Full wwPDB X-ray Structure Validation Report ⓘ

Dec 18, 2023 – 02:24 PM EST

PDB ID	:	8SF6
Title	:	Promiscuous amino acid gamma synthase from Caldicellulosiruptor hydrothermalis in closed conformation
Authors	:	Buller, A.R.; Zmich, A.P.; Bingman, C.A.
Deposited on	:	2023-04-10
Resolution	:	1.70 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
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.

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

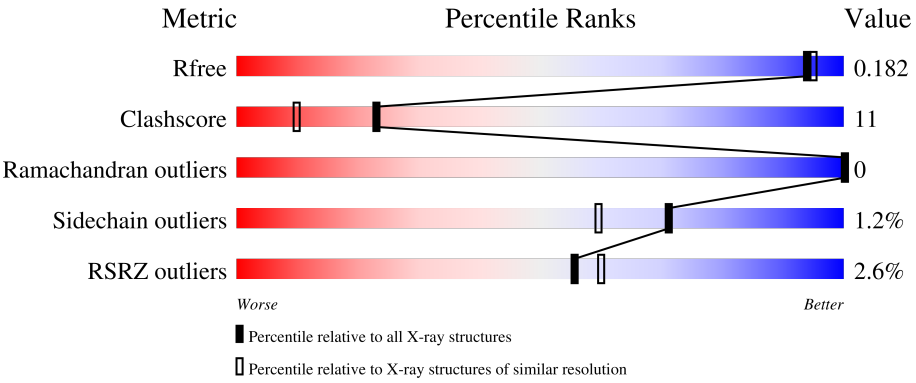
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	433	2% 73% 24%
1	B	433	3% 76% 21%
1	C	433	3% 73% 24%
1	D	433	3% 71% 26%
1	E	433	3% 74% 24%

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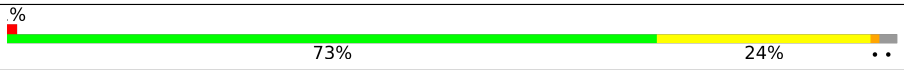
Mol	Chain	Length	Quality of chain
1	F	433	
1	G	433	
1	H	433	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 28751 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 O-acetylhomoserine/O-acetylserine sulfhydrylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	P	S	0	6	0
			3342	2157	550	629	1	5			
1	B	424	Total	C	N	O	P	S	0	4	0
			3332	2151	552	623	1	5			
1	C	423	Total	C	N	O	P	S	0	4	0
			3328	2150	551	621	1	5			
1	D	424	Total	C	N	O	P	S	0	2	0
			3322	2143	548	624	1	6			
1	E	425	Total	C	N	O	P	S	0	4	0
			3328	2150	553	619	1	5			
1	F	423	Total	C	N	O	P	S	0	1	0
			3283	2122	541	614	1	5			
1	G	423	Total	C	N	O	P	S	0	3	0
			3317	2140	547	624	1	5			
1	H	425	Total	C	N	O	P	S	0	2	0
			3305	2135	544	620	1	5			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	426	LEU	-	expression tag	UNP E4QC33
A	427	GLU	-	expression tag	UNP E4QC33
A	428	HIS	-	expression tag	UNP E4QC33
A	429	HIS	-	expression tag	UNP E4QC33
A	430	HIS	-	expression tag	UNP E4QC33
A	431	HIS	-	expression tag	UNP E4QC33
A	432	HIS	-	expression tag	UNP E4QC33
A	433	HIS	-	expression tag	UNP E4QC33
B	426	LEU	-	expression tag	UNP E4QC33
B	427	GLU	-	expression tag	UNP E4QC33
B	428	HIS	-	expression tag	UNP E4QC33
B	429	HIS	-	expression tag	UNP E4QC33
B	430	HIS	-	expression tag	UNP E4QC33

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Chain	Residue	Modelled	Actual	Comment	Reference
B	431	HIS	-	expression tag	UNP E4QC33
B	432	HIS	-	expression tag	UNP E4QC33
B	433	HIS	-	expression tag	UNP E4QC33
C	426	LEU	-	expression tag	UNP E4QC33
C	427	GLU	-	expression tag	UNP E4QC33
C	428	HIS	-	expression tag	UNP E4QC33
C	429	HIS	-	expression tag	UNP E4QC33
C	430	HIS	-	expression tag	UNP E4QC33
C	431	HIS	-	expression tag	UNP E4QC33
C	432	HIS	-	expression tag	UNP E4QC33
C	433	HIS	-	expression tag	UNP E4QC33
D	426	LEU	-	expression tag	UNP E4QC33
D	427	GLU	-	expression tag	UNP E4QC33
D	428	HIS	-	expression tag	UNP E4QC33
D	429	HIS	-	expression tag	UNP E4QC33
D	430	HIS	-	expression tag	UNP E4QC33
D	431	HIS	-	expression tag	UNP E4QC33
D	432	HIS	-	expression tag	UNP E4QC33
D	433	HIS	-	expression tag	UNP E4QC33
E	426	LEU	-	expression tag	UNP E4QC33
E	427	GLU	-	expression tag	UNP E4QC33
E	428	HIS	-	expression tag	UNP E4QC33
E	429	HIS	-	expression tag	UNP E4QC33
E	430	HIS	-	expression tag	UNP E4QC33
E	431	HIS	-	expression tag	UNP E4QC33
E	432	HIS	-	expression tag	UNP E4QC33
E	433	HIS	-	expression tag	UNP E4QC33
F	426	LEU	-	expression tag	UNP E4QC33
F	427	GLU	-	expression tag	UNP E4QC33
F	428	HIS	-	expression tag	UNP E4QC33
F	429	HIS	-	expression tag	UNP E4QC33
F	430	HIS	-	expression tag	UNP E4QC33
F	431	HIS	-	expression tag	UNP E4QC33
F	432	HIS	-	expression tag	UNP E4QC33
F	433	HIS	-	expression tag	UNP E4QC33
G	426	LEU	-	expression tag	UNP E4QC33
G	427	GLU	-	expression tag	UNP E4QC33
G	428	HIS	-	expression tag	UNP E4QC33
G	429	HIS	-	expression tag	UNP E4QC33
G	430	HIS	-	expression tag	UNP E4QC33
G	431	HIS	-	expression tag	UNP E4QC33
G	432	HIS	-	expression tag	UNP E4QC33

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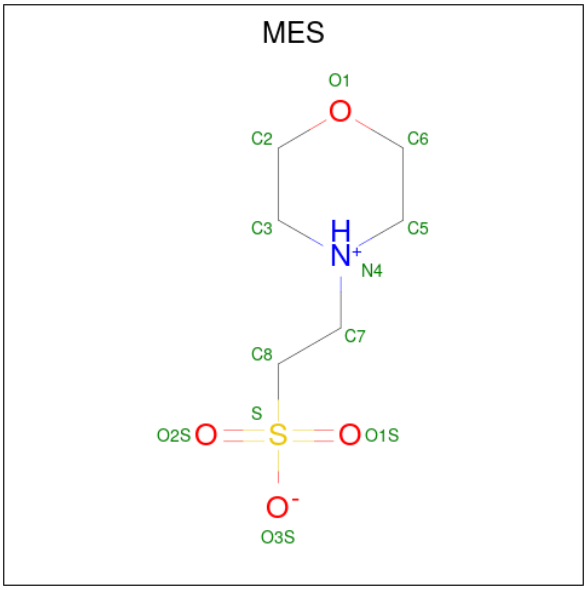
Chain	Residue	Modelled	Actual	Comment	Reference
G	433	HIS	-	expression tag	UNP E4QC33
H	426	LEU	-	expression tag	UNP E4QC33
H	427	GLU	-	expression tag	UNP E4QC33
H	428	HIS	-	expression tag	UNP E4QC33
H	429	HIS	-	expression tag	UNP E4QC33
H	430	HIS	-	expression tag	UNP E4QC33
H	431	HIS	-	expression tag	UNP E4QC33
H	432	HIS	-	expression tag	UNP E4QC33
H	433	HIS	-	expression tag	UNP E4QC33

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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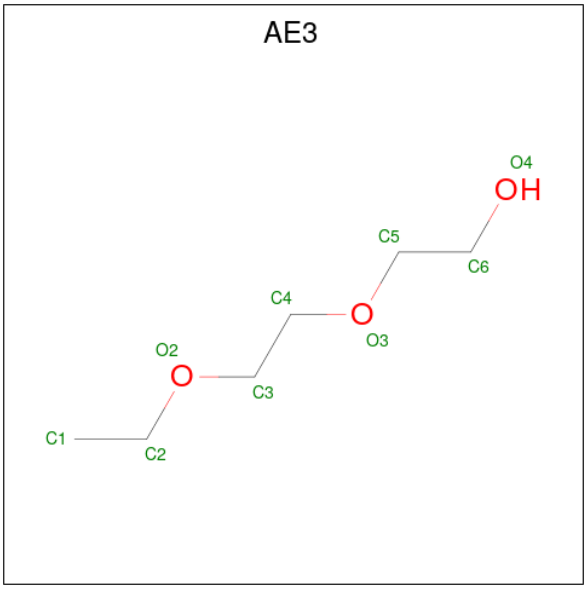
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total C N O S 12 6 1 4 1	0	0
2	H	1	Total C N O S 12 6 1 4 1	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Na 2 2	0	0
3	B	2	Total Na 2 2	0	0
3	C	4	Total Na 4 4	0	0
3	D	2	Total Na 2 2	0	0
3	G	2	Total Na 2 2	0	0
3	H	1	Total Na 1 1	0	0

- Molecule 4 is 2-(2-ETHOXYETHOXY)ETHANOL (three-letter code: AE3) (formula: $C_6H_{14}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C O 9 6 3	0	0

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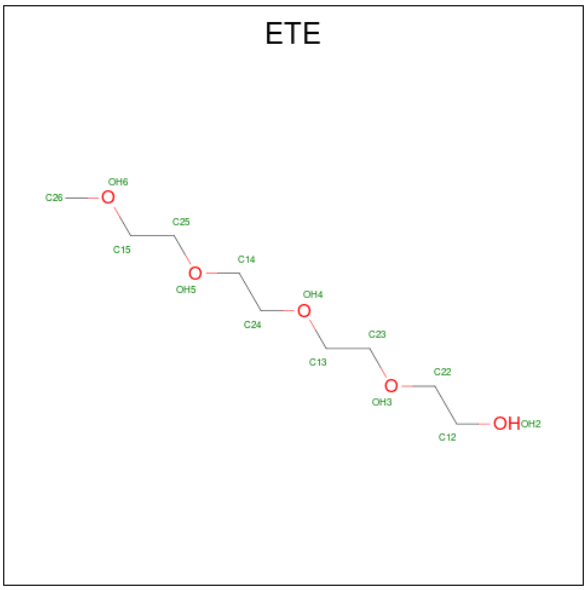
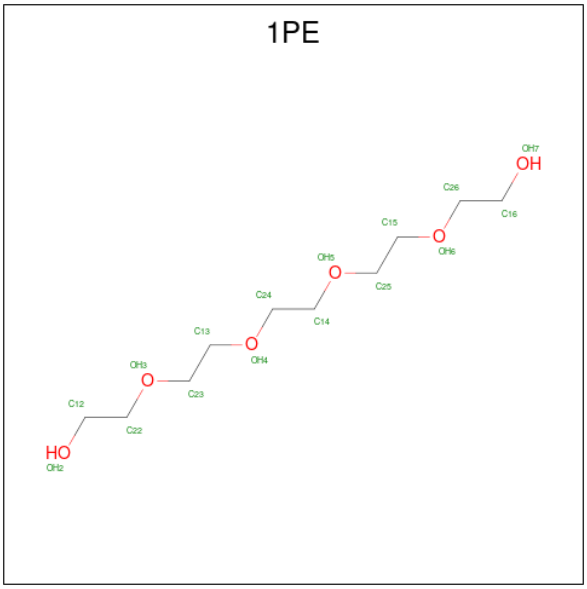
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C O 9 6 3	0	0

- Molecule 5 is 2-{2-[2-2-(METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: ETE) (formula: $C_9H_{20}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total C O 14 9 5	0	0

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	1	Total C O 16 10 6	0	0
6	H	1	Total C O 16 10 6	0	0

- Molecule 7 is water.

