



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 08:32 am GMT

PDB ID : 1PJQ  
Title : Structure and function of CysG, the multifunctional methyltransferase/dehydrogenase/ferrochelatase for siroheme synthesis  
Authors : Stroupe, M.E.; Leech, H.K.; Daniels, D.S.; Warren, M.J.; Getzoff, E.D.  
Deposited on : 2003-06-03  
Resolution : 2.21 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

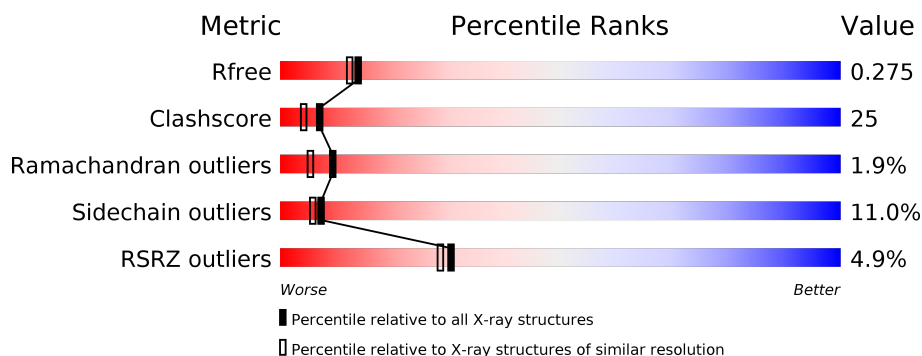
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.21 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	4744 (2.24-2.20)
Clashscore	112137	5509 (2.24-2.20)
Ramachandran outliers	110173	5427 (2.24-2.20)
Sidechain outliers	110143	5428 (2.24-2.20)
RSRZ outliers	101464	4776 (2.24-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	457	
1	B	457	

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
1	SEP	B	128	-	-	X	-
2	ACT	A	504	-	-	X	X
2	ACT	A	505	-	-	X	-
3	PGE	A	502	-	-	X	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7503 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.

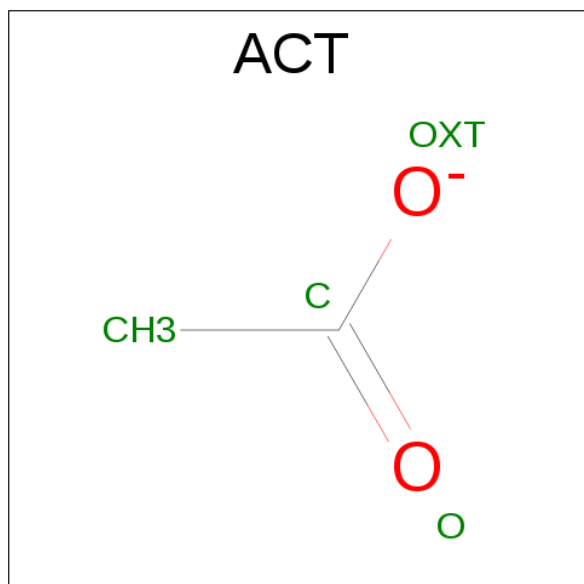
- Molecule 1 is a protein called Siroheme synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	P	S	0	13	0
			3581	2249	650	663	1	18			
1	B	455	Total	C	N	O	P	S	0	4	0
			3548	2228	643	659	1	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	128	SEP	SER	MODIFIED RESIDUE	UNP P25924
B	128	SEP	SER	MODIFIED RESIDUE	UNP P25924

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



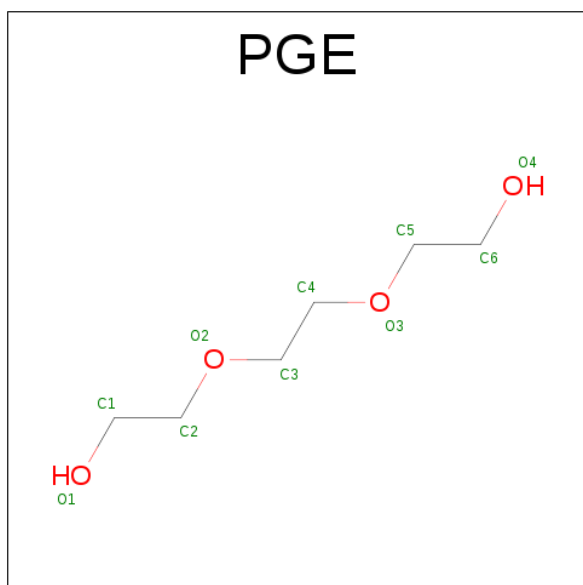
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		

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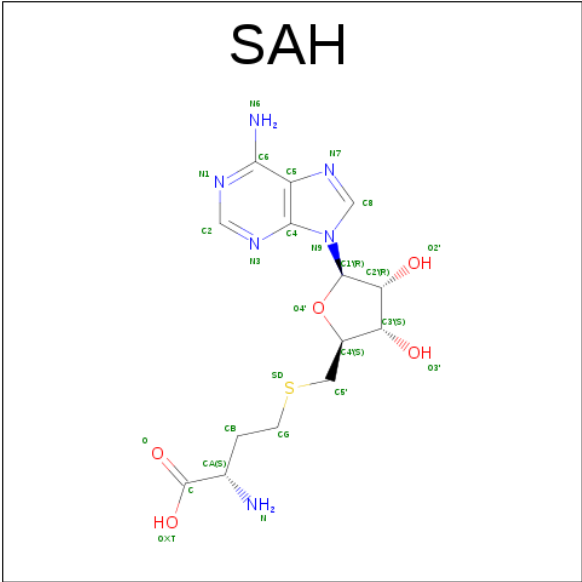
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula:  $C_{14}H_{20}N_6O_5S$ ).

