:B:297:ILE:HG12	2.55	0.42
1:C:356:SER:O	1:C:360:ARG:HG3	2.20	0.42
1:E:190:SER:O	1:E:191:GLU:HB2	2.20	0.42
1:F:54:PHE:HE2	1:F:288:PHE:CE1	2.38	0.42
1:B:252:ILE:CG2	1:B:307:GLN:NE2	2.82	0.42
1:C:76:LEU:HD22	1:C:150:MET:SD	2.60	0.42
1:D:116:GLU:O	1:D:119:ARG:CD	2.63	0.42
1:D:220:TYR:OH	1:D:246:PHE:HB2	2.20	0.42
1:E:334:VAL:O	1:E:338:ILE:HG13	2.20	0.42
1:B:306:ASN:OD1	1:B:308:GLN:N	2.50	0.41
1:C:269:HIS:O	1:C:273:VAL:HG23	2.20	0.41
1:F:242:LYS:O	1:F:244:GLY:N	2.53	0.41
1:A:179:VAL:HB	2:A:401:8PH:H19	2.02	0.41
1:E:211:LEU:HD13	1:E:293:GLN:HE22	1.85	0.41
2:B:401:8PH:H21	2:B:402:8PH:H22	2.03	0.41
1:E:50:THR:OG1	1:E:73:TYR:HE1	2.01	0.41
1:F:100:PHE:HA	1:F:103:PHE:CE2	2.55	0.41
1:D:326:MET:HE1	1:D:333:ALA:HA	2.01	0.41
1:F:229:GLU:HB3	1:F:243:LEU:HD23	2.03	0.41
1:B:342:MET:HE2	1:B:342:MET:HA	2.00	0.41
1:C:194:ASP:OD2	1:C:195:PRO:HD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:233:GLN:HA	1:E:236:TRP:CE2	2.56	0.41
1:E:291:ILE:HB	1:E:292:PRO:HD3	2.02	0.41
1:F:80:ASP:OD1	2:F:401:8PH:H7	2.19	0.41
1:B:255:ALA:HB1	1:B:310:PHE:CZ	2.56	0.41
1:C:252:ILE:HG23	1:C:253:ASP:N	2.36	0.41
1:D:349:ILE:HA	1:D:350:PRO:HD3	1.91	0.41
1:D:248:LEU:HA	1:D:249:PRO:HD2	1.90	0.41
1:D:57:VAL:HG11	1:D:288:PHE:HA	2.03	0.41
1:F:153:GLY:HA3	1:F:174:TYR:CG	2.56	0.41
1:C:77:ARG:HA	1:C:77:ARG:HD2	1.92	0.41
1:D:159:ASP:CG	1:D:160:LYS:H	2.22	0.41
1:D:245:ASP:C	1:D:247:ALA:N	2.75	0.41
1:E:149:ARG:HH21	1:E:185:ARG:HH12	1.69	0.41
1:E:221:LEU:HG	1:E:225:GLN:OE1	2.21	0.41
1:B:220:TYR:HB2	1:B:231:TRP:CZ2	2.56	0.40
1:C:51:SER:OG	1:C:54:PHE:HB2	2.22	0.40
1:D:218:ARG:HG2	1:D:218:ARG:O	2.20	0.40
1:F:183:LEU:HD13	2:F:401:8PH:H26	2.02	0.40
1:C:233:GLN:HA	1:C:236:TRP:NE1	2.37	0.40
1:D:111:PHE:HB3	1:D:122:LEU:HB3	2.03	0.40
1:D:77:ARG:HA	1:D:77:ARG:HD3	1.97	0.40
1:F:252:ILE:HG22	1:F:253:ASP:OD2	2.21	0.40
1:A:105:TYR:O	1:A:107:PRO:HD3	2.21	0.40
1:B:163:THR:HA	1:B:233:GLN:HB3	2.04	0.40
1:D:163:THR:CA	1:D:233:GLN:HE21	2.35	0.40
1:A:251:ASN:O	1:A:252:ILE:C	2.60	0.40
1:B:146:ILE:HG22	1:B:150:MET:HE3	2.02	0.40
1:B:180:GLY:HA2	2:B:401:8PH:H27	2.03	0.40
1:C:262:LEU:O	1:C:265:ASN:HB3	2.21	0.40
1:F:97:LEU:HD12	1:F:158:LEU:HD11	2.04	0.40
1:A:42:THR:HG22	1:A:46:TYR:CE2	2.57	0.40
1:C:353:ASN:HD22	1:C:355:SER:H	1.70	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	332/360 (92%)	314 (95%)	15 (4%)	3 (1%)	20	36
1	B	332/360 (92%)	312 (94%)	18 (5%)	2 (1%)	28	48
1	C	332/360 (92%)	317 (96%)	12 (4%)	3 (1%)	20	36
1	D	332/360 (92%)	311 (94%)	17 (5%)	4 (1%)	15	27
1	E	332/360 (92%)	318 (96%)	10 (3%)	4 (1%)	15	27
1	F	332/360 (92%)	305 (92%)	21 (6%)	6 (2%)	10	17
All	All	1992/2160 (92%)	1877 (94%)	93 (5%)	22 (1%)	17	29