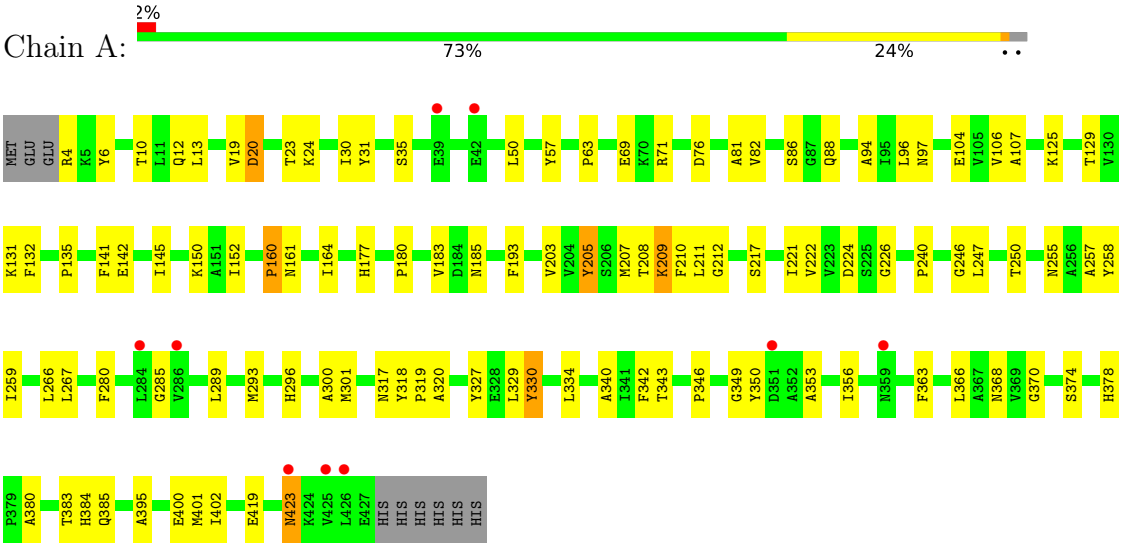
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	264	Total O 264 264	0	0
7	B	284	Total O 284 284	0	0
7	C	259	Total O 259 259	0	0
7	D	237	Total O 237 237	0	0
7	E	251	Total O 251 251	0	0
7	F	156	Total O 156 156	0	0
7	G	284	Total O 284 284	0	0
7	H	286	Total O 286 286	0	0

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 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.

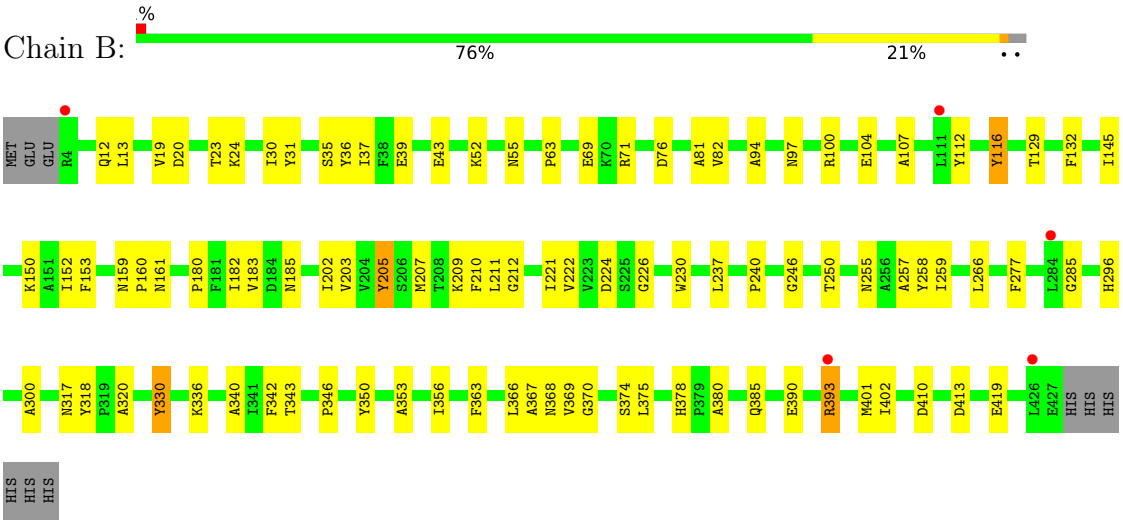
• Molecule 1: O-acetylhomoserine/O-acetylserine sulfhydrylase

Chain A:



• Molecule 1: O-acetylhomoserine/O-acetylserine sulfhydrylase

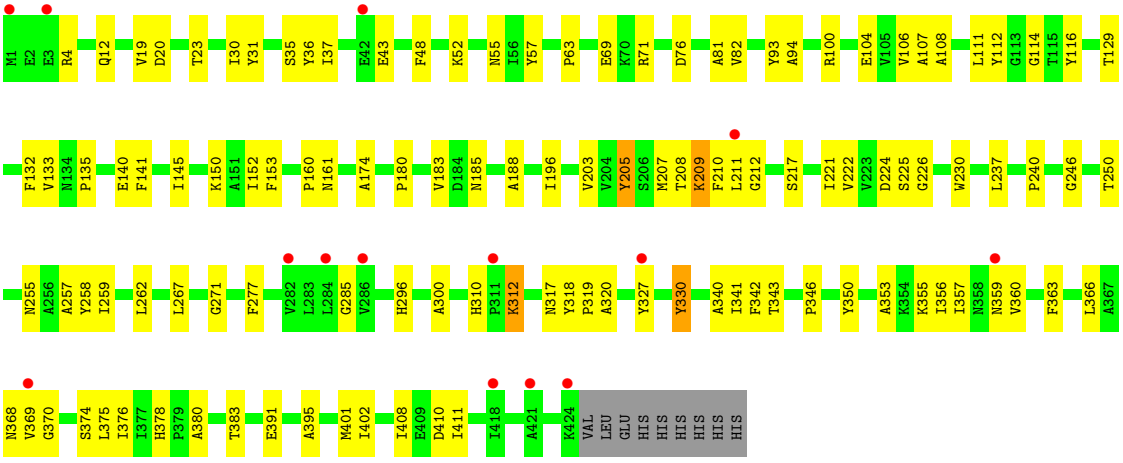
Chain B:



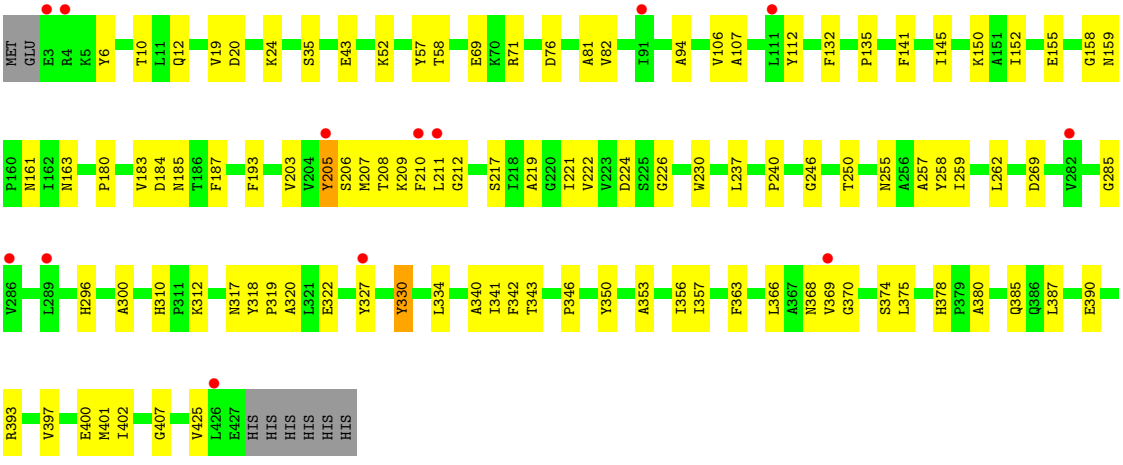
• Molecule 1: O-acetylhomoserine/O-acetylserine sulfhydrylase

Chain C:

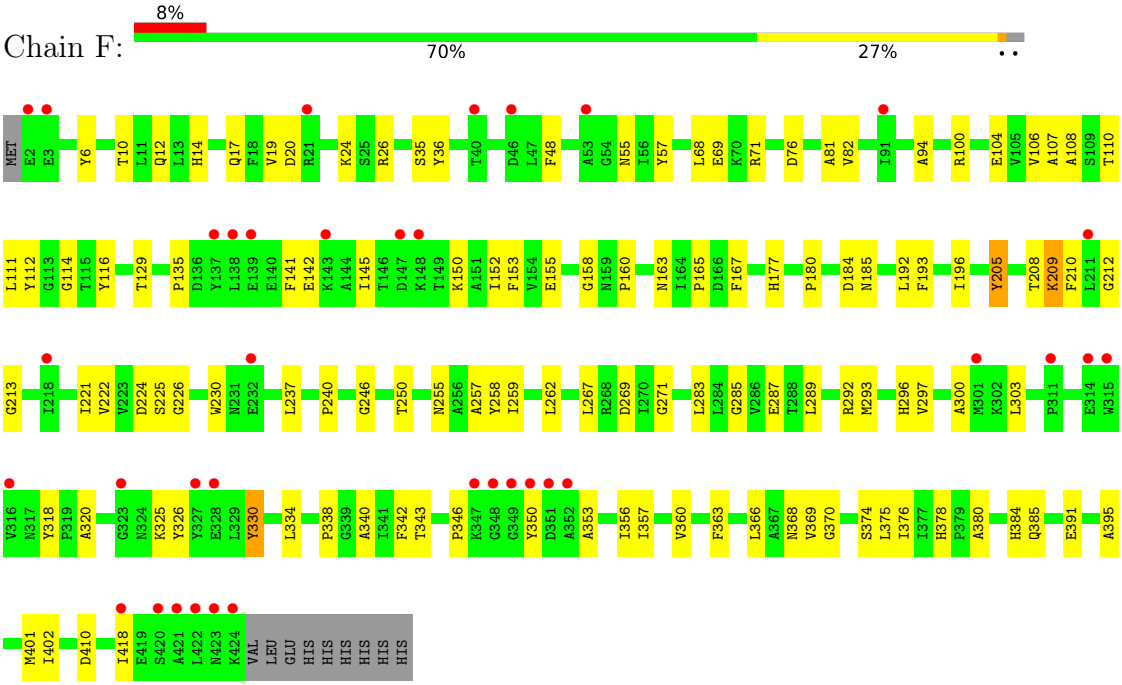
• Molecule 1: O-acetylhomoserine/O-acetylserine sulfhydrylase



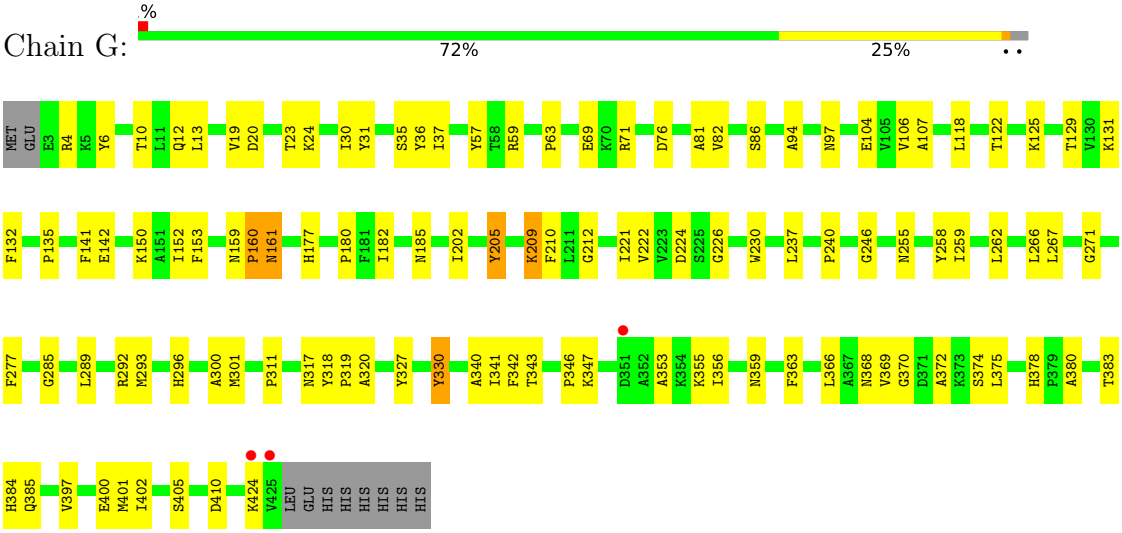
• Molecule 1: O-acetylhomoserine/O-acetylserine sulfhydrylase