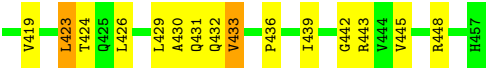


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	147	Total	O	0	0
			147	147		
5	B	179	Total	O	0	0
			179	179		







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.73Å 121.49Å 130.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.21 19.97 – 2.21	Depositor EDS
% Data completeness (in resolution range)	98.8 (19.97-2.21) 98.9 (19.97-2.21)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.16 (at 2.21Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.235 , 0.273 0.239 , 0.275	Depositor DCC
$R_{free}$ test set	4891 reflections (10.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.1	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 56.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7503	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, SAH, PGE, SEP

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	0.53	4/3627 (0.1%)	0.84	13/4903 (0.3%)
1	B	0.46	0/3594	0.85	12/4861 (0.2%)
All	All	0.49	4/7221 (0.1%)	0.85	25/9764 (0.3%)

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	3
1	B	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	375	LYS	CA-CB	-7.08	1.38	1.53
1	A	375	LYS	N-CA	6.88	1.60	1.46
1	A	276	CYS	N-CA	-6.62	1.33	1.46
1	A	375	LYS	CA-C	6.57	1.70	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	276	CYS	N-CA-CB	-12.98	87.23	110.60
1	A	375	LYS	CB-CA-C	10.45	131.30	110.40
1	B	350	ALA	N-CA-C	9.13	135.66	111.00
1	A	400	GLN	CB-CA-C	-9.13	92.14	110.40
1	B	375	LYS	N-CA-C	8.63	134.30	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	370	ASN	N-CA-C	-8.53	87.97	111.00
1	A	374[A]	GLU	CA-C-N	-7.88	99.87	117.20
1	A	374[B]	GLU	CA-C-N	-7.88	99.87	117.20
1	B	375	LYS	CA-C-N	-7.82	100.00	117.20
1	B	351	GLN	N-CA-C	7.74	131.89	111.00
1	A	347	ARG	N-CA-C	7.61	131.54	111.00
1	B	369	GLU	N-CA-CB	7.31	123.76	110.60
1	A	276	CYS	N-CA-C	6.94	129.75	111.00
1	B	369	GLU	CA-C-N	-6.55	102.79	117.20
1	B	350	ALA	N-CA-CB	-6.46	101.06	110.10
1	A	276	CYS	O-C-N	6.43	132.99	122.70
1	B	352	SER	N-CA-C	-6.22	94.20	111.00
1	B	360	LEU	N-CA-C	-6.20	94.25	111.00
1	B	263	ALA	N-CA-C	-6.09	94.56	111.00
1	A	374[A]	GLU	C-N-CA	-5.36	108.31	121.70
1	A	374[B]	GLU	C-N-CA	-5.36	108.31	121.70
1	A	375	LYS	N-CA-CB	5.31	120.15	110.60
1	B	374	GLU	N-CA-C	5.24	125.13	111.00
1	A	401	ALA	CA-C-N	-5.13	105.91	117.20
1	A	401	ALA	N-CA-CB	-5.10	102.95	110.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	275	HIS	Mainchain
1	A	374[A]	GLU	Mainchain
1	A	374[B]	GLU	Mainchain
1	B	374	GLU	Mainchain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3581	0	3611	232	0
1	B	3548	0	3584	157	0
2	A	8	0	6	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4	0	3	1	0
3	A	10	0	13	8	0
4	B	26	0	19	0	0
5	A	147	0	0	9	0
5	B	179	0	0	4	0
All	All	7503	0	7236	367	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 25.