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	318	LEU
1	A	320	GLN
1	B	318	LEU
1	C	318	LEU
1	D	318	LEU
1	F	318	LEU
1	D	85	ASP
1	D	246	PHE
1	E	200	ASP
1	F	243	LEU
1	E	54	PHE
1	E	107	PRO
1	E	328	ALA
1	F	252	ILE
1	A	252	ILE
1	B	249	PRO
1	D	252	ILE
1	F	308	GLN
1	C	54	PHE
1	F	119	ARG
1	F	107	PRO
1	C	63	GLY

### 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	297/320 (93%)	283 (95%)	14 (5%)	30	54
1	B	297/320 (93%)	285 (96%)	12 (4%)	36	62
1	C	297/320 (93%)	284 (96%)	13 (4%)	33	57
1	D	297/320 (93%)	277 (93%)	20 (7%)	19	35
1	E	297/320 (93%)	282 (95%)	15 (5%)	28	50
1	F	297/320 (93%)	278 (94%)	19 (6%)	20	38
All	All	1782/1920 (93%)	1689 (95%)	93 (5%)	27	49

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	PHE
1	A	115	LYS
1	A	120	GLN
1	A	203	ARG
1	A	233	GLN
1	A	281	ARG
1	A	295	MET
1	A	316	ILE
1	A	323	THR
1	A	326	MET
1	A	327	ASP
1	A	344	GLU
1	A	351	ASP
1	A	357	SER
1	B	54	PHE
1	B	77	ARG
1	B	110	ARG
1	B	137	GLU
1	B	196	LEU
1	B	203	ARG
1	B	233	GLN
1	B	238	ARG

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Mol	Chain	Res	Type
1	B	249	PRO
1	B	316	ILE
1	B	340	GLN
1	B	352	SER
1	C	49	GLN
1	C	52	ARG
1	C	110	ARG
1	C	119	ARG
1	C	129	SER
1	C	203	ARG
1	C	233	GLN
1	C	280	LEU
1	C	295	MET
1	C	297	ILE
1	C	315	LEU
1	C	316	ILE
1	C	318	LEU
1	D	52	ARG
1	D	54	PHE
1	D	83	GLU
1	D	119	ARG
1	D	159	ASP
1	D	166	GLN
1	D	203	ARG
1	D	219	ASP
1	D	225	GLN
1	D	233	GLN
1	D	242	LYS
1	D	314	VAL
1	D	315	LEU
1	D	316	ILE
1	D	318	LEU
1	D	326	MET
1	D	327	ASP
1	D	351	ASP
1	D	352	SER
1	D	361	GLN
1	E	52	ARG
1	E	54	PHE
1	E	80	ASP
1	E	83	GLU
1	E	86	MET