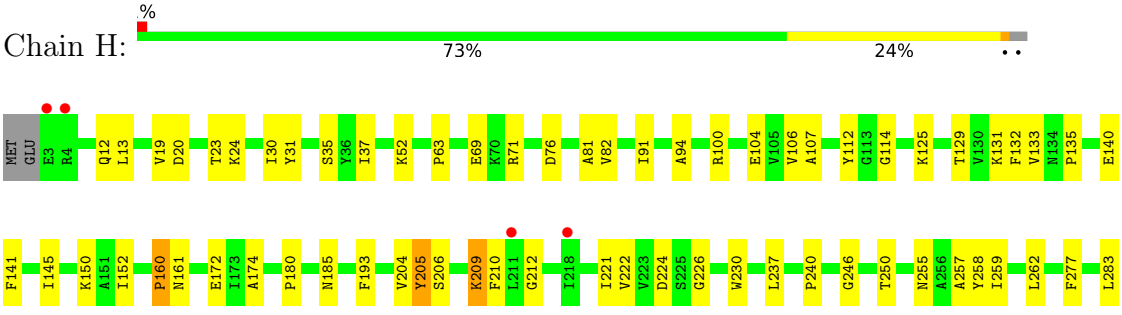
• Molecule 1: O-acetylhomoserine/O-acetylserine sulfhydrylase

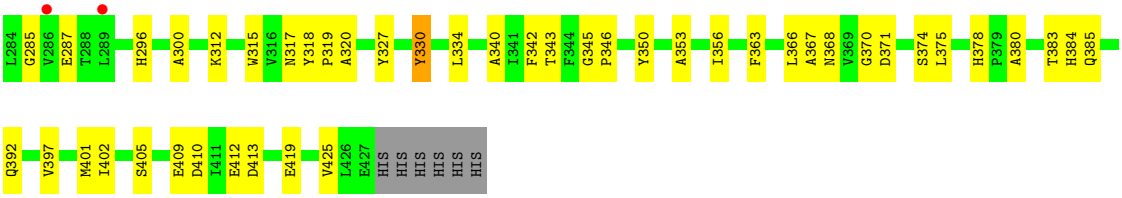


• Molecule 1: O-acetylhomoserine/O-acetylserine sulfhydrylase



• Molecule 1: O-acetylhomoserine/O-acetylserine sulfhydrylase




L284
G285
V286
E287
T288
L289
H296
A300
K312
W315
V316
N317
Y318
P319
A320
Y327
Y330
L334
A340
I341
F342
T343
F344
G345
P346
Y350
A353
I356
F363
L366
A367
N368
V369
G370
D371
S374
L375
H378
P379
A380
T383
H384
Q385

Q392
V397
M401
I402
S405
E409
D410
I411
E412
D413
E419
V425
L426
E427
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	279.09Å 133.12Å 115.79Å 90.00° 94.87° 90.00°	Depositor
Resolution (Å)	39.92 – 1.70 39.93 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.2 (39.92-1.70) 97.2 (39.93-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.04 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.154 , 0.179 0.159 , 0.182	Depositor DCC
R_{free} test set	22101 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	27.8	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 28.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	28751	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NA, MES, ETE, AE3, LLP, 1PE

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	0.87	0/3400	1.02	1/4619 (0.0%)
1	B	0.92	0/3387	1.04	3/4601 (0.1%)
1	C	0.89	3/3386 (0.1%)	1.03	3/4598 (0.1%)
1	D	0.89	0/3374	1.00	1/4582 (0.0%)
1	E	0.88	1/3389 (0.0%)	0.99	1/4603 (0.0%)
1	F	0.75	0/3335	0.95	0/4536
1	G	0.91	1/3372 (0.0%)	1.03	1/4582 (0.0%)
1	H	0.96	0/3360	1.04	0/4568
All	All	0.88	5/27003 (0.0%)	1.01	10/36689 (0.0%)

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
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
All	All	0	8

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	206	SER	CA-CB	-5.37	1.44	1.52
1	C	374	SER	CA-CB	-5.32	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	405	SER	CA-CB	-5.32	1.45	1.52
1	E	206	SER	CA-CB	-5.19	1.45	1.52
1	C	290	SER	CA-CB	-5.18	1.45	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	423	ASN	CB-CA-C	8.23	126.87	110.40
1	B	116	TYR	CB-CG-CD1	-7.13	116.72	121.00
1	G	292	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	C	116	TYR	CB-CG-CD2	-6.14	117.31	121.00
1	D	93	TYR	CB-CG-CD2	-6.13	117.32	121.00
1	C	393	ARG	NE-CZ-NH1	-5.87	117.36	120.30
1	B	393[A]	ARG	NE-CZ-NH1	-5.73	117.43	120.30
1	B	393[B]	ARG	NE-CZ-NH1	-5.73	117.43	120.30
1	C	58	THR	CA-CB-OG1	-5.39	97.68	109.00
1	E	58	THR	CA-CB-OG1	-5.18	98.12	109.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	205	TYR	Peptide
1	B	205	TYR	Peptide
1	C	205	TYR	Peptide
1	D	205	TYR	Peptide
1	E	205	TYR	Peptide
1	F	205	TYR	Peptide
1	G	205	TYR	Peptide
1	H	205	TYR	Peptide

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	3342	0	3313	81	0
1	B	3332	0	3310	75	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3328	0	3320	71	0
1	D	3322	0	3297	91	0
1	E	3328	0	3314	75	0
1	F	3283	0	3239	85	0
1	G	3317	0	3286	83	0
1	H	3305	0	3266	90	0
2	A	12	0	13	3	0
2	B	12	0	13	1	0
2	C	12	0	13	1	0
2	D	12	0	13	1	0
2	E	12	0	13	2	0
2	F	12	0	13	2	0
2	G	12	0	13	3	0
2	H	12	0	13	2	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	4	0	0	0	0
3	D	2	0	0	0	0
3	G	2	0	0	0	0
3	H	1	0	0	0	0
4	D	9	0	14	0	0
4	E	9	0	14	0	0
5	E	14	0	20	1	0
6	H	32	0	44	1	0
7	A	264	0	0	1	0
7	B	284	0	0	5	0
7	C	259	0	0	4	0
7	D	237	0	0	1	0
7	E	251	0	0	3	0
7	F	156	0	0	3	0
7	G	284	0	0	1	0
7	H	286	0	0	6	0
All	All	28751	0	26541	606	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 11.