All (367) 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:B:127:SER:C	1:B:128:SEP:N	1.67	1.43
1:A:374[A]:GLU:HG2	1:A:375:LYS:N	1.36	1.33
1:B:128:SEP:CB	1:B:128:SEP:OG	1.83	1.27
1:A:302:GLY:HA3	2:A:505:ACT:H2	1.25	1.13
1:A:374[B]:GLU:HG2	1:A:375:LYS:N	1.68	1.07
1:B:346:HIS:CE1	1:B:347:ARG:HD3	1.89	1.06
1:B:256:MET:O	1:B:259:VAL:HG12	1.60	1.01
1:A:284:GLN:HA	1:A:287:LEU:HD21	1.42	1.00
1:A:137[A]:ARG:NH2	1:B:176:ARG:HH12	1.65	0.95
1:A:346:HIS:HE1	1:A:347:ARG:HH21	1.00	0.95
1:A:142:LYS:NZ	3:A:502:PGE:H2	1.82	0.95
1:A:346:HIS:CE1	1:A:347:ARG:HH21	1.84	0.94
1:B:349:TYR:H	1:B:349:TYR:HD1	1.15	0.93
1:B:236:LEU:HD21	1:B:240:GLN:HE21	1.34	0.93
1:B:365:GLU:HG3	1:B:366:LEU:N	1.80	0.93
1:A:374[B]:GLU:CG	1:A:375:LYS:N	2.26	0.92
1:A:407:LEU:HD22	1:A:439:ILE:HG12	1.50	0.91
1:B:265:ARG:HH11	1:B:265:ARG:HG3	1.35	0.91
1:B:374:GLU:HG3	1:B:375:LYS:HE2	1.52	0.90
1:B:227:ASP:HB3	1:B:230:LEU:HD22	1.53	0.89
1:A:352:SER:HB3	1:A:376:GLN:HG2	1.52	0.89
1:A:287:LEU:H	1:A:287:LEU:HD23	1.38	0.88
1:B:412:THR:H	1:B:416:GLN:HE21	1.22	0.86
1:B:284[A]:GLN:HG3	1:B:288:ARG:HH21	1.43	0.84
1:A:268:VAL:O	1:A:268:VAL:HG12	1.75	0.83
1:A:142:LYS:HZ3	3:A:502:PGE:H2	1.43	0.83
1:A:401:ALA:O	1:A:422:VAL:HG12	1.80	0.82
1:B:162:ARG:HG3	1:B:166:LYS:HE2	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374[B]:GLU:HG3	1:A:376:GLN:H	1.45	0.81
1:B:290:ALA:HB3	1:B:322:ILE:HD13	1.63	0.81
1:A:331[B]:THR:HG23	1:A:334:SER:H	1.46	0.80
1:B:128:SEP:CB	1:B:132:SER:H	1.97	0.78
1:B:407:LEU:CD2	1:B:439:ILE:HG12	2.14	0.78
1:A:137[A]:ARG:HH22	1:B:176:ARG:HH12	1.32	0.78
1:A:303:ASP:H	2:A:505:ACT:CH3	1.96	0.77
1:B:365:GLU:HG3	1:B:366:LEU:H	1.46	0.77
1:A:302:GLY:CA	2:A:505:ACT:H2	2.09	0.77
1:A:128:SEP:HB3	1:A:132:SER:H	1.48	0.76
1:A:401:ALA:O	1:A:422:VAL:CG1	2.33	0.76
1:B:409:GLU:HB2	1:B:433:VAL:CG1	2.15	0.76
1:A:412:THR:H	1:A:416:GLN:HE21	1.33	0.76
1:A:370:ASN:HD21	1:B:370:ASN:HA	1.49	0.76
1:B:284[A]:GLN:HG3	1:B:288:ARG:NH2	2.01	0.75
1:A:287:LEU:N	1:A:287:LEU:HD23	2.01	0.75
1:A:366:LEU:HD12	1:A:371:LEU:HD11	1.69	0.75
1:B:284[A]:GLN:CG	1:B:288:ARG:HH21	1.99	0.75
1:A:112:ILE:HD12	1:A:129:GLY:HA2	1.69	0.75
1:A:356:VAL:HG12	1:A:357:THR:CG2	2.17	0.74
1:A:142:LYS:HZ3	3:A:502:PGE:H42	1.52	0.74
1:A:213:ASP:OD1	1:A:215:ARG:HG2	1.86	0.74
1:B:395:ILE:HG23	1:B:423:LEU:HD13	1.69	0.74
1:A:382[B]:MET:HB2	1:A:437:ALA:O	1.88	0.74
1:A:356:VAL:O	1:A:381[B]:TYR:HB2	1.87	0.74
1:B:351:GLN:HA	1:B:351:GLN:OE1	1.88	0.74
1:B:127:SER:C	1:B:128:SEP:H	1.89	0.73
1:B:365:GLU:CG	1:B:366:LEU:N	2.52	0.73
1:B:281:GLU:O	1:B:285:ILE:HG13	1.87	0.73
1:B:346:HIS:HE1	1:B:347:ARG:HD3	1.48	0.72
1:B:66:ASP:O	1:B:69:LEU:HB2	1.88	0.72
1:A:227:ASP:H	1:A:412:THR:CG2	2.03	0.72
1:A:137[A]:ARG:NH2	1:B:176:ARG:NH1	2.37	0.71
1:B:309:ARG:HH11	1:B:309:ARG:HB3	1.56	0.71