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Mol	Chain	Res	Type
1	E	121	VAL
1	E	203	ARG
1	E	233	GLN
1	E	281	ARG
1	E	295	MET
1	E	316	ILE
1	E	324	LEU
1	E	325	MET
1	E	340	GLN
1	E	344	GLU
1	F	54	PHE
1	F	77	ARG
1	F	83	GLU
1	F	90	VAL
1	F	110	ARG
1	F	115	LYS
1	F	119	ARG
1	F	120	GLN
1	F	203	ARG
1	F	233	GLN
1	F	248	LEU
1	F	252	ILE
1	F	262	LEU
1	F	281	ARG
1	F	295	MET
1	F	316	ILE
1	F	347	HIS
1	F	352	SER
1	F	364	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	59	GLN
1	A	161	HIS
1	A	215	ASN
1	A	225	GLN
1	A	233	GLN
1	A	251	ASN
1	A	257	GLN
1	A	293	GLN

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Mol	Chain	Res	Type
1	A	369	GLN
1	B	48	ASN
1	B	59	GLN
1	B	225	GLN
1	B	233	GLN
1	B	251	ASN
1	B	257	GLN
1	B	293	GLN
1	B	307	GLN
1	B	353	ASN
1	C	48	ASN
1	C	59	GLN
1	C	120	GLN
1	C	134	ASN
1	C	225	GLN
1	C	233	GLN
1	C	257	GLN
1	C	293	GLN
1	D	48	ASN
1	D	59	GLN
1	D	101	HIS
1	D	224	GLN
1	D	225	GLN
1	D	233	GLN
1	D	251	ASN
1	D	293	GLN
1	D	353	ASN
1	E	49	GLN
1	E	140	GLN
1	E	215	ASN
1	E	257	GLN
1	E	293	GLN
1	E	353	ASN
1	F	48	ASN
1	F	49	GLN
1	F	59	GLN
1	F	101	HIS
1	F	120	GLN
1	F	225	GLN
1	F	233	GLN
1	F	251	ASN
1	F	257	GLN

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Mol	Chain	Res	Type
1	F	308	GLN
1	F	340	GLN
1	F	369	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 ⓘ

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	8PH	A	401	-	25,26,26	2.28	9 (36%)	31,37,37	1.30	5 (16%)
2	8PH	A	402	-	7,7,26	0.34	0	6,6,37	0.72	0
2	8PH	A	403	-	17,18,26	2.73	9 (52%)	23,29,37	1.43	4 (17%)
2	8PH	B	401	-	25,26,26	2.26	9 (36%)	31,37,37	1.33	5 (16%)
2	8PH	B	402	-	8,8,26	0.34	0	7,7,37	0.80	0
2	8PH	C	401	-	25,26,26	2.25	9 (36%)	31,37,37	1.32	5 (16%)
2	8PH	D	401	-	25,26,26	2.27	9 (36%)	31,37,37	1.25	4 (12%)
2	8PH	E	401	-	25,26,26	2.28	9 (36%)	31,37,37	1.27	4 (12%)
2	8PH	F	401	-	25,26,26	2.29	9 (36%)	31,37,37	1.28	5 (16%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	8PH	F	402	-	25,26,26	2.31	9 (36%)	31,37,37	1.33	4 (12%)

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	8PH	A	401	-	-	0/33/33/33	0/1/1/1
2	8PH	A	402	-	-	0/5/5/33	0/0/0/1
2	8PH	A	403	-	-	0/25/25/33	0/1/1/1
2	8PH	B	401	-	-	0/33/33/33	0/1/1/1
2	8PH	B	402	-	-	0/6/6/33	0/0/0/1
2	8PH	C	401	-	-	0/33/33/33	0/1/1/1
2	8PH	D	401	-	-	0/33/33/33	0/1/1/1
2	8PH	E	401	-	-	0/33/33/33	0/1/1/1
2	8PH	F	401	-	-	0/33/33/33	0/1/1/1
2	8PH	F	402	-	-	0/33/33/33	0/1/1/1