All (606) 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:H:410:ASP:OD1	1:H:412:GLU:OE1	1.99	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:161:ASN:O	1:E:317:ASN:ND2	2.21	0.74
1:F:353:ALA:HA	1:F:402:ILE:HD11	1.71	0.71
1:F:210:PHE:CE1	1:F:370:GLY:HA2	2.26	0.71
1:E:210:PHE:CE1	1:E:370:GLY:HA2	2.27	0.70
1:E:353:ALA:HA	1:E:402:ILE:HD11	1.72	0.70
1:D:210:PHE:CE1	1:D:370:GLY:HA2	2.28	0.69
1:G:226:GLY:HA2	1:G:255[A]:ASN:O	1.93	0.69
1:A:210:PHE:CE1	1:A:370:GLY:HA2	2.29	0.68
1:C:210:PHE:CE1	1:C:370:GLY:HA2	2.31	0.66
1:G:311:PRO:O	1:G:347:LYS:HE2	1.96	0.65
1:A:185:ASN:HB3	1:A:205:TYR:CE2	2.32	0.64
1:E:43:GLU:HG3	1:E:52:LYS:HE3	1.78	0.64
1:B:210:PHE:CE1	1:B:370:GLY:HA2	2.33	0.64
1:C:311:PRO:O	1:C:347:LYS:HE2	1.98	0.64
1:A:57:TYR:OH	1:F:208:THR:HG21	1.99	0.63
1:B:368:ASN:HB2	1:H:35:SER:OG	1.99	0.63
1:E:185:ASN:HB3	1:E:205:TYR:CE1	2.33	0.63
1:G:185:ASN:HB3	1:G:205:TYR:CE1	2.34	0.63
1:C:150:LYS:O	1:C:180:PRO:HD2	1.99	0.63
1:F:230:TRP:CD2	1:F:237:LEU:HD13	2.34	0.62
1:D:366:LEU:C	1:D:366:LEU:HD12	2.20	0.62
1:C:353:ALA:HA	1:C:402:ILE:HD11	1.82	0.62
1:H:419:GLU:OE2	7:H:601:HOH:O	2.16	0.62
1:A:353:ALA:HA	1:A:402:ILE:HD11	1.83	0.61
1:G:210:PHE:CE1	1:G:370:GLY:HA2	2.35	0.61
1:C:185:ASN:HB3	1:C:205:TYR:CE1	2.36	0.61
1:C:226:GLY:HA2	1:C:255:ASN:O	2.02	0.60
1:F:185:ASN:HB3	1:F:205:TYR:CE2	2.37	0.59
1:F:76:ASP:OD2	1:F:205:TYR:OH	2.21	0.58
1:B:277:PHE:CE1	1:D:277:PHE:HE1	2.21	0.58
1:D:161:ASN:O	1:D:317:ASN:ND2	2.36	0.58
1:G:353:ALA:HA	1:G:402:ILE:HD11	1.85	0.58
1:B:353:ALA:HA	1:B:402:ILE:HD11	1.86	0.58
1:A:296:HIS:HB3	1:A:340:ALA:CB	2.33	0.57
1:F:150:LYS:O	1:F:180:PRO:HD2	2.04	0.57
1:B:39:GLU:HG2	7:B:738:HOH:O	2.04	0.57
1:F:94:ALA:HA	1:F:258:TYR:OH	2.03	0.57
1:F:366:LEU:HD12	1:F:366:LEU:C	2.23	0.57
1:B:296:HIS:HB3	1:B:340:ALA:CB	2.34	0.57
1:C:12:GLN:O	1:C:71:ARG:HD3	2.03	0.57
1:C:383:THR:HA	2:C:501:MES:H31	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:353:ALA:HA	1:H:402:ILE:HD11	1.87	0.57
1:C:224:ASP:CB	1:C:259:ILE:HB	2.34	0.57
1:A:366:LEU:HD12	1:A:366:LEU:C	2.25	0.57
1:A:385:GLN:HG3	7:A:638:HOH:O	2.04	0.57
1:D:353:ALA:HA	1:D:402:ILE:HD11	1.86	0.57
1:B:35:SER:OG	1:H:368:ASN:HB2	2.05	0.56
1:D:145:ILE:HD11	1:D:152:ILE:HD11	1.87	0.56
1:E:76:ASP:OD2	1:E:205:TYR:OH	2.21	0.56
1:C:240:PRO:HB3	1:C:246:GLY:HA2	1.87	0.56
1:F:106:VAL:O	1:F:152:ILE:HA	2.05	0.56
1:B:185:ASN:HB3	1:B:205:TYR:CE2	2.40	0.56
1:H:161:ASN:O	1:H:317:ASN:ND2	2.39	0.56
1:D:368:ASN:HB2	1:G:35:SER:OG	2.05	0.56
1:H:145:ILE:HD11	1:H:152:ILE:HD11	1.86	0.56
1:B:390:GLU:OE1	1:C:124[B]:ARG:NH1	2.23	0.56
1:E:94:ALA:HA	1:E:258:TYR:OH	2.06	0.56
1:F:350:TYR:CE1	1:F:378:HIS:CE1	2.94	0.56
1:F:226:GLY:O	1:F:255:ASN:HB2	2.06	0.55
1:A:35[B]:SER:OG	1:F:368:ASN:HB2	2.06	0.55
1:B:23:THR:HG21	1:G:31:TYR:CZ	2.41	0.55
1:A:368:ASN:HB2	1:F:35:SER:OG	2.07	0.55
1:B:82:VAL:HG23	1:B:259:ILE:HG13	1.89	0.55
1:D:35:SER:OG	1:G:368:ASN:HB2	2.07	0.55
1:D:31:TYR:CZ	1:H:23:THR:HG21	2.42	0.55
1:H:419:GLU:HG3	7:H:641:HOH:O	2.07	0.55
1:D:355:LYS:O	1:D:359:ASN:ND2	2.40	0.55
1:E:112:TYR:CE1	2:E:501:MES:H82	2.42	0.55
1:C:145:ILE:HD11	1:C:152:ILE:HD11	1.88	0.55
1:G:104:GLU:HA	1:G:129:THR:O	2.06	0.55
1:B:76:ASP:OD2	1:B:205:TYR:OH	2.25	0.54
1:A:94:ALA:HA	1:A:258:TYR:OH	2.07	0.54
1:D:76:ASP:OD2	1:D:205:TYR:OH	2.23	0.54
1:B:107:ALA:O	1:B:132:PHE:HA	2.08	0.54
1:D:94:ALA:HA	1:D:258:TYR:OH	2.08	0.54
1:H:210:PHE:CE1	1:H:370:GLY:HA2	2.42	0.54
1:B:366:LEU:C	1:B:366:LEU:HD12	2.28	0.54
1:H:343:THR:HB	1:H:401:MET:HG3	1.88	0.54
1:D:226:GLY:HA2	1:D:255:ASN:O	2.07	0.54
1:F:363:PHE:CE2	1:F:374:SER:HB3	2.43	0.54
1:H:212:GLY:O	1:H:285:GLY:HA3	2.08	0.54
1:H:343:THR:HA	1:H:402:ILE:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:GLN:O	1:B:71:ARG:HD3	2.08	0.54
1:E:317:ASN:HB3	1:E:343:THR:OG1	2.08	0.54
1:F:224:ASP:CB	1:F:259:ILE:HB	2.38	0.54
1:F:224:ASP:HB2	1:F:259:ILE:HB	1.89	0.54
1:G:161:ASN:O	1:G:317:ASN:ND2	2.40	0.54
1:A:210:PHE:CD1	1:A:370:GLY:HA2	2.43	0.54
1:C:366:LEU:HD12	1:C:366:LEU:C	2.28	0.54
1:A:224:ASP:CB	1:A:259:ILE:HB	2.38	0.54
1:D:104:GLU:HA	1:D:129:THR:O	2.08	0.54
1:A:161:ASN:O	1:A:317:ASN:ND2	2.41	0.54
1:D:82:VAL:HG23	1:D:259:ILE:HG13	1.89	0.54
1:F:385:GLN:HG3	7:F:632:HOH:O	2.08	0.53
1:G:383:THR:HA	2:G:501:MES:H31	1.90	0.53
1:B:31:TYR:CZ	1:G:23:THR:HG21	2.44	0.53
1:F:378:HIS:CE1	1:F:380:ALA:HB3	2.44	0.53
1:A:224:ASP:HB2	1:A:259:ILE:HB	1.89	0.53
1:B:393[A]:ARG:NH1	7:B:610:HOH:O	2.41	0.53
1:F:300:ALA:CB	1:F:340:ALA:HA	2.38	0.53
1:H:185:ASN:HB3	1:H:205:TYR:CE2	2.44	0.53
1:C:336:LYS:HE3	7:C:607:HOH:O	2.07	0.53
1:E:226:GLY:HA2	1:E:255:ASN:O	2.08	0.53
1:D:318:TYR:CD1	1:D:342:PHE:HB3	2.43	0.53
1:D:357:ILE:CD1	1:D:378:HIS:HB2	2.39	0.53
1:F:296:HIS:HB3	1:F:340:ALA:CB	2.39	0.53
1:E:82:VAL:HG23	1:E:259:ILE:HG13	1.91	0.53
1:F:210:PHE:CD1	1:F:370:GLY:HA2	2.43	0.53
1:H:100:ARG:HD3	7:H:862:HOH:O	2.09	0.53
1:D:320:ALA:HA	1:D:330:TYR:CD2	2.44	0.53
1:E:145:ILE:HD11	1:E:152:ILE:HD11	1.89	0.53
1:H:82:VAL:HG23	1:H:259:ILE:HG13	1.90	0.53
1:H:378:HIS:CE1	1:H:380:ALA:HB3	2.43	0.53
1:A:82:VAL:HG23	1:A:259:ILE:HG13	1.91	0.53
1:B:30:ILE:HB	1:G:30:ILE:HB	1.91	0.53
1:E:19:VAL:CG1	1:E:24:LYS:HA	2.39	0.53
1:G:81:ALA:HA	1:G:222:VAL:O	2.09	0.53
1:H:366:LEU:HD12	1:H:366:LEU:C	2.30	0.53
1:A:208:THR:HG21	1:F:57:TYR:OH	2.09	0.52
1:D:196:ILE:HD13	1:D:225:SER:HA	1.91	0.52
1:E:318:TYR:CD1	1:E:342:PHE:HB3	2.44	0.52
1:G:366:LEU:C	1:G:366:LEU:HD12	2.30	0.52
1:H:296:HIS:HB3	1:H:340:ALA:CB	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:82:VAL:HG23	1:F:259:ILE:HG13	1.91	0.52
1:C:212:GLY:O	1:C:285:GLY:HA3	2.08	0.52
1:D:185:ASN:HB3	1:D:205:TYR:CE2	2.45	0.52
1:E:205:TYR:HB2	1:E:221:ILE:HG22	1.92	0.52
1:E:385:GLN:HG3	7:E:626:HOH:O	2.08	0.52
1:B:23:THR:HB	1:G:63:PRO:HG3	1.90	0.52
1:F:14:HIS:HD2	7:F:751:HOH:O	1.91	0.52
1:F:104:GLU:HA	1:F:129:THR:O	2.10	0.52
1:A:363:PHE:CE2	1:A:374:SER:HB3	2.45	0.52
1:C:35:SER:OG	1:E:368:ASN:HB2	2.10	0.52
1:D:30:ILE:HB	1:H:30:ILE:HB	1.92	0.52
1:G:107:ALA:O	1:G:132:PHE:HA	2.09	0.52
1:C:355:LYS:O	1:C:359:ASN:ND2	2.43	0.52
1:D:320:ALA:HA	1:D:330:TYR:CE2	2.44	0.52
1:C:4:ARG:NH2	7:C:610:HOH:O	2.43	0.51
1:F:296:HIS:HB3	1:F:340:ALA:HB2	1.92	0.51
1:H:224:ASP:CB	1:H:259:ILE:HB	2.40	0.51
1:B:19:VAL:HG21	1:G:37:ILE:HG13	1.92	0.51
1:B:226:GLY:HA2	1:B:255:ASN:O	2.10	0.51
1:D:210:PHE:CD1	1:D:370:GLY:HA2	2.45	0.51
1:E:341:ILE:HD11	1:E:369:VAL:HB	1.93	0.51
1:A:81:ALA:HA	1:A:222:VAL:O	2.11	0.51
1:A:296:HIS:HB3	1:A:340:ALA:HB2	1.92	0.51
1:F:196:ILE:HD13	1:F:225:SER:HA	1.92	0.51
1:H:385:GLN:HG3	7:H:679:HOH:O	2.09	0.51
1:A:50:LEU:HD12	1:A:247:LEU:HD13	1.93	0.51
1:D:346:PRO:HB3	1:D:356:ILE:CD1	2.40	0.51
1:G:230:TRP:CD2	1:G:237:LEU:HD13	2.46	0.51
1:E:296:HIS:HB3	1:E:340:ALA:HB2	1.93	0.51
1:G:300:ALA:CB	1:G:340:ALA:HA	2.41	0.51
1:G:320:ALA:HA	1:G:330:TYR:CE2	2.46	0.51
1:C:224:ASP:HB2	1:C:259:ILE:HB	1.93	0.51
1:D:310:HIS:CE1	1:D:312:LYS:HB2	2.46	0.51
1:H:205:TYR:HB2	1:H:221:ILE:HG22	1.93	0.51
1:B:240:PRO:HB3	1:B:246:GLY:HA2	1.92	0.51
1:B:31:TYR:CD2	1:B:63:PRO:HG2	2.46	0.50
1:C:161:ASN:O	1:C:317:ASN:ND2	2.44	0.50
1:A:226:GLY:HA2	1:A:255:ASN:O	2.11	0.50
1:D:296:HIS:HB3	1:D:340:ALA:HB2	1.93	0.50
1:A:350:TYR:CE1	1:A:378:HIS:CE1	2.99	0.50
1:B:81:ALA:HA	1:B:222:VAL:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:ASP:CB	1:B:259:ILE:HB	2.41	0.50
1:D:224:ASP:CB	1:D:259:ILE:HB	2.41	0.50
1:E:69:GLU:HA	1:E:221:ILE:HD11	1.93	0.50
1:E:363:PHE:CE2	1:E:374:SER:HB3	2.46	0.50
1:A:76:ASP:OD2	1:A:205:TYR:OH	2.22	0.50
1:C:94:ALA:HA	1:C:258:TYR:OH	2.12	0.50
1:C:300:ALA:CB	1:C:340:ALA:HA	2.41	0.50
1:E:366:LEU:HD11	1:E:375:LEU:HD22	1.93	0.50
1:E:366:LEU:C	1:E:366:LEU:HD12	2.32	0.50
1:G:82:VAL:HG23	1:G:259:ILE:HG13	1.92	0.50
1:C:368:ASN:HB2	1:E:35:SER:OG	2.11	0.50
1:E:224:ASP:CB	1:E:259:ILE:HB	2.41	0.50
1:F:12:GLN:O	1:F:71:ARG:HD3	2.12	0.50
1:F:226:GLY:HA2	1:F:255:ASN:O	2.12	0.50
1:G:224:ASP:CB	1:G:259:ILE:HB	2.42	0.50
1:A:383:THR:HA	2:A:501:MES:H52	1.94	0.50
1:G:363:PHE:CE2	1:G:374:SER:HB3	2.47	0.50
1:G:205:TYR:HB2	1:G:221:ILE:HG22	1.93	0.50
1:G:343:THR:HA	1:G:402:ILE:O	2.12	0.50
1:H:224:ASP:HB2	1:H:259:ILE:HB	1.92	0.50
1:C:210:PHE:CD1	1:C:370:GLY:HA2	2.47	0.49
1:F:240:PRO:HB3	1:F:246:GLY:HA2	1.94	0.49
1:H:12:GLN:O	1:H:71:ARG:HD3	2.12	0.49
1:H:346:PRO:HB3	1:H:356:ILE:CD1	2.42	0.49
1:C:296:HIS:HB3	1:C:340:ALA:CB	2.42	0.49
1:H:107:ALA:O	1:H:132:PHE:HA	2.12	0.49
1:C:81:ALA:HA	1:C:222:VAL:O	2.12	0.49
1:G:296:HIS:HB3	1:G:340:ALA:CB	2.41	0.49
1:H:150:LYS:O	1:H:180:PRO:HD2	2.12	0.49
1:H:230:TRP:CD2	1:H:237:LEU:HD13	2.47	0.49
1:D:296:HIS:HB3	1:D:340:ALA:CB	2.43	0.49
1:G:355:LYS:O	1:G:359:ASN:ND2	2.45	0.49
1:C:301:MET:HE1	1:C:320:ALA:HB1	1.94	0.49
1:D:383:THR:HA	2:D:501:MES:H52	1.94	0.49
1:H:226:GLY:HA2	1:H:255:ASN:O	2.11	0.49
1:B:205:TYR:HB2	1:B:221:ILE:HG22	1.94	0.49
1:C:346:PRO:HB3	1:C:356:ILE:CD1	2.43	0.49
1:H:69:GLU:HA	1:H:221:ILE:HD11	1.95	0.49
1:B:330:TYR:CD1	1:B:330:TYR:C	2.84	0.49
1:G:378:HIS:CE1	1:G:380:ALA:HB3	2.48	0.49
1:A:57:TYR:CD2	2:F:501:MES:H51	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ASN:HB2	1:A:395:ALA:O	2.13	0.49