1:A:112:ILE:CD1	1:A:129:GLY:HA2	2.21	0.70
1:A:366:LEU:HD12	1:A:371:LEU:CD1	2.21	0.70
1:B:443:ARG:HG2	1:B:443:ARG:HH21	1.55	0.70
1:B:346:HIS:ND1	1:B:347:ARG:HD3	2.06	0.70
1:A:287:LEU:CD2	1:A:287:LEU:H	2.03	0.70
1:A:142:LYS:HZ1	3:A:502:PGE:H2	1.58	0.69
1:B:412:THR:H	1:B:416:GLN:NE2	1.88	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:VAL:HG12	1:A:357:THR:HG22	1.73	0.69
1:A:412:THR:H	1:A:416:GLN:NE2	1.90	0.69
1:A:283:ASN:O	1:A:287:LEU:CD2	2.39	0.69
1:B:100:CYS:H	1:B:110:SER:HB2	1.57	0.69
1:B:419:VAL:CG1	1:B:429:LEU:HD22	2.23	0.69
1:A:420[A]:HIS:CD2	1:A:421:GLY:N	2.60	0.69
1:A:447:LEU:HD23	1:A:447:LEU:H	1.57	0.68
1:A:122:LEU:HD21	1:B:139:LEU:HD11	1.75	0.68
1:A:418:VAL:H	1:A:457:HIS:CE1	2.11	0.68
1:A:420[A]:HIS:HD2	1:A:421:GLY:N	1.92	0.67
1:B:128:SEP:HB2	1:B:132:SER:H	1.59	0.67
1:A:227:ASP:H	1:A:412:THR:HG23	1.59	0.67
1:A:249:ARG:HG3	1:A:249:ARG:HH11	1.58	0.67
1:A:348:ASP:N	1:A:348:ASP:OD1	2.27	0.67
1:B:375:LYS:HD3	5:B:552:HOH:O	1.94	0.67
1:B:223:ALA:HB2	1:B:299:LEU:HD22	1.78	0.65
1:B:419:VAL:HG12	1:B:429:LEU:HD22	1.76	0.65
1:B:374:GLU:HG2	1:B:375:LYS:HG2	1.78	0.65
1:B:407:LEU:HD21	1:B:439:ILE:HG12	1.79	0.65
1:B:128:SEP:HB3	1:B:132:SER:H	1.60	0.65
1:A:277:VAL:HG12	1:A:281:GLU:HG2	1.78	0.65
1:A:352:SER:OG	1:B:354:ARG:HD3	1.97	0.64
1:A:309:ARG:HG2	1:A:312:GLU:OE1	1.97	0.64
1:B:367:ASP:OD1	1:B:367:ASP:N	2.20	0.64
1:A:419:VAL:HG21	1:A:429:LEU:HB3	1.80	0.63
1:B:162:ARG:O	1:B:166:LYS:HD2	1.97	0.63
1:B:403:MET:HE1	1:B:442:GLY:HA2	1.78	0.63
1:A:164:ARG:HD2	1:A:208:PHE:CE2	2.34	0.63
1:A:399:MET:SD	1:A:423:LEU:HD11	2.38	0.63
1:A:429:LEU:O	1:A:432:GLN:HB2	1.98	0.63
1:A:85:VAL:HG22	1:A:88:ARG:HH21	1.64	0.63
5:A:617:HOH:O	1:B:318:CYS:HB2	1.99	0.63
1:A:384[B]:LEU:HD22	1:A:435:SER:OG	1.99	0.63
1:A:400:GLN:O	1:A:402:ASP:N	2.32	0.63
1:B:409:GLU:HB2	1:B:433:VAL:HG12	1.79	0.63
1:A:278:PRO:O	1:A:280:GLU:N	2.32	0.63
1:A:354:ARG:NH2	1:B:354:ARG:NH2	2.46	0.62
1:B:100:CYS:H	1:B:110:SER:CB	2.13	0.62
1:A:371:LEU:O	1:A:378:LEU:HD11	1.99	0.62
1:B:368:TRP:HH2	1:B:390:ILE:HG12	1.65	0.62
1:A:275:HIS:CG	1:A:276:CYS:H	2.11	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ARG:HH11	1:A:187:ARG:HG3	1.64	0.62
1:A:374[B]:GLU:CG	1:A:376:GLN:H	2.13	0.62
1:A:331[B]:THR:CG2	1:A:334:SER:H	2.12	0.62
1:B:256:MET:O	1:B:259:VAL:CG1	2.44	0.62
1:A:307:PHE:CB	2:A:505:ACT:H3	2.30	0.62
1:A:231:LEU:O	1:B:233:LEU:HD13	1.99	0.61
1:A:346:HIS:CE1	1:A:347:ARG:HD2	2.35	0.61
1:A:176:ARG:NH1	1:A:295:ARG:HD2	2.16	0.61
1:B:265:ARG:NH1	1:B:265:ARG:HG3	2.11	0.60
1:A:137[A]:ARG:HG2	1:A:137[A]:ARG:HH21	1.66	0.60
1:A:268:VAL:HA	1:A:277:VAL:HG21	1.83	0.60
1:A:277:VAL:O	1:A:282:ILE:HG13	2.01	0.60
1:B:162:ARG:CG	1:B:166:LYS:HE2	2.29	0.60
1:A:261[B]:ARG:NH1	5:A:627:HOH:O	2.33	0.60
1:A:303:ASP:H	2:A:505:ACT:H1	1.66	0.60
1:B:29:ARG:O	1:B:33:GLU:HG3	2.01	0.60