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	402	8PH	PAZ-OAC	-3.51	1.48	1.54
2	A	401	8PH	PAZ-OAC	-3.51	1.48	1.54
2	F	401	8PH	PAZ-OAC	-3.48	1.48	1.54
2	A	403	8PH	PAZ-OAC	-3.46	1.48	1.54
2	E	401	8PH	PAZ-OAC	-3.43	1.48	1.54
2	B	401	8PH	PAZ-OAC	-3.43	1.48	1.54
2	D	401	8PH	PAZ-OAC	-3.41	1.48	1.54
2	C	401	8PH	PAZ-OAC	-3.38	1.48	1.54
2	F	402	8PH	CAI-NAV	-2.49	1.33	1.37
2	E	401	8PH	CAJ-NAW	-2.47	1.33	1.37
2	F	401	8PH	CAI-NAV	-2.43	1.33	1.37
2	E	401	8PH	CAI-NAV	-2.40	1.33	1.37
2	B	401	8PH	CAJ-NAW	-2.39	1.33	1.37
2	B	401	8PH	CAI-NAV	-2.35	1.33	1.37
2	F	401	8PH	CAJ-NAW	-2.34	1.33	1.37
2	D	401	8PH	CAI-NAV	-2.32	1.33	1.37
2	D	401	8PH	CAJ-NAW	-2.32	1.33	1.37
2	A	401	8PH	CAJ-NAW	-2.31	1.33	1.37
2	C	401	8PH	CAI-NAV	-2.31	1.33	1.37
2	A	401	8PH	CAI-NAV	-2.27	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	402	8PH	CAJ-NAW	-2.27	1.33	1.37
2	A	403	8PH	CAI-NAV	-2.25	1.33	1.37
2	A	403	8PH	CAJ-NAW	-2.24	1.33	1.37
2	C	401	8PH	CAJ-NAW	-2.20	1.33	1.37
2	A	401	8PH	PAY-CAX	2.57	1.86	1.85
2	C	401	8PH	PAY-CAX	2.64	1.87	1.85
2	C	401	8PH	PAZ-CAX	2.71	1.87	1.85
2	F	401	8PH	PAY-CAX	2.72	1.87	1.85
2	B	401	8PH	PAY-CAX	2.75	1.87	1.85
2	A	403	8PH	PAZ-CAX	2.75	1.87	1.85
2	B	401	8PH	PAZ-CAX	2.78	1.87	1.85
2	D	401	8PH	PAY-CAX	2.79	1.87	1.85
2	E	401	8PH	PAY-CAX	2.79	1.87	1.85
2	D	401	8PH	PAZ-CAX	2.82	1.87	1.85
2	A	403	8PH	PAY-CAX	2.82	1.87	1.85