1:F:357:ILE:HG12	1:F:376:ILE:HG12	1.95	0.49
1:H:106:VAL:O	1:H:152:ILE:HA	2.13	0.49
1:B:230:TRP:CD2	1:B:237:LEU:HD13	2.48	0.49
1:B:277:PHE:CE1	1:D:277:PHE:CE1	3.00	0.49
1:E:150:LYS:O	1:E:180:PRO:HD2	2.13	0.49
1:A:69:GLU:HA	1:A:221:ILE:HD11	1.95	0.48
1:A:164:ILE:O	1:A:329:LEU:HD13	2.12	0.48
7:D:673:HOH:O	1:G:385:GLN:HG3	2.13	0.48
1:E:317:ASN:O	1:E:342:PHE:HB2	2.13	0.48
1:C:301:MET:HE2	7:C:606:HOH:O	2.14	0.48
1:F:112:TYR:CE2	1:F:114:GLY:HA3	2.49	0.48
1:G:94:ALA:HA	1:G:258:TYR:OH	2.13	0.48
1:B:366:LEU:HD11	1:B:375:LEU:HD22	1.94	0.48
1:B:385:GLN:HG3	7:B:690:HOH:O	2.13	0.48
1:F:6:TYR:HB3	1:F:10:THR:HB	1.95	0.48
1:B:104:GLU:HA	1:B:129:THR:O	2.13	0.48
1:F:19:VAL:CG1	1:F:24:LYS:HA	2.44	0.48
1:G:142:GLU:OE2	1:G:177:HIS:NE2	2.46	0.48
1:A:76:ASP:CG	1:A:205:TYR:HH	2.15	0.48
1:B:250:THR:HA	1:B:257:ALA:HB2	1.96	0.48
1:G:160:PRO:HD3	1:G:384:HIS:CE1	2.49	0.48
1:G:317:ASN:HB3	1:G:343:THR:OG1	2.13	0.48
1:F:346:PRO:HB3	1:F:356:ILE:CD1	2.43	0.48
1:B:210:PHE:CD1	1:B:370:GLY:HA2	2.49	0.48
1:C:82:VAL:HG23	1:C:259:ILE:HG13	1.96	0.48
1:C:202:ILE:HD13	1:C:258:TYR:CZ	2.49	0.48
1:D:240:PRO:HB3	1:D:246:GLY:HA2	1.96	0.48
1:H:94:ALA:HA	1:H:258:TYR:OH	2.14	0.48
1:A:346:PRO:HB3	1:A:356:ILE:CD1	2.43	0.48
1:F:81:ALA:HA	1:F:222:VAL:O	2.14	0.48
1:A:378:HIS:CE1	1:A:380:ALA:HB3	2.49	0.48
1:D:37:ILE:HG13	1:H:19:VAL:HG21	1.94	0.48
1:D:300:ALA:CB	1:D:340:ALA:HA	2.44	0.48
1:E:107:ALA:O	1:E:132:PHE:HA	2.13	0.48
1:H:81:ALA:HA	1:H:222:VAL:O	2.14	0.48
1:A:193:PHE:HB2	1:A:334:LEU:HD23	1.96	0.47
1:C:208:THR:HG21	1:E:57:TYR:OH	2.14	0.47
1:F:209:LLP:HD3	1:F:369:VAL:HG22	1.96	0.47
1:G:76:ASP:OD2	1:G:205:TYR:OH	2.28	0.47
1:G:301:MET:HE1	7:G:604:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:GLY:O	1:A:285:GLY:HA3	2.14	0.47
1:B:94:ALA:HA	1:B:258:TYR:OH	2.14	0.47
1:F:142:GLU:CD	1:F:177:HIS:HE2	2.16	0.47
1:A:104:GLU:HA	1:A:129:THR:O	2.13	0.47
1:A:343:THR:HA	1:A:402:ILE:O	2.14	0.47
1:F:300:ALA:HB2	1:F:340:ALA:HA	1.96	0.47
1:A:12:GLN:O	1:A:71:ARG:HD3	2.14	0.47
1:A:320:ALA:HA	1:A:330:TYR:CE2	2.49	0.47
1:B:336:LYS:HE2	7:B:815:HOH:O	2.14	0.47
1:B:350:TYR:CE1	1:B:378:HIS:CE1	3.02	0.47
1:H:319:PRO:O	1:H:327:TYR:HA	2.14	0.47
1:A:160:PRO:HD3	1:A:384:HIS:CE1	2.50	0.47
1:D:341:ILE:HD11	1:D:369:VAL:HB	1.96	0.47
1:E:255:ASN:HB3	5:E:502:ETE:OH5	2.14	0.47
1:E:346:PRO:HD2	1:E:400:GLU:O	2.14	0.47
1:G:366:LEU:HD11	1:G:375:LEU:HD22	1.95	0.47
1:H:363:PHE:CE2	1:H:374:SER:HB3	2.50	0.47
1:A:343:THR:HB	1:A:401:MET:HG3	1.96	0.47
1:B:320:ALA:HA	1:B:330:TYR:CE2	2.50	0.47
1:B:346:PRO:HB3	1:B:356:ILE:CD1	2.44	0.47
1:C:6:TYR:HB3	1:C:10:THR:HB	1.94	0.47
1:D:330:TYR:CD1	1:D:330:TYR:C	2.88	0.47
1:F:267:LEU:O	1:F:271:GLY:HA2	2.14	0.47
1:G:224:ASP:HB2	1:G:259:ILE:HB	1.97	0.47
1:B:104:GLU:HG2	1:B:129:THR:HB	1.97	0.47
1:C:107:ALA:O	1:C:132:PHE:HA	2.14	0.47
1:G:6:TYR:HB3	1:G:10:THR:HB	1.96	0.47
1:G:210:PHE:CD1	1:G:370:GLY:HA2	2.49	0.47
1:G:12:GLN:O	1:G:71:ARG:HD3	2.15	0.47
1:G:150:LYS:O	1:G:180:PRO:HD2	2.14	0.47
1:H:160:PRO:HD3	1:H:384:HIS:CE1	2.50	0.47
1:B:296:HIS:HB3	1:B:340:ALA:HB2	1.95	0.47
1:C:160:PRO:HD3	1:C:384:HIS:CE1	2.49	0.47
1:D:116:TYR:OH	1:D:391:GLU:HG2	2.14	0.47
1:D:208:THR:HG21	1:G:57:TYR:OH	2.15	0.47
1:H:210:PHE:CD1	1:H:370:GLY:HA2	2.50	0.47
1:A:205:TYR:HB2	1:A:221:ILE:HG22	1.97	0.47
1:C:343:THR:HB	1:C:401:MET:HG3	1.97	0.47
1:D:106:VAL:O	1:D:152:ILE:HA	2.15	0.47
1:E:310:HIS:CE1	1:E:312:LYS:HB2	2.50	0.47
1:C:319:PRO:O	1:C:327:TYR:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:ASP:CG	1:D:205:TYR:HH	2.18	0.46
1:E:212:GLY:O	1:E:285:GLY:HA3	2.15	0.46
1:E:346:PRO:HG3	1:E:356:ILE:HD12	1.97	0.46
1:B:363:PHE:CE2	1:B:374:SER:HB3	2.51	0.46
1:G:277:PHE:CE1	1:H:277:PHE:HE1	2.33	0.46
1:H:250:THR:HA	1:H:257:ALA:HB2	1.97	0.46
1:A:150:LYS:O	1:A:180:PRO:HD2	2.15	0.46
1:G:212:GLY:O	1:G:285:GLY:HA3	2.16	0.46
1:G:341:ILE:HD11	1:G:369:VAL:HB	1.97	0.46
1:D:81:ALA:HA	1:D:222:VAL:O	2.15	0.46
1:F:343:THR:HA	1:F:402:ILE:O	2.15	0.46
1:A:330:TYR:CD1	1:A:330:TYR:C	2.89	0.46
1:D:212:GLY:O	1:D:285:GLY:HA3	2.16	0.46
1:E:226:GLY:O	1:E:255:ASN:HB2	2.16	0.46
1:G:277:PHE:CE1	1:H:277:PHE:CE1	3.04	0.46
1:C:320:ALA:HA	1:C:330:TYR:CE2	2.51	0.46
1:F:158:GLY:HA3	1:F:163:ASN:OD1	2.16	0.46
1:C:250:THR:HA	1:C:257:ALA:HB2	1.97	0.46
1:F:145:ILE:HD11	1:F:152:ILE:HD11	1.97	0.46
1:F:330:TYR:CD1	1:F:330:TYR:C	2.90	0.46
1:A:107:ALA:O	1:A:132:PHE:HA	2.16	0.46
1:B:212:GLY:O	1:B:285:GLY:HA3	2.15	0.46
1:E:193:PHE:HB2	1:E:334:LEU:HD23	1.97	0.46
1:E:250:THR:HA	1:E:257:ALA:HB2	1.98	0.46
1:F:112:TYR:CE1	2:F:501:MES:H82	2.50	0.46
1:H:133:VAL:HB	1:H:140:GLU:HB3	1.98	0.46
1:A:19:VAL:HG12	1:A:24:LYS:HA	1.97	0.46
1:B:182:ILE:HG12	1:B:202:ILE:HB	1.98	0.46
1:E:81:ALA:HA	1:E:222:VAL:O	2.15	0.46
1:F:212:GLY:O	1:F:285:GLY:HA3	2.16	0.46
1:F:343:THR:HB	1:F:401:MET:HG3	1.98	0.46
1:G:13:LEU:HD12	1:H:409:GLU:HG3	1.98	0.46
1:G:135:PRO:HA	1:G:141:PHE:CE2	2.51	0.46
1:H:76:ASP:OD2	1:H:205:TYR:OH	2.32	0.46
1:H:172:GLU:HG2	7:H:659:HOH:O	2.15	0.46
1:A:97:ASN:N	1:A:266:LEU:HD11	2.30	0.45
1:A:104:GLU:HG2	1:A:129:THR:HB	1.98	0.45
1:A:193:PHE:HB2	1:A:334:LEU:CD2	2.46	0.45
1:B:419:GLU:HG3	7:B:716:HOH:O	2.16	0.45
1:C:378:HIS:CE1	1:C:380:ALA:HB3	2.51	0.45
1:E:193:PHE:HB2	1:E:334:LEU:CD2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:226:GLY:HA2	1:G:255[B]:ASN:O	2.15	0.45
1:H:312:LYS:CE	1:H:425:VAL:O	2.64	0.45
1:A:96:LEU:C	1:A:266:LEU:HD11	2.37	0.45
1:C:76:ASP:OD2	1:C:205:TYR:OH	2.29	0.45
1:A:19:VAL:CG1	1:A:24:LYS:HA	2.46	0.45
1:D:161:ASN:HB2	1:D:395:ALA:O	2.15	0.45
1:A:320:ALA:HA	1:A:330:TYR:CD2	2.52	0.45
1:C:317:ASN:HB3	1:C:343:THR:OG1	2.17	0.45
1:E:155:GLU:HG2	1:E:184:ASP:HB3	1.99	0.45
1:F:184:ASP:OD2	1:F:209:LLP:N1	2.49	0.45
1:G:69:GLU:HA	1:G:221:ILE:HD11	1.99	0.45
1:H:193:PHE:HB2	1:H:334:LEU:CD2	2.46	0.45
1:E:296:HIS:HB3	1:E:340:ALA:CB	2.47	0.45
1:E:319:PRO:O	1:E:327:TYR:HA	2.17	0.45
1:C:57:TYR:CD2	2:E:501:MES:H51	2.51	0.45
1:E:106:VAL:O	1:E:152:ILE:HA	2.16	0.45
1:G:372:ALA:HB1	1:H:13:LEU:HD21	1.98	0.45
1:D:23:THR:HG21	1:H:31:TYR:CZ	2.51	0.45
1:E:350:TYR:CE1	1:E:378:HIS:CE1	3.05	0.45
1:F:116:TYR:OH	1:F:391:GLU:HG2	2.16	0.45
1:B:97:ASN:N	1:B:266:LEU:HD11	2.32	0.45
1:B:100:ARG:HB2	1:H:125:LYS:O	2.17	0.45
1:B:112:TYR:CE1	2:B:501:MES:H82	2.52	0.45
1:D:57:TYR:CD2	2:G:501:MES:H61	2.52	0.45
1:D:360:VAL:HG21	1:D:376:ILE:HG21	1.99	0.45
1:C:209:LLP:HD3	1:C:369:VAL:HG22	1.98	0.45
1:A:31:TYR:CG	1:A:63:PRO:HG2	2.52	0.45
1:A:319:PRO:O	1:A:327:TYR:HA	2.17	0.45
1:B:367:ALA:O	1:B:368:ASN:HB2	2.16	0.45
1:E:300:ALA:CB	1:E:340:ALA:HA	2.48	0.45
1:F:68:LEU:HA	1:F:283:LEU:HD21	1.99	0.45
1:F:250:THR:HA	1:F:257:ALA:HB2	1.99	0.45
1:H:19:VAL:CG1	1:H:24:LYS:HA	2.47	0.45
1:B:207:MET:HA	1:B:211:LEU:HB2	1.99	0.44
1:B:343:THR:HB	1:B:401:MET:HG3	1.99	0.44
1:D:346:PRO:HG3	1:D:356:ILE:HD12	1.99	0.44
1:D:378:HIS:CE1	1:D:380:ALA:HB3	2.52	0.44
1:E:6:TYR:HB3	1:E:10:THR:HB	1.98	0.44
1:E:135:PRO:HA	1:E:141:PHE:CE2	2.52	0.44
1:E:230:TRP:CD2	1:E:237:LEU:HD13	2.52	0.44
1:F:357:ILE:CD1	1:F:378:HIS:HB2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:277:PHE:HE1	1:H:277:PHE:CE1	2.36	0.44
1:H:296:HIS:HE1	1:H:371:ASP:O	1.99	0.44
1:H:318:TYR:CD1	1:H:342:PHE:HB3	2.51	0.44
1:H:375:LEU:HB2	1:H:405:SER:HB3	2.00	0.44
1:A:300:ALA:CB	1:A:340:ALA:HA	2.48	0.44
1:B:37:ILE:HG13	1:G:19:VAL:HG21	1.99	0.44
1:C:142:GLU:CD	1:C:177:HIS:HE2	2.19	0.44
1:C:385:GLN:HG3	7:C:671:HOH:O	2.16	0.44
1:D:69:GLU:HA	1:D:221:ILE:HD11	1.98	0.44
1:E:343:THR:HB	1:E:401:MET:HG3	1.99	0.44
1:F:107:ALA:HA	1:F:153:PHE:O	2.18	0.44
1:D:135:PRO:HA	1:D:141:PHE:CE2	2.53	0.44
1:D:363:PHE:CD2	1:D:374:SER:HB3	2.53	0.44
1:F:213:GLY:HA3	1:F:292:ARG:NH1	2.33	0.44
1:H:104:GLU:HG2	1:H:129:THR:HB	1.98	0.44
1:E:343:THR:HA	1:E:402:ILE:O	2.17	0.44
1:H:112:TYR:CE1	2:H:501:MES:H82	2.53	0.44
1:C:320:ALA:HA	1:C:330:TYR:CD2	2.53	0.44
1:D:363:PHE:CE2	1:D:374:SER:HB3	2.53	0.44
1:F:76:ASP:CG	1:F:205:TYR:HH	2.19	0.44
1:G:267:LEU:O	1:G:271:GLY:HA2	2.17	0.44
1:B:150:LYS:O	1:B:180:PRO:HD2	2.18	0.44
1:C:205:TYR:HB2	1:C:221:ILE:HG22	2.00	0.44
1:C:341:ILE:HD11	1:C:369:VAL:HB	1.98	0.44
1:E:159:ASN:HB2	1:E:187:PHE:CZ	2.52	0.44
1:F:192:LEU:HD11	1:F:297:VAL:CG1	2.47	0.44
1:G:19:VAL:CG1	1:G:24:LYS:HA	2.47	0.44
1:A:50:LEU:HD12	1:A:247:LEU:CD1	2.48	0.44
1:A:183:VAL:O	1:A:203:VAL:HA	2.18	0.44
1:C:86:SER:HB2	1:C:209:LLP:OP2	2.18	0.44
1:D:300:ALA:HB2	1:D:340:ALA:HA	2.00	0.44
1:E:341:ILE:CD1	1:E:369:VAL:HB	2.48	0.44
1:G:106:VAL:O	1:G:152:ILE:HA	2.17	0.44
1:G:240:PRO:HB3	1:G:246:GLY:HA2	2.00	0.44
1:A:20:ASP:OD2	1:A:23:THR:OG1	2.35	0.44
1:B:13:LEU:HD11	1:D:408:ILE:HG13	2.00	0.44
1:G:318:TYR:CD1	1:G:342:PHE:HB3	2.53	0.44
1:A:207:MET:HA	1:A:211:LEU:HB2	1.99	0.43
1:B:224:ASP:OD2	1:B:258:TYR:HB3	2.17	0.43
1:C:41:PRO:HG3	1:E:357:ILE:HB	1.99	0.43
1:C:207:MET:HA	1:C:211:LEU:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:ASP:HB2	1:D:259:ILE:HB	2.00	0.43
1:F:363:PHE:CD2	1:F:374:SER:HB3	2.53	0.43
1:C:330:TYR:CD1	1:C:330:TYR:C	2.91	0.43
1:G:104:GLU:HG2	1:G:129:THR:HB	1.99	0.43
1:B:318:TYR:CD1	1:B:342:PHE:HB3	2.53	0.43
1:B:343:THR:HA	1:B:402:ILE:O	2.18	0.43