1:A:140[A]:ARG:HG2	1:A:140[A]:ARG:HH11	1.67	0.60
1:A:346:HIS:ND1	1:A:347:ARG:HD2	2.17	0.60
1:B:196:ASP:O	1:B:200:VAL:HG23	2.01	0.60
1:B:238:GLN:HE22	1:B:295:ARG:HH21	1.48	0.60
1:B:160:GLN:O	1:B:161:LEU:HD23	2.02	0.59
1:A:112:ILE:HG13	1:B:7:PHE:HB2	1.84	0.59
1:B:166:LYS:HA	1:B:175:ARG:HD3	1.83	0.59
1:A:384[B]:LEU:CD2	1:A:435:SER:OG	2.50	0.59
1:A:268:VAL:O	1:A:268:VAL:CG1	2.48	0.59
1:A:357:THR:HG21	5:A:633:HOH:O	2.02	0.58
1:A:220:LEU:HD23	1:A:298:ARG:HB3	1.84	0.58
1:A:425:GLN:O	1:A:428:GLU:HG3	2.02	0.58
1:A:261[B]:ARG:HD2	5:A:506:HOH:O	2.02	0.58
1:A:450:LYS:O	1:A:451:LEU:HD23	2.04	0.58
1:B:443:ARG:HG2	1:B:443:ARG:NH2	2.15	0.58
1:A:356:VAL:HG12	1:A:357:THR:HG23	1.86	0.57
1:B:368:TRP:CD1	1:B:393:LYS:HD3	2.39	0.57
1:A:171:THR:OG1	1:A:174:GLU:HG2	2.04	0.57
1:A:307:PHE:HB2	2:A:505:ACT:CH3	2.35	0.57
1:B:368:TRP:NE1	1:B:393:LYS:HD3	2.20	0.57
1:A:357:THR:C	1:B:351:GLN:HG3	2.25	0.57
1:B:267:PHE:HE2	1:B:271[A]:ARG:HG3	1.70	0.57
1:A:380:PHE:O	1:A:438:LEU:HD23	2.05	0.56
1:A:261[B]:ARG:NH2	1:B:30:LEU:HD13	2.21	0.56
1:A:223:ALA:HB2	1:A:299:LEU:HD22	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:ALA:CB	1:B:322:ILE:HD13	2.33	0.56
1:B:412:THR:N	1:B:416:GLN:HE21	2.00	0.56
1:A:261[B]:ARG:CZ	1:B:30:LEU:HD13	2.35	0.56
1:A:277:VAL:HB	1:A:282:ILE:HG13	1.87	0.56
1:B:122:LEU:HD13	1:B:123:MET:N	2.20	0.56
1:B:298:ARG:NH1	1:B:313:GLU:OE2	2.39	0.56
1:A:283:ASN:O	1:A:287:LEU:HD22	2.04	0.55
1:A:351:GLN:HB2	1:B:357:THR:HG22	1.88	0.55
1:B:401:ALA:HB1	1:B:424:THR:HG23	1.86	0.55
1:B:391:GLN:O	1:B:395:ILE:HG12	2.06	0.55
1:B:346:HIS:H	1:B:350:ALA:HB2	1.72	0.55
1:A:400:GLN:O	1:A:401:ALA:C	2.44	0.55
1:A:117:ILE:HD13	1:A:143:LEU:CB	2.37	0.55
1:A:374[A]:GLU:HG2	1:A:376:GLN:H	1.72	0.55
1:A:117:ILE:CD1	1:A:143:LEU:HB2	2.37	0.54
1:A:418:VAL:N	1:A:457:HIS:CE1	2.75	0.54
1:B:117:ILE:HD12	1:B:117:ILE:N	2.22	0.54
1:A:383[B]:GLY:HA3	5:A:633:HOH:O	2.08	0.54
1:A:400:GLN:HB3	1:A:402:ASP:OD2	2.08	0.54
1:A:391:GLN:NE2	1:A:423:LEU:O	2.40	0.54
1:A:354:ARG:NH2	1:A:370:ASN:OD1	2.40	0.54
1:A:374[B]:GLU:HG3	1:A:376:GLN:N	2.19	0.54
1:B:239:ILE:HD11	1:B:299:LEU:HD21	1.90	0.54
1:B:404:PRO:HB2	1:B:445:VAL:HB	1.90	0.54
1:A:307:PHE:HB2	2:A:505:ACT:H3	1.89	0.53
1:A:41:ASN:OD1	1:A:65:PHE:HA	2.07	0.53
1:A:146:LEU:C	1:A:146:LEU:HD23	2.28	0.53
1:B:400:GLN:HG3	5:B:682:HOH:O	2.08	0.53
1:B:66:ASP:HB3	1:B:69:LEU:HD22	1.89	0.53
1:B:311:GLY:O	1:B:315:GLU:HG2	2.08	0.53
1:B:351:GLN:OE1	1:B:351:GLN:CA	2.56	0.53
1:A:346:HIS:CE1	1:A:347:ARG:CD	2.91	0.53
1:A:227:ASP:N	1:A:412:THR:HG23	2.23	0.53
1:A:346:HIS:HE1	1:A:347:ARG:NH2	1.86	0.53
1:B:265:ARG:CG	1:B:265:ARG:HH11	2.13	0.53
1:A:456:ASN:O	1:A:457:HIS:HB2	2.09	0.53
1:A:277:VAL:O	1:A:278:PRO:C	2.47	0.53
1:A:115:SER:HB3	1:A:140[A]:ARG:HD3	1.91	0.52
1:A:140[B]:ARG:NH2	1:A:144:GLU:HG3	2.25	0.52