2	F	402	8PH	PAY-CAX	2.93	1.87	1.85
2	E	401	8PH	PAZ-CAX	2.96	1.87	1.85
2	F	401	8PH	PAZ-CAX	2.99	1.87	1.85
2	F	402	8PH	PAZ-CAX	3.03	1.87	1.85
2	A	401	8PH	PAZ-CAX	3.14	1.87	1.85
2	B	401	8PH	PAY-OAF	3.54	1.61	1.54
2	A	401	8PH	PAY-OAF	3.58	1.61	1.54
2	C	401	8PH	PAZ-OAG	3.58	1.61	1.54
2	B	401	8PH	PAY-OAE	3.58	1.61	1.54
2	A	403	8PH	PAY-OAE	3.59	1.61	1.54
2	B	401	8PH	PAZ-OAG	3.59	1.61	1.54
2	D	401	8PH	PAZ-OAG	3.59	1.61	1.54
2	F	402	8PH	PAY-OAE	3.60	1.61	1.54
2	A	401	8PH	PAY-OAE	3.60	1.61	1.54
2	F	401	8PH	PAZ-OAG	3.61	1.61	1.54
2	F	401	8PH	PAY-OAE	3.61	1.61	1.54
2	A	403	8PH	PAY-OAF	3.61	1.61	1.54
2	C	401	8PH	PAY-OAE	3.61	1.61	1.54
2	F	402	8PH	PAY-OAF	3.62	1.61	1.54
2	E	401	8PH	PAZ-OAG	3.62	1.61	1.54
2	C	401	8PH	PAY-OAF	3.62	1.61	1.54
2	A	401	8PH	PAZ-OAG	3.62	1.61	1.54
2	E	401	8PH	PAY-OAF	3.63	1.61	1.54
2	D	401	8PH	PAY-OAE	3.63	1.61	1.54
2	F	401	8PH	PAY-OAF	3.63	1.61	1.54
2	F	402	8PH	PAZ-OAG	3.63	1.61	1.54
2	E	401	8PH	PAY-OAE	3.63	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	8PH	PAY-OAF	3.64	1.61	1.54
2	A	403	8PH	PAZ-OAG	3.65	1.61	1.54
2	A	403	8PH	PAZ-OAH	6.79	1.61	1.50
2	E	401	8PH	PAZ-OAH	6.80	1.61	1.50
2	D	401	8PH	PAZ-OAH	6.82	1.61	1.50
2	F	401	8PH	PAZ-OAH	6.83	1.61	1.50
2	C	401	8PH	PAZ-OAH	6.85	1.61	1.50
2	A	401	8PH	PAZ-OAH	6.86	1.61	1.50
2	B	401	8PH	PAZ-OAH	6.86	1.61	1.50
2	F	402	8PH	PAZ-OAH	6.91	1.61	1.50