1:E:296:HIS:CE1	1:E:407:GLY:HA2	2.54	0.43
1:F:155:GLU:HG2	1:F:184:ASP:HB3	2.00	0.43
1:F:287:GLU:OE2	7:F:601:HOH:O	2.21	0.43
1:F:320:ALA:HA	1:F:330:TYR:CD2	2.54	0.43
1:H:383:THR:HA	2:H:501:MES:H52	2.01	0.43
1:D:250:THR:HA	1:D:257:ALA:HB2	2.00	0.43
1:G:4:ARG:HH22	1:H:413:ASP:HA	1.83	0.43
1:A:250:THR:HA	1:A:257:ALA:HB2	1.99	0.43
1:B:43:GLU:HG3	1:B:52:LYS:HD3	2.00	0.43
1:C:301:MET:HE1	1:C:320:ALA:CB	2.48	0.43
1:F:289:LEU:HD12	1:F:293:MET:HG2	2.00	0.43
1:F:360:VAL:HG21	1:F:376:ILE:HG21	1.99	0.43
1:G:317:ASN:O	1:G:342:PHE:HB2	2.17	0.43
1:B:277:PHE:HE1	1:D:277:PHE:CE1	2.37	0.43
1:D:108:ALA:O	1:D:111:LEU:HG	2.18	0.43
1:H:315:TRP:CE2	1:H:345:GLY:HA3	2.54	0.43
1:D:43:GLU:OE2	1:D:52:LYS:HE2	2.19	0.43
1:D:48:PHE:HE1	2:G:501:MES:H22	1.83	0.43
1:F:69:GLU:HA	1:F:221:ILE:HD11	2.00	0.43
1:F:160:PRO:HD3	1:F:384:HIS:CE1	2.54	0.43
1:A:6:TYR:HB3	1:A:10:THR:HB	2.00	0.43
1:A:259:ILE:HD12	1:A:259:ILE:HA	1.74	0.43
1:D:150:LYS:O	1:D:180:PRO:HD2	2.19	0.43
1:D:267:LEU:O	1:D:271:GLY:HA2	2.19	0.43
1:H:19:VAL:HG12	1:H:24:LYS:HA	1.99	0.43
1:H:350:TYR:CE1	1:H:378:HIS:CE1	3.07	0.43
1:H:367:ALA:O	1:H:368:ASN:HB2	2.19	0.43
1:C:363:PHE:CE2	1:C:374:SER:HB3	2.54	0.43
1:D:107:ALA:O	1:D:132:PHE:HA	2.19	0.43
1:D:185:ASN:OD1	1:D:188:ALA:HB3	2.19	0.43
1:E:19:VAL:HG12	1:E:24:LYS:HA	2.00	0.43
1:E:378:HIS:CE1	1:E:380:ALA:HB3	2.54	0.43
1:F:165:PRO:HD2	1:F:167:PHE:CZ	2.53	0.43
1:G:346:PRO:HB3	1:G:356:ILE:CD1	2.49	0.43
1:H:141:PHE:O	1:H:145:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:LYS:O	1:G:36:TYR:HA	2.19	0.43
1:C:289:LEU:O	1:C:293:MET:HG2	2.18	0.43
1:D:36:TYR:CG	1:D:55:ASN:HB3	2.54	0.43
1:D:112:TYR:CE2	1:D:114:GLY:HA3	2.54	0.43
1:E:12:GLN:O	1:E:71:ARG:HD3	2.18	0.43
1:G:118:LEU:HD12	1:G:122:THR:HB	2.00	0.43
1:C:106:VAL:O	1:C:152:ILE:HA	2.19	0.42
1:C:318:TYR:CD1	1:C:342:PHE:HB3	2.54	0.42
1:E:183:VAL:O	1:E:203:VAL:HA	2.19	0.42
1:G:296:HIS:HB3	1:G:340:ALA:HB2	2.01	0.42
1:D:346:PRO:HB3	1:D:356:ILE:HD11	2.01	0.42
1:E:387:LEU:N	1:E:387:LEU:HD12	2.35	0.42
1:E:425:VAL:HG12	7:E:787:HOH:O	2.19	0.42
1:G:262:LEU:C	1:G:262:LEU:HD23	2.39	0.42
1:H:300:ALA:CB	1:H:340:ALA:HA	2.49	0.42
1:F:36:TYR:CG	1:F:55:ASN:HB3	2.53	0.42
1:F:135:PRO:HA	1:F:141:PHE:CE2	2.54	0.42
1:G:380:ALA:HA	1:G:397:VAL:HG11	2.01	0.42
1:H:193:PHE:HB2	1:H:334:LEU:HD23	2.01	0.42
1:A:142:GLU:CD	1:A:177:HIS:HE2	2.23	0.42
1:A:301:MET:HE3	1:A:301:MET:O	2.20	0.42
1:C:226:GLY:O	1:C:255:ASN:HB2	2.19	0.42
1:D:116:TYR:CD1	1:D:116:TYR:C	2.92	0.42
1:E:240:PRO:HB3	1:E:246:GLY:HA2	2.01	0.42
1:H:135:PRO:HA	1:H:141:PHE:CE2	2.54	0.42
1:A:211:LEU:HA	1:A:211:LEU:HD23	1.79	0.42
1:B:145:ILE:HD11	1:B:152:ILE:HD11	2.02	0.42
1:B:226:GLY:O	1:B:255:ASN:HB2	2.19	0.42
1:B:259:ILE:HD12	1:B:259:ILE:HA	1.86	0.42
1:C:97:ASN:N	1:C:266:LEU:HD11	2.34	0.42
1:E:208:THR:HA	1:E:217:SER:O	2.20	0.42
1:D:208:THR:HA	1:D:217:SER:O	2.19	0.42
1:F:303:LEU:HD11	1:F:418:ILE:HG21	2.00	0.42
1:G:97:ASN:N	1:G:266:LEU:HD11	2.35	0.42
1:G:343:THR:HB	1:G:401:MET:HG3	2.02	0.42
1:A:88:GLN:HB3	1:F:269:ASP:O	2.20	0.42
1:B:317:ASN:O	1:B:342:PHE:HB2	2.19	0.42
1:F:17:GLN:NE2	1:F:26:ARG:O	2.53	0.42
1:G:86:SER:HB2	1:G:209:LLP:OP2	2.19	0.42
1:G:159:ASN:HA	1:G:160:PRO:HA	1.92	0.42
1:H:320:ALA:HA	1:H:330:TYR:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:LEU:HD23	1:A:13:LEU:HA	1.90	0.42
1:C:69:GLU:HA	1:C:221:ILE:HD11	2.02	0.42
1:D:350:TYR:CE1	1:D:378:HIS:CE1	3.08	0.42
1:F:76:ASP:OD2	1:F:205:TYR:CE1	2.73	0.42
1:F:366:LEU:HD11	1:F:375:LEU:HD13	2.01	0.42
1:A:82:VAL:CG1	1:A:267:LEU:HD22	2.49	0.42
1:B:161:ASN:O	1:B:317:ASN:ND2	2.52	0.42
1:D:63:PRO:HG3	1:H:23:THR:HB	2.02	0.42
1:D:133:VAL:HB	1:D:140:GLU:HB3	2.01	0.42
1:G:259:ILE:HA	1:G:259:ILE:HD12	1.80	0.42
1:H:320:ALA:HA	1:H:330:TYR:CD2	2.55	0.42
1:A:240:PRO:HB3	1:A:246:GLY:CA	2.50	0.42
1:B:69:GLU:HA	1:B:221:ILE:HD11	2.02	0.42
1:E:390:GLU:OE1	1:E:393[B]:ARG:NH1	2.53	0.42
1:H:91:ILE:HG12	1:H:204:VAL:HG21	2.02	0.42
1:H:366:LEU:HD11	1:H:375:LEU:HD22	2.01	0.42
2:A:501:MES:H21	1:F:57:TYR:CD2	2.55	0.41
1:C:88:GLN:HB3	1:E:269:ASP:O	2.20	0.41
1:D:23:THR:HB	1:H:63:PRO:HG3	2.01	0.41
1:D:237:LEU:HA	1:D:237:LEU:HD23	1.79	0.41
1:F:110:THR:HA	1:F:395:ALA:HA	2.01	0.41
1:H:317:ASN:HB3	1:H:343:THR:OG1	2.20	0.41
1:C:104:GLU:HA	1:C:129:THR:O	2.19	0.41
1:D:152:ILE:HD12	1:D:174:ALA:HB2	2.03	0.41
1:D:207:MET:HA	1:D:211:LEU:HB2	2.01	0.41
1:F:193:PHE:HB2	1:F:334:LEU:HD23	2.03	0.41
1:F:318:TYR:CD1	1:F:342:PHE:HB3	2.55	0.41
1:G:19:VAL:HG12	1:G:24:LYS:HA	2.03	0.41
1:G:289:LEU:O	1:G:293:MET:HG2	2.20	0.41
1:A:31:TYR:CD2	1:A:63:PRO:HG2	2.55	0.41
1:B:413:ASP:HA	1:D:4:ARG:HH22	1.85	0.41
1:F:108:ALA:O	1:F:111:LEU:HG	2.19	0.41
1:H:380:ALA:HA	1:H:397:VAL:HG11	2.02	0.41
1:A:318:TYR:CD1	1:A:342:PHE:HB3	2.55	0.41
1:B:116:TYR:CD1	1:B:116:TYR:C	2.93	0.41
1:B:300:ALA:CB	1:B:340:ALA:HA	2.50	0.41
1:B:369:VAL:HA	1:B:375:LEU:HD12	2.03	0.41
1:D:319:PRO:O	1:D:327:TYR:HA	2.21	0.41
1:E:210:PHE:CD1	1:E:370:GLY:HA2	2.56	0.41
1:H:363:PHE:CD2	1:H:374:SER:HB3	2.55	0.41
1:H:392:GLN:HB3	1:H:397:VAL:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:VAL:O	1:A:152:ILE:HA	2.20	0.41
1:C:357:ILE:CD1	1:C:378:HIS:HB2	2.50	0.41
1:D:259:ILE:HD12	1:D:259:ILE:HA	1.77	0.41
1:H:112:TYR:CE2	1:H:114:GLY:HA3	2.56	0.41
1:H:283:LEU:O	1:H:287:GLU:HG3	2.19	0.41
1:A:208:THR:HA	1:A:217:SER:O	2.20	0.41
1:D:100:ARG:HB2	1:G:125:LYS:O	2.21	0.41
1:G:107:ALA:HA	1:G:153:PHE:O	2.20	0.41
1:G:319:PRO:O	1:G:327:TYR:HA	2.20	0.41
1:G:372:ALA:CB	1:H:13:LEU:HD21	2.50	0.41
1:D:366:LEU:HD11	1:D:375:LEU:HD13	2.02	0.41
1:D:411:ILE:HD12	1:D:411:ILE:HA	1.87	0.41
1:E:76:ASP:OD2	1:E:205:TYR:CE2	2.73	0.41
1:E:158:GLY:HA3	1:E:163:ASN:OD1	2.21	0.41
1:E:262:LEU:HD23	1:E:262:LEU:C	2.41	0.41
1:F:262:LEU:C	1:F:262:LEU:HD23	2.41	0.41
1:H:296:HIS:HB3	1:H:340:ALA:HB2	2.03	0.41
1:A:349:GLY:HA2	1:A:400:GLU:HB2	2.03	0.41
1:C:118:LEU:HD12	1:C:122:THR:HB	2.01	0.41
1:D:209:LLP:NZ	1:D:209:LLP:O3	2.47	0.41
1:E:224:ASP:HB2	1:E:259:ILE:HB	2.03	0.41
1:H:206:SER:HB2	1:H:209:LLP:OP4	2.21	0.41
1:A:30:ILE:HG12	1:A:280:PHE:CG	2.56	0.41
2:A:501:MES:H62	1:F:48:PHE:HE1	1.85	0.41
1:D:104:GLU:HG2	1:D:129:THR:HB	2.03	0.41
1:D:262:LEU:C	1:D:262:LEU:HD23	2.41	0.41
1:E:207:MET:HA	1:E:211:LEU:HB2	2.02	0.41
1:F:325:LYS:HD2	1:F:326:TYR:CZ	2.55	0.41
1:H:152:ILE:HD12	1:H:174:ALA:HB2	2.03	0.41
6:H:503:1PE:H122	7:H:807:HOH:O	2.20	0.41
1:A:145:ILE:HD11	1:A:152:ILE:HD11	2.03	0.41
1:D:183:VAL:O	1:D:203:VAL:HA	2.21	0.41
1:E:300:ALA:HB2	1:E:340:ALA:HA	2.03	0.41
1:F:320:ALA:HA	1:F:330:TYR:CE2	2.55	0.41
1:G:346:PRO:HD2	1:G:400:GLU:O	2.21	0.41
1:A:135:PRO:HA	1:A:141:PHE:CE2	2.57	0.40
1:A:419:GLU:HG2	1:A:423:ASN:HD22	1.86	0.40
1:B:36:TYR:CG	1:B:55:ASN:HB3	2.56	0.40
1:B:107:ALA:HA	1:B:153:PHE:O	2.21	0.40
1:B:183:VAL:O	1:B:203:VAL:HA	2.22	0.40
1:D:19:VAL:HG21	1:H:37:ILE:HG13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:343:THR:HB	1:D:401:MET:HG3	2.03	0.40
1:H:330:TYR:CD1	1:H:330:TYR:C	2.94	0.40
1:A:317:ASN:HB3	1:A:343:THR:OG1	2.21	0.40
1:B:378:HIS:CE1	1:B:380:ALA:HB3	2.56	0.40
1:C:155:GLU:HG2	1:C:184:ASP:HB3	2.03	0.40
1:C:161:ASN:HB2	1:C:395:ALA:O	2.20	0.40
1:D:107:ALA:HA	1:D:153:PHE:O	2.21	0.40
1:E:322:GLU:HG2	7:E:826:HOH:O	2.21	0.40
1:G:59:ARG:HH21	1:G:59:ARG:HD2	1.69	0.40
1:A:125:LYS:HG2	1:F:100:ARG:CZ	2.51	0.40
1:A:289:LEU:O	1:A:293:MET:HG2	2.21	0.40
1:A:317:ASN:O	1:A:342:PHE:HB2	2.21	0.40
1:D:230:TRP:CD2	1:D:237:LEU:HD13	2.56	0.40
1:E:380:ALA:HA	1:E:397:VAL:HG11	2.03	0.40
1:A:86:SER:HB2	1:A:209:LLP:OP1	2.21	0.40
1:B:159:ASN:HA	1:B:160:PRO:HA	1.90	0.40
1:C:107:ALA:HA	1:C:153:PHE:O	2.20	0.40
1:C:138:LEU:HD13	1:C:169:ALA:HB1	2.04	0.40
1:C:375:LEU:HB2	1:C:405:SER:HB3	2.03	0.40
1:G:182:ILE:HG12	1:G:202:ILE:HB	2.02	0.40
1:G:277:PHE:HE1	1:H:277:PHE:CZ	2.40	0.40
1:H:230:TRP:CG	1:H:237:LEU:HD13	2.56	0.40
1:H:262:LEU:HD23	1:H:262:LEU:C	2.41	0.40
1:C:193:PHE:HB2	1:C:334:LEU:CD2	2.52	0.40
1:D:12:GLN:O	1:D:71:ARG:HD3	2.21	0.40
1:D:341:ILE:CD1	1:D:369:VAL:HB	2.50	0.40
1:E:207:MET:HB2	1:E:219:ALA:HB3	2.03	0.40
1:E:320:ALA:HA	1:E:330:TYR:CE2	2.56	0.40
1:F:19:VAL:HG12	1:F:24:LYS:HA	2.03	0.40
1:F:318:TYR:CE1	1:F:338:PRO:HG2	2.57	0.40
1:H:240:PRO:HB3	1:H:246:GLY:HA2	2.02	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	427/433 (99%)	417 (98%)	10 (2%)	0	100	100
1	B	425/433 (98%)	415 (98%)	10 (2%)	0	100	100
1	C	424/433 (98%)	414 (98%)	10 (2%)	0	100	100
1	D	423/433 (98%)	413 (98%)	10 (2%)	0	100	100
1	E	426/433 (98%)	414 (97%)	12 (3%)	0	100	100
1	F	421/433 (97%)	411 (98%)	10 (2%)	0	100	100
1	G	423/433 (98%)	415 (98%)	8 (2%)	0	100	100
1	H	424/433 (98%)	414 (98%)	10 (2%)	0	100	100
All	All	3393/3464 (98%)	3313 (98%)	80 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	349/358 (98%)	344 (99%)	5 (1%)	67	53
1	B	347/358 (97%)	344 (99%)	3 (1%)	78	70
1	C	348/358 (97%)	345 (99%)	3 (1%)	78	70
1	D	346/358 (97%)	341 (99%)	5 (1%)	67	53
1	E	346/358 (97%)	344 (99%)	2 (1%)	86	80
1	F	338/358 (94%)	335 (99%)	3 (1%)	78	70
1	G	346/358 (97%)	339 (98%)	7 (2%)	55	38
1	H	342/358 (96%)	337 (98%)	5 (2%)	65	51
All	All	2762/2864 (96%)	2729 (99%)	33 (1%)	71	59