1:B:374:GLU:CG	1:B:375:LYS:HE2	2.32	0.52
1:B:346:HIS:O	1:B:350:ALA:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ILE:HG13	1:A:38:LEU:HD21	1.92	0.52
1:A:81:ASP:H	2:A:504:ACT:H3	1.74	0.52
1:B:128:SEP:O1P	2:B:503:ACT:H1	2.09	0.52
1:B:164:ARG:HD2	1:B:208:PHE:CE2	2.45	0.52
1:A:117:ILE:HD13	1:A:143:LEU:HB3	1.92	0.51
1:B:288:ARG:HH11	1:B:288:ARG:HG2	1.74	0.51
1:A:135:LEU:HG	1:B:183:PHE:CD2	2.45	0.51
1:A:198:LYS:HG2	5:A:603:HOH:O	2.11	0.51
1:B:403:MET:CE	1:B:442:GLY:HA2	2.41	0.51
1:A:168:GLN:HE21	1:A:168:GLN:HA	1.75	0.51
1:A:45:PHE:CE1	1:A:60:LEU:HD22	2.45	0.51
1:A:374[A]:GLU:CG	1:A:375:LYS:N	2.19	0.51
1:A:374[B]:GLU:O	1:A:375:LYS:HB2	2.10	0.51
1:A:403:MET:O	1:A:422:VAL:HG13	2.11	0.50
5:A:526:HOH:O	1:B:9:GLN:HG3	2.10	0.50
1:A:277:VAL:HG12	1:A:281:GLU:CG	2.39	0.50
1:A:347:ARG:HG2	1:A:348:ASP:OD1	2.11	0.50
1:A:350:ALA:HA	1:A:375:LYS:O	2.11	0.50
1:B:309:ARG:HH11	1:B:309:ARG:CB	2.22	0.50
1:A:374[A]:GLU:O	1:A:375:LYS:HB2	2.10	0.50
1:A:150:HIS:CD2	1:A:153:GLN:HE22	2.29	0.50
1:A:307:PHE:CB	2:A:505:ACT:CH3	2.90	0.50
1:A:373:ALA:O	1:A:374[B]:GLU:HB2	2.11	0.50
1:A:303:ASP:N	2:A:505:ACT:CH3	2.72	0.50
1:A:445:VAL:O	1:A:445:VAL:HG12	2.12	0.49
1:B:166:LYS:HA	1:B:175:ARG:HH11	1.78	0.49
1:A:123[B]:MET:CE	1:B:1:MET:HG3	2.42	0.49
1:B:349:TYR:N	1:B:349:TYR:CD1	2.66	0.49
1:A:134:VAL:O	1:A:138:LEU:HG	2.12	0.49
1:A:354:ARG:HH22	1:B:354:ARG:NH2	2.08	0.49
1:A:377[A]:THR:HG23	1:A:377[A]:THR:O	2.13	0.49
1:A:150:HIS:HB3	1:A:153:GLN:NE2	2.27	0.49
1:A:344:LEU:O	1:A:377[A]:THR:HG21	2.13	0.49
1:B:265:ARG:NH1	1:B:265:ARG:CG	2.74	0.49
1:A:241:GLN:HE21	1:A:295:ARG:HH12	1.60	0.49
1:A:241:GLN:HE21	1:A:295:ARG:NH1	2.10	0.49
1:B:17:ILE:HD11	1:B:31:LEU:HD22	1.95	0.48
1:A:289:GLU:OE2	1:A:294:LYS:HD2	2.13	0.48
1:A:284:GLN:CA	1:A:287:LEU:HD21	2.28	0.48
1:A:309:ARG:O	1:A:313:GLU:HG3	2.13	0.48
1:A:268:VAL:HG13	1:A:282:ILE:HG12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:LEU:HD23	1:A:378:LEU:HD22	1.96	0.48
1:B:291:GLN:HG3	1:B:322:ILE:HD11	1.95	0.48
1:A:365:GLU:O	1:A:366:LEU:HD23	2.14	0.48
1:B:73[B]:CYS:SG	1:B:75:LEU:O	2.72	0.48
1:B:309:ARG:NH1	1:B:312:GLU:OE1	2.47	0.47
1:A:97:ARG:NE	1:B:72:SER:HA	2.28	0.47
1:A:277:VAL:HB	1:A:282:ILE:CG1	2.44	0.47
1:B:349:TYR:N	1:B:349:TYR:HD1	1.97	0.47
1:B:359:HIS:CG	1:B:386:GLN:NE2	2.82	0.47
1:A:303:ASP:H	2:A:505:ACT:H2	1.75	0.47
1:B:287:LEU:HD12	1:B:316:THR:O	2.14	0.47
1:B:250:LEU:HD21	1:B:436:PRO:HG3	1.96	0.47
1:A:356:VAL:CG1	1:A:357:THR:N	2.76	0.47
1:B:401:ALA:HB1	1:B:424:THR:CG2	2.44	0.47
1:A:187:ARG:HG3	1:A:187:ARG:NH1	2.28	0.47
1:B:31:LEU:HD23	1:B:38:LEU:HD13	1.96	0.47
1:A:58:LEU:C	1:A:58:LEU:HD12	2.35	0.47
1:A:11:ARG:HE	1:A:11:ARG:HB2	1.33	0.47
1:A:346:HIS:ND1	1:A:347:ARG:CD	2.77	0.47
1:A:400:GLN:HB3	1:A:400:GLN:HE21	1.45	0.47