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	8PH	OAG-PAZ-OAH	-3.19	105.92	113.05
2	F	402	8PH	OAG-PAZ-OAH	-3.15	106.00	113.05
2	D	401	8PH	OAG-PAZ-OAH	-3.13	106.05	113.05
2	A	403	8PH	OAG-PAZ-OAH	-3.10	106.11	113.05
2	B	401	8PH	OAG-PAZ-OAH	-3.06	106.20	113.05
2	E	401	8PH	OAG-PAZ-OAH	-3.04	106.24	113.05
2	C	401	8PH	OAG-PAZ-OAH	-3.03	106.26	113.05
2	F	401	8PH	OAG-PAZ-OAH	-3.03	106.26	113.05
2	A	401	8PH	PAZ-CAX-PAY	-2.63	107.84	112.70
2	F	401	8PH	PAZ-CAX-PAY	-2.22	108.59	112.70
2	C	401	8PH	PAZ-CAX-PAY	-2.20	108.62	112.70
2	B	401	8PH	PAZ-CAX-PAY	-2.13	108.77	112.70
2	E	401	8PH	PAZ-CAX-OAD	2.21	112.45	107.24
2	D	401	8PH	PAZ-CAX-OAD	2.40	112.91	107.24
2	E	401	8PH	PAY-CAX-OAD	2.45	113.03	107.24
2	D	401	8PH	PAY-CAX-OAD	2.49	113.12	107.24
2	A	401	8PH	PAZ-CAX-OAD	2.53	113.21	107.24
2	B	401	8PH	PAZ-CAX-OAD	2.59	113.34	107.24
2	A	403	8PH	PAY-CAX-OAD	2.60	113.37	107.24
2	A	403	8PH	PAZ-CAX-OAD	2.61	113.39	107.24
2	F	401	8PH	PAZ-CAX-OAD	2.61	113.39	107.24
2	A	401	8PH	PAY-CAX-OAD	2.61	113.40	107.24
2	C	401	8PH	PAZ-CAX-OAD	2.62	113.43	107.24
2	F	402	8PH	PAZ-CAX-OAD	2.67	113.54	107.24
2	C	401	8PH	PAY-CAX-OAD	2.70	113.62	107.24
2	B	401	8PH	PAY-CAX-OAD	2.72	113.65	107.24
2	F	402	8PH	PAY-CAX-OAD	2.75	113.72	107.24
2	F	401	8PH	PAY-CAX-OAD	2.82	113.90	107.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	8PH	OAC-PAZ-CAX	2.87	112.39	106.04
2	E	401	8PH	OAC-PAZ-CAX	2.90	112.44	106.04
2	D	401	8PH	OAC-PAZ-CAX	2.98	112.62	106.04
2	A	403	8PH	OAC-PAZ-CAX	3.01	112.69	106.04
2	A	401	8PH	OAC-PAZ-CAX	3.03	112.74	106.04
2	C	401	8PH	OAC-PAZ-CAX	3.04	112.76	106.04
2	B	401	8PH	OAC-PAZ-CAX	3.05	112.78	106.04
2	F	402	8PH	OAC-PAZ-CAX	3.13	112.95	106.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	8PH	1	0
2	A	402	8PH	1	0
2	A	403	8PH	1	0
2	B	401	8PH	6	0
2	B	402	8PH	2	0
2	C	401	8PH	4	0
2	D	401	8PH	2	0
2	E	401	8PH	4	0
2	F	401	8PH	4	0
2	F	402	8PH	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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	334/360 (92%)	-0.09	15 (4%)	34 36	17, 32, 68, 114	0
1	B	334/360 (92%)	0.16	26 (7%)	14 14	20, 36, 74, 119	0
1	C	334/360 (92%)	-0.04	14 (4%)	37 39	19, 35, 63, 107	0
1	D	334/360 (92%)	0.28	30 (8%)	10 10	22, 48, 86, 123	0
1	E	334/360 (92%)	0.28	23 (6%)	18 18	28, 48, 85, 123	0
1	F	334/360 (92%)	0.55	32 (9%)	9 8	28, 56, 95, 137	0
All	All	2004/2160 (92%)	0.19	140 (6%)	17 17	17, 41, 86, 137	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	321	ALA	14.7
1	F	320	GLN	14.6
1	F	319	GLY	10.1
1	B	321	ALA	9.6
1	D	319	GLY	9.2
1	F	323	THR	9.1
1	E	323	THR	8.2
1	D	321	ALA	7.8
1	F	322	VAL	7.5
1	E	320	GLN	7.0
1	F	318	LEU	6.9
1	A	320	GLN	6.8
1	B	317	ARG	6.6
1	B	319	GLY	6.5
1	B	320	GLN	6.3
1	F	315	LEU	6.1
1	B	318	LEU	6.0
1	E	315	LEU	5.9
1	C	321	ALA	5.7