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	20	ASP
1	A	131	LYS
1	A	160	PRO
1	A	330	TYR
1	B	20	ASP
1	B	330	TYR
1	B	410	ASP
1	C	20	ASP
1	C	330	TYR
1	C	379	PRO
1	D	20	ASP
1	D	160	PRO
1	D	312	LYS
1	D	330	TYR
1	D	410	ASP
1	E	20	ASP
1	E	330	TYR
1	F	20	ASP
1	F	330	TYR
1	F	410	ASP
1	G	20	ASP
1	G	131	LYS
1	G	160	PRO
1	G	161	ASN
1	G	330	TYR
1	G	410	ASP
1	G	424	LYS
1	H	20	ASP
1	H	52	LYS
1	H	131	LYS
1	H	160	PRO
1	H	330	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	LLP	H	209	1	23,24,25	1.02	1 (4%)	25,32,34	0.91	1 (4%)
1	LLP	C	209	1	23,24,25	0.93	0	25,32,34	0.88	1 (4%)
1	LLP	G	209	1	23,24,25	1.27	4 (17%)	25,32,34	0.91	2 (8%)
1	LLP	D	209	1	23,24,25	1.03	1 (4%)	25,32,34	0.98	1 (4%)
1	LLP	A	209	1	23,24,25	1.05	2 (8%)	25,32,34	0.92	1 (4%)
1	LLP	B	209	1	23,24,25	0.94	0	25,32,34	0.94	1 (4%)
1	LLP	E	209	1	23,24,25	0.93	1 (4%)	25,32,34	0.86	1 (4%)
1	LLP	F	209	1	23,24,25	0.81	0	25,32,34	1.08	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	H	209	1	-	4/16/17/19	0/1/1/1
1	LLP	C	209	1	-	2/16/17/19	0/1/1/1
1	LLP	G	209	1	-	2/16/17/19	0/1/1/1
1	LLP	D	209	1	-	2/16/17/19	0/1/1/1
1	LLP	A	209	1	-	3/16/17/19	0/1/1/1
1	LLP	B	209	1	-	3/16/17/19	0/1/1/1
1	LLP	E	209	1	-	4/16/17/19	0/1/1/1
1	LLP	F	209	1	-	2/16/17/19	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	209	LLP	C4-C5	-2.94	1.38	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	209	LLP	C4-C5	-2.72	1.38	1.42
1	G	209	LLP	C3-C2	-2.51	1.38	1.40
1	D	209	LLP	C4-C5	-2.36	1.39	1.42
1	H	209	LLP	C4-C4'	-2.28	1.42	1.46
1	A	209	LLP	C4-C5	-2.26	1.39	1.42
1	G	209	LLP	C4-C4'	-2.23	1.42	1.46
1	A	209	LLP	O3-C3	-2.21	1.31	1.37
1	G	209	LLP	P-OP3	-2.14	1.46	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	209	LLP	OP3-P-OP4	-3.11	98.45	106.73
1	B	209	LLP	OP2-P-OP4	-3.06	98.59	106.73
1	A	209	LLP	OP2-P-OP4	-3.01	98.74	106.73
1	G	209	LLP	OP3-P-OP4	-2.87	99.10	106.73
1	C	209	LLP	OP4-P-OP1	-2.60	99.17	106.47
1	E	209	LLP	OP4-P-OP1	-2.43	99.67	106.47
1	H	209	LLP	OP4-P-OP1	-2.41	99.71	106.47
1	D	209	LLP	C4-C3-C2	-2.32	118.75	120.19
1	G	209	LLP	OP3-P-OP2	2.01	115.31	107.64