1:A:270:LYS:O	1:A:271:ARG:C	2.53	0.47
1:A:356:VAL:HG12	1:A:357:THR:N	2.29	0.47
1:B:430:ALA:C	1:B:432:GLN:H	2.18	0.46
1:A:435:SER:HB3	1:A:436:PRO:HA	1.97	0.46
1:B:198:LYS:HD2	5:B:649:HOH:O	2.16	0.46
1:A:331[B]:THR:OG1	2:A:505:ACT:OXT	2.26	0.46
1:B:236:LEU:C	1:B:236:LEU:HD23	2.35	0.46
1:B:149:GLN:NE2	5:B:530:HOH:O	2.49	0.46
1:B:286:LEU:HD21	1:B:298:ARG:HD2	1.98	0.46
1:B:80:THR:H	1:B:86:ASN:HD21	1.64	0.46
1:A:306:ILE:HD12	1:A:331[A]:THR:HG21	1.98	0.46
1:A:356:VAL:C	1:A:357:THR:HG23	2.35	0.46
1:A:447:LEU:HD12	1:A:451:LEU:HD11	1.98	0.46
1:B:263:ALA:O	1:B:265:ARG:NH1	2.49	0.46
1:B:400:GLN:O	1:B:403:MET:HB2	2.16	0.46
1:B:164:ARG:HD3	1:B:168:GLN:NE2	2.32	0.45
1:B:405:VAL:HG12	1:B:406:ALA:N	2.32	0.45
1:A:118:ASP:O	1:A:119:ARG:HD3	2.16	0.45
1:A:142:LYS:HZ3	3:A:502:PGE:C2	2.24	0.45
1:B:176:ARG:O	1:B:180:GLU:HG3	2.16	0.45
1:A:303:ASP:N	2:A:505:ACT:H2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:HIS:CD2	1:A:153:GLN:NE2	2.85	0.45
1:A:422:VAL:HG12	1:A:423:LEU:N	2.32	0.45
1:A:117:ILE:HD11	1:A:143:LEU:HB2	1.99	0.45
1:A:142:LYS:NZ	3:A:502:PGE:H42	2.26	0.45
1:A:124:VAL:HG21	1:A:147:LEU:HD11	1.98	0.44
1:A:384[A]:LEU:HD12	1:A:384[A]:LEU:HA	1.73	0.44
1:A:409:GLU:OE1	1:A:434:GLU:HG2	2.17	0.44
1:B:339:TYR:CD2	1:B:412:THR:HA	2.53	0.44
1:A:3:HIS:CE1	1:B:9:GLN:HG2	2.52	0.44
1:A:117:ILE:HD13	1:A:143:LEU:HB2	1.98	0.44
1:A:153:GLN:OE1	1:A:193:ALA:HA	2.18	0.44
1:B:177:ARG:NH2	1:B:213:ASP:OD2	2.48	0.44
1:A:381[B]:TYR:O	1:A:383[B]:GLY:N	2.50	0.44
1:A:452:ASN:ND2	5:A:519:HOH:O	2.45	0.44
1:B:185:ASN:HD22	1:B:207:LEU:HD21	1.82	0.44
1:B:339:TYR:HB3	1:B:416:GLN:HE22	1.83	0.44
1:B:9:GLN:HE22	1:B:11:ARG:HG3	1.83	0.44
1:A:137[A]:ARG:HG2	1:A:137[A]:ARG:NH2	2.32	0.44
1:A:356:VAL:HG21	1:A:371:LEU:HD21	1.99	0.44
1:B:162:ARG:O	1:B:166:LYS:CD	2.63	0.44
1:A:139:LEU:CD2	3:A:502:PGE:H5	2.48	0.44
1:A:117:ILE:CD1	1:A:143:LEU:CB	2.96	0.44
1:A:400:GLN:O	1:A:402:ASP:OD2	2.36	0.44
1:A:237:GLN:O	1:A:241:GLN:HG2	2.18	0.43
1:A:261[A]:ARG:NH1	1:B:140:ARG:CZ	2.81	0.43
1:A:374[A]:GLU:CG	1:A:376:GLN:H	2.30	0.43
1:A:411:GLY:O	1:A:412:THR:HG22	2.17	0.43
1:A:177:ARG:NH1	1:A:213:ASP:HB3	2.33	0.43
1:A:448:ARG:O	1:A:452:ASN:HB2	2.18	0.43
1:A:80:THR:HA	2:A:504:ACT:H2	2.00	0.43
1:A:227:ASP:H	1:A:412:THR:HG21	1.82	0.43
1:B:340:SER:O	1:B:448:ARG:HG3	2.19	0.43
1:A:220:LEU:HD12	1:A:314:LEU:HD11	2.01	0.43
1:A:279:GLN:NE2	1:A:309:ARG:HD3	2.33	0.43
1:A:269:GLY:HA2	1:A:276:CYS:SG	2.58	0.42
1:A:425:GLN:HA	1:A:428:GLU:HG3	2.01	0.42
1:B:267:PHE:CE2	1:B:271[A]:ARG:HG3	2.53	0.42
1:A:425:GLN:C	1:A:428:GLU:HG3	2.39	0.42
1:A:322:ILE:HA	1:A:323:PRO:HD3	1.90	0.42
1:A:122:LEU:HD12	1:B:127:SER:O	2.19	0.42
1:A:420[B]:HIS:N	1:A:420[B]:HIS:ND1	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:LYS:HG3	1:B:175:ARG:NH1	2.34	0.42
1:B:395:ILE:HG22	1:B:399:MET:O	2.19	0.42