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Mol	Chain	Res	Type	RSRZ
1	C	317	ARG	5.7
1	D	318	LEU	5.4
1	A	321	ALA	5.3
1	E	36	LEU	4.9
1	A	315	LEU	4.9
1	F	36	LEU	4.9
1	D	323	THR	4.8
1	E	319	GLY	4.7
1	F	313	ALA	4.7
1	F	161	HIS	4.6
1	D	317	ARG	4.6
1	D	322	VAL	4.4
1	C	322	VAL	4.4
1	B	322	VAL	4.4
1	C	36	LEU	4.3
1	E	322	VAL	4.2
1	F	316	ILE	4.2
1	D	316	ILE	4.2
1	B	316	ILE	4.1
1	F	351	ASP	4.1
1	B	315	LEU	4.0
1	D	241	LYS	4.0
1	D	320	GLN	4.0
1	E	318	LEU	4.0
1	E	159	ASP	4.0
1	D	160	LYS	3.9
1	D	36	LEU	3.9
1	B	351	ASP	3.7
1	F	37	SER	3.7
1	A	36	LEU	3.7
1	E	321	ALA	3.7
1	E	324	LEU	3.6
1	A	322	VAL	3.6
1	F	317	ARG	3.5
1	B	323	THR	3.5
1	F	241	LYS	3.5
1	D	315	LEU	3.5
1	E	86	MET	3.5
1	B	36	LEU	3.5
1	D	90	VAL	3.5
1	F	352	SER	3.4
1	F	347	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	317	ARG	3.4
1	C	320	GLN	3.3
1	A	324	LEU	3.3
1	C	313	ALA	3.3
1	B	324	LEU	3.3
1	E	37	SER	3.3
1	C	316	ILE	3.2
1	A	312	GLY	3.2
1	C	318	LEU	3.2
1	F	112	MET	3.2
1	E	87	THR	3.1
1	D	352	SER	3.1
1	D	52	ARG	3.0
1	D	159	ASP	3.0
1	B	259	LEU	3.0
1	E	326	MET	3.0
1	D	115	LYS	2.9
1	B	312	GLY	2.9
1	B	313	ALA	2.9
1	D	347	HIS	2.9
1	E	52	ARG	2.9
1	B	241	LYS	2.8
1	A	313	ALA	2.8
1	D	166	GLN	2.8
1	D	91	GLU	2.8
1	F	369	GLN	2.7
1	F	76	LEU	2.7
1	E	312	GLY	2.7
1	F	225	GLN	2.7
1	D	263	ILE	2.7
1	A	317	ARG	2.7
1	A	318	LEU	2.7
1	F	159	ASP	2.6
1	F	217	ILE	2.6
1	E	369	GLN	2.6
1	C	315	LEU	2.6
1	C	37	SER	2.6
1	B	350	PRO	2.6
1	D	262	LEU	2.6
1	C	225	GLN	2.6
1	B	52	ARG	2.6
1	F	88	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	159	ASP	2.5
1	A	323	THR	2.5
1	A	228	ARG	2.5
1	B	314	VAL	2.5
1	C	319	GLY	2.5
1	F	52	ARG	2.4
1	C	228	ARG	2.4
1	D	231	TRP	2.4
1	F	324	LEU	2.4
1	B	250	GLU	2.4
1	B	263	ILE	2.4
1	E	313	ALA	2.4
1	F	226	GLY	2.3
1	E	107	PRO	2.3
1	D	119	ARG	2.3
1	E	281	ARG	2.3
1	B	228	ARG	2.3
1	F	250	GLU	2.3
1	F	108	ASP	2.2
1	D	226	GLY	2.2
1	A	351	ASP	2.2
1	A	248	LEU	2.2
1	D	117	LYS	2.2
1	D	311	LYS	2.1
1	F	231	TRP	2.1
1	A	314	VAL	2.1
1	B	262	LEU	2.1
1	B	347	HIS	2.1
1	E	316	ILE	2.1
1	F	281	ARG	2.1
1	F	87	THR	2.1
1	D	369	GLN	2.1
1	C	323	THR	2.0
1	D	37	SER	2.0
1	B	242	LYS	2.0
1	D	259	LEU	2.0
1	E	108	ASP	2.0

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

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



### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	8PH	A	402	8/26	0.92	0.30	3.94	36,38,40,42	0
2	8PH	D	401	26/26	0.77	0.25	3.52	52,103,114,115	0
2	8PH	C	401	26/26	0.82	0.23	2.76	33,86,96,97	0
2	8PH	E	401	26/26	0.64	0.33	2.74	47,93,106,106	0
2	8PH	A	401	26/26	0.89	0.18	2.59	27,54,69,70	0
2	8PH	F	401	26/26	0.82	0.24	1.83	50,92,102,102	0
2	8PH	A	403	18/26	0.80	0.19	1.00	101,106,107,107	0
2	8PH	B	402	9/26	0.92	0.20	0.78	38,38,40,42	0
2	8PH	B	401	26/26	0.87	0.17	0.77	31,81,93,94	0
2	8PH	F	402	26/26	0.74	0.33	0.70	62,101,110,110	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.