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	209	LLP	O-C-CA-CB
1	B	209	LLP	O-C-CA-CB
1	C	209	LLP	O-C-CA-CB
1	D	209	LLP	O-C-CA-CB
1	E	209	LLP	O-C-CA-CB
1	F	209	LLP	O-C-CA-CB
1	G	209	LLP	O-C-CA-CB
1	H	209	LLP	O-C-CA-CB
1	E	209	LLP	C4-C4'-NZ-CE
1	F	209	LLP	C4-C4'-NZ-CE
1	G	209	LLP	C4-C4'-NZ-CE
1	C	209	LLP	C4-C4'-NZ-CE
1	D	209	LLP	C4-C4'-NZ-CE
1	H	209	LLP	CG-CD-CE-NZ
1	B	209	LLP	C4-C4'-NZ-CE
1	H	209	LLP	C4-C4'-NZ-CE

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Mol	Chain	Res	Type	Atoms
1	A	209	LLP	C4-C4'-NZ-CE
1	B	209	LLP	CG-CD-CE-NZ
1	H	209	LLP	CA-CB-CG-CD
1	E	209	LLP	CA-CB-CG-CD
1	E	209	LLP	CG-CD-CE-NZ
1	A	209	LLP	CG-CD-CE-NZ

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	H	209	LLP	1	0
1	C	209	LLP	2	0
1	G	209	LLP	1	0
1	D	209	LLP	1	0
1	A	209	LLP	1	0
1	F	209	LLP	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 26 ligands modelled in this entry, 13 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	MES	E	501	-	12,12,12	0.62	0	14,16,16	0.84	0
6	1PE	H	502	-	15,15,15	0.49	0	14,14,14	0.48	0
2	MES	C	501	-	12,12,12	0.85	0	14,16,16	1.15	1 (7%)
2	MES	F	501	-	12,12,12	0.65	0	14,16,16	0.79	0
4	AE3	D	502	-	8,8,8	0.53	0	7,7,7	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	AE3	E	503	-	8,8,8	0.58	0	7,7,7	0.35	0
2	MES	A	501	-	12,12,12	0.79	0	14,16,16	0.85	0
2	MES	D	501	-	12,12,12	0.70	0	14,16,16	0.88	1 (7%)
5	ETE	E	502	-	13,13,13	0.64	0	12,12,12	0.42	0
2	MES	G	501	-	12,12,12	0.80	0	14,16,16	1.22	1 (7%)
2	MES	B	501	-	12,12,12	0.84	0	14,16,16	1.07	0
6	1PE	H	503	-	15,15,15	0.42	0	14,14,14	0.57	0
2	MES	H	501	-	12,12,12	0.84	0	14,16,16	0.87	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MES	E	501	-	-	6/6/14/14	0/1/1/1
6	1PE	H	502	-	-	6/13/13/13	-
2	MES	C	501	-	-	2/6/14/14	0/1/1/1
2	MES	F	501	-	-	6/6/14/14	0/1/1/1
4	AE3	D	502	-	-	3/6/6/6	-
4	AE3	E	503	-	-	3/6/6/6	-
2	MES	A	501	-	-	0/6/14/14	0/1/1/1
2	MES	D	501	-	-	0/6/14/14	0/1/1/1
5	ETE	E	502	-	-	4/11/11/11	-
2	MES	G	501	-	-	0/6/14/14	0/1/1/1
2	MES	B	501	-	-	6/6/14/14	0/1/1/1
6	1PE	H	503	-	-	6/13/13/13	-
2	MES	H	501	-	-	6/6/14/14	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	501	MES	O1S-S-C8	-2.96	103.35	106.92
2	C	501	MES	O1S-S-C8	-2.79	103.55	106.92
2	D	501	MES	O2S-S-C8	-2.50	103.90	106.92

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	501	MES	C8-C7-N4-C3
2	E	501	MES	N4-C7-C8-S
2	F	501	MES	C8-C7-N4-C5
2	F	501	MES	C7-C8-S-O1S
2	F	501	MES	C7-C8-S-O2S
2	H	501	MES	N4-C7-C8-S
6	H	502	1PE	C25-C15-OH6-C26
5	E	502	ETE	OH2-C12-C22-OH3
5	E	502	ETE	OH6-C15-C25-OH5
6	H	503	1PE	C25-C15-OH6-C26
6	H	502	1PE	OH6-C15-C25-OH5
2	B	501	MES	C7-C8-S-O3S
2	E	501	MES	C7-C8-S-O3S
2	F	501	MES	C7-C8-S-O3S
2	H	501	MES	C7-C8-S-O3S
6	H	502	1PE	OH2-C12-C22-OH3
6	H	503	1PE	OH7-C16-C26-OH6
6	H	503	1PE	OH5-C14-C24-OH4
4	D	502	AE3	O3-C5-C6-O4
6	H	502	1PE	OH7-C16-C26-OH6
4	E	503	AE3	O2-C3-C4-O3
4	E	503	AE3	C1-C2-O2-C3
2	B	501	MES	N4-C7-C8-S
2	F	501	MES	N4-C7-C8-S
2	B	501	MES	C8-C7-N4-C3
2	B	501	MES	C8-C7-N4-C5
2	C	501	MES	C8-C7-N4-C5
2	E	501	MES	C8-C7-N4-C5
2	F	501	MES	C8-C7-N4-C3
2	H	501	MES	C8-C7-N4-C3
2	H	501	MES	C8-C7-N4-C5
6	H	502	1PE	C23-C13-OH4-C24
6	H	503	1PE	C15-C25-OH5-C14
4	D	502	AE3	C1-C2-O2-C3
4	E	503	AE3	C4-C3-O2-C2
2	B	501	MES	C7-C8-S-O1S
2	B	501	MES	C7-C8-S-O2S
2	E	501	MES	C7-C8-S-O1S
2	E	501	MES	C7-C8-S-O2S
2	H	501	MES	C7-C8-S-O1S
4	D	502	AE3	C6-C5-O3-C4
5	E	502	ETE	C23-C13-OH4-C24
5	E	502	ETE	C15-C25-OH5-C14

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Mol	Chain	Res	Type	Atoms
6	H	502	1PE	OH4-C13-C23-OH3
2	C	501	MES	C8-C7-N4-C3
6	H	503	1PE	C24-C14-OH5-C25
2	H	501	MES	C7-C8-S-O2S
6	H	503	1PE	OH6-C15-C25-OH5

There are no ring outliers.

10 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	501	MES	2	0
2	C	501	MES	1	0
2	F	501	MES	2	0
2	A	501	MES	3	0
2	D	501	MES	1	0
5	E	502	ETE	1	0
2	G	501	MES	3	0
2	B	501	MES	1	0
6	H	503	1PE	1	0
2	H	501	MES	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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^2)	Q<0.9
1	A	423/433 (97%)	-0.00	9 (2%)	63	67	22, 30, 47, 68	0
1	B	423/433 (97%)	-0.11	5 (1%)	79	82	21, 29, 42, 67	0
1	C	422/433 (97%)	-0.06	3 (0%)	87	90	22, 30, 46, 72	0
1	D	423/433 (97%)	0.09	14 (3%)	46	51	21, 31, 49, 83	0
1	E	424/433 (97%)	0.09	13 (3%)	49	53	22, 31, 47, 75	0
1	F	422/433 (97%)	0.38	36 (8%)	10	12	25, 38, 55, 84	0
1	G	422/433 (97%)	-0.13	3 (0%)	87	90	21, 29, 44, 77	0
1	H	424/433 (97%)	-0.08	6 (1%)	75	79	21, 28, 42, 77	0
All	All	3383/3464 (97%)	0.02	89 (2%)	56	60	21, 30, 48, 84	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	425	VAL	7.0
1	A	426	LEU	5.9
1	E	426	LEU	4.7
1	F	421	ALA	4.5
1	A	425	VAL	4.1
1	D	1	MET	3.9
1	G	425	VAL	3.8
1	F	424	LYS	3.7
1	F	138	LEU	3.6
1	B	4	ARG	3.5
1	F	327	TYR	3.5
1	E	211	LEU	3.5
1	F	422	LEU	3.4
1	H	211	LEU	3.4
1	E	3	GLU	3.3
1	F	418	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	91	ILE	3.1
1	A	39	GLU	3.1
1	F	350	TYR	3.0
1	D	369	VAL	3.0
1	F	139	GLU	3.0
1	F	349	GLY	3.0
1	F	351	ASP	2.9
1	F	323	GLY	2.9
1	D	311	PRO	2.9
1	F	137	TYR	2.9
1	C	424	LYS	2.8
1	B	426	LEU	2.8
1	F	348	GLY	2.8
1	F	311	PRO	2.7
1	H	3	GLU	2.7
1	D	424	LYS	2.6
1	D	286	VAL	2.6
1	F	347	LYS	2.6
1	F	218	ILE	2.6
1	D	421	ALA	2.6
1	D	418	ILE	2.5
1	E	4	ARG	2.5
1	F	301	MET	2.5
1	H	286	VAL	2.5
1	F	21	ARG	2.4
1	F	232	GLU	2.4
1	F	314	GLU	2.4
1	D	284	LEU	2.4
1	E	210	PHE	2.4
1	D	359	ASN	2.4
1	B	111	LEU	2.4
1	B	284	LEU	2.4
1	H	218	ILE	2.4
1	F	423	ASN	2.4
1	A	351	ASP	2.4
1	F	211	LEU	2.3
1	F	147	ASP	2.3
1	E	327	TYR	2.3
1	F	53	ALA	2.3
1	F	40	THR	2.3
1	F	352	ALA	2.3
1	F	143	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	369	VAL	2.2
1	F	316	VAL	2.2
1	E	111	LEU	2.2
1	F	328	GLU	2.2
1	F	2	GLU	2.2
1	G	424	LYS	2.2
1	C	4	ARG	2.1
1	E	282	VAL	2.1
1	E	286	VAL	2.1
1	D	211	LEU	2.1
1	G	351	ASP	2.1
1	E	205	TYR	2.1
1	A	42	GLU	2.1
1	B	393[A]	ARG	2.1
1	D	3	GLU	2.1
1	A	284	LEU	2.1
1	D	42	GLU	2.1
1	F	3	GLU	2.1
1	F	315	TRP	2.1
1	E	289	LEU	2.1
1	F	46	ASP	2.0
1	D	282	VAL	2.0
1	F	91	ILE	2.0
1	A	359	ASN	2.0
1	F	148	LYS	2.0
1	H	4	ARG	2.0
1	F	420	SER	2.0
1	D	327	TYR	2.0
1	A	286	VAL	2.0
1	H	289	LEU	2.0
1	A	423	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
1	LLP	A	209	24/25	0.98	0.11	24,28,30,32	0
1	LLP	B	209	24/25	0.98	0.12	21,25,28,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	LLP	C	209	24/25	0.98	0.10	22,25,29,29	0
1	LLP	D	209	24/25	0.98	0.14	24,27,32,33	0
1	LLP	E	209	24/25	0.98	0.18	24,29,32,33	0
1	LLP	F	209	24/25	0.98	0.14	29,33,36,39	0
1	LLP	H	209	24/25	0.98	0.12	22,26,30,32	0
1	LLP	G	209	24/25	0.99	0.12	21,25,28,28	0

6.3 Carbohydrates (i)

There are no monosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å^2)	Q<0.9
5	ETE	E	502	14/14	0.73	0.28	55,72,82,83	0
4	AE3	E	503	9/9	0.79	0.15	55,62,71,72	0
3	NA	A	503	1/1	0.81	0.30	55,55,55,55	0
6	1PE	H	502	16/16	0.82	0.24	48,66,69,72	0
4	AE3	D	502	9/9	0.83	0.20	57,72,83,84	0
6	1PE	H	503	16/16	0.84	0.18	54,63,80,81	0
3	NA	C	503	1/1	0.85	0.21	49,49,49,49	0
3	NA	G	502	1/1	0.88	0.20	63,63,63,63	0
3	NA	G	503	1/1	0.91	0.21	47,47,47,47	1
3	NA	B	503	1/1	0.91	0.17	56,56,56,56	0
3	NA	C	504	1/1	0.93	0.19	45,45,45,45	1
3	NA	H	504	1/1	0.95	0.29	44,44,44,44	0
3	NA	B	502	1/1	0.95	0.27	47,47,47,47	0
3	NA	D	504	1/1	0.95	0.15	51,51,51,51	0
3	NA	D	503	1/1	0.96	0.23	39,39,39,39	0
2	MES	F	501	12/12	0.96	0.14	38,48,52,53	0
2	MES	H	501	12/12	0.96	0.14	34,37,41,48	0
3	NA	A	502	1/1	0.96	0.30	50,50,50,50	0
2	MES	E	501	12/12	0.96	0.16	35,39,42,45	0
2	MES	A	501	12/12	0.97	0.11	34,37,39,47	0
2	MES	B	501	12/12	0.97	0.13	30,34,38,43	0
2	MES	G	501	12/12	0.97	0.13	28,34,38,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MES	C	501	12/12	0.97	0.12	33,35,37,42	0
2	MES	D	501	12/12	0.98	0.13	38,39,44,51	0
3	NA	C	505	1/1	0.98	0.19	51,51,51,51	0
3	NA	C	502	1/1	0.99	0.22	41,41,41,41	0

6.5 Other polymers (i)

There are no such residues in this entry.