1:A:249:ARG:HG3	1:A:249:ARG:NH1	2.30	0.42
1:A:357:THR:O	1:B:351:GLN:HG3	2.19	0.42
1:A:275:HIS:CE1	1:A:278:PRO:HG3	2.55	0.42
1:A:406:ALA:C	1:A:407:LEU:HD23	2.40	0.42
1:B:96:ARG:HG3	1:B:98:ILE:HD12	2.00	0.42
1:A:281:GLU:O	1:A:285:ILE:HG13	2.20	0.42
1:B:9:GLN:HE21	1:B:9:GLN:C	2.22	0.42
1:A:132:SER:HB3	1:A:135:LEU:HB2	2.01	0.42
1:A:377[A]:THR:CG2	1:A:377[A]:THR:O	2.68	0.42
1:A:353:VAL:HG22	1:A:377[A]:THR:HG22	2.01	0.42
1:B:346:HIS:HE1	1:B:347:ARG:CD	2.25	0.42
1:B:309:ARG:HH11	1:B:309:ARG:CG	2.32	0.41
1:B:394:LEU:HD23	1:B:399:MET:SD	2.59	0.41
1:A:268:VAL:CG1	1:A:282:ILE:CD1	2.98	0.41
1:B:128:SEP:O	1:B:131:THR:OG1	2.17	0.41
1:B:291:GLN:CG	1:B:322:ILE:HD11	2.50	0.41
1:A:156:ARG:HD3	5:A:595:HOH:O	2.20	0.41
1:A:247:TYR:N	1:A:247:TYR:CD2	2.87	0.41
1:A:422:VAL:O	1:A:423:LEU:C	2.58	0.41
1:B:359:HIS:HB2	1:B:386:GLN:HG3	2.02	0.41
1:B:385:ASN:HD22	1:B:385:ASN:HA	1.59	0.41
1:A:140[A]:ARG:CG	1:A:140[A]:ARG:HH11	2.32	0.41
1:A:247:TYR:H	1:A:247:TYR:HD2	1.68	0.41
1:B:375:LYS:HG2	1:B:375:LYS:H	1.63	0.41
1:B:409:GLU:HB2	1:B:433:VAL:HG11	2.00	0.41
1:A:300:LYS:NZ	1:A:300:LYS:HB3	2.35	0.41
1:A:385[A]:ASN:OD1	1:A:385[A]:ASN:O	2.39	0.41
1:A:37:ARG:HH21	1:A:37:ARG:CG	2.34	0.41
1:B:346:HIS:O	1:B:350:ALA:CB	2.69	0.41
1:A:444:VAL:O	1:A:447:LEU:HD23	2.20	0.41
1:A:139:LEU:HD21	3:A:502:PGE:H5	2.03	0.41
1:B:371:LEU:C	1:B:373:ALA:H	2.24	0.41
1:A:116:ILE:HG22	1:A:117:ILE:N	2.36	0.41
1:A:391:GLN:HG3	1:A:392:GLU:N	2.36	0.41
1:A:260:ARG:NE	1:A:262:ASP:OD2	2.54	0.40
1:A:269:GLY:C	1:A:271:ARG:H	2.24	0.40
1:B:309:ARG:HH12	1:B:312:GLU:CD	2.23	0.40
1:A:275:HIS:ND1	1:A:276:CYS:N	2.59	0.40
1:B:128:SEP:HB2	1:B:132:SER:N	2.32	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:ALA:HB1	1:B:351:GLN:H	1.64	0.40
1:B:55:GLU:HG3	1:B:57:MET:HG2	2.03	0.40
1:B:9:GLN:HE21	1:B:9:GLN:CA	2.33	0.40
1:A:268:VAL:CG1	1:A:282:ILE:HG12	2.51	0.40
1:B:260:ARG:O	1:B:261:ARG:C	2.60	0.40
1:A:261[A]:ARG:HH12	1:B:140:ARG:CZ	2.35	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	454/457 (99%)	419 (92%)	23 (5%)	12 (3%)	6	3
1	B	454/457 (99%)	428 (94%)	20 (4%)	6 (1%)	14	10
All	All	908/914 (99%)	847 (93%)	43 (5%)	18 (2%)	9	5

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	LYS
1	A	279	GLN
1	A	347	ARG
1	A	375	LYS
1	A	382[A]	MET
1	A	382[B]	MET
1	A	400	GLN
1	A	401	ALA
1	B	374	GLU
1	B	375	LYS
1	A	315	GLU
1	A	195	ALA

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Mol	Chain	Res	Type
1	A	278	PRO
1	A	366	LEU
1	B	360	LEU
1	B	261	ARG
1	B	347	ARG
1	B	370	ASN

### 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	379/372 (102%)	341 (90%)	38 (10%)	9	7
1	B	375/372 (101%)	329 (88%)	46 (12%)	5	4
All	All	754/744 (101%)	670 (89%)	84 (11%)	7	5

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	37	ARG
1	A	38	LEU
1	A	43	LEU
1	A	111	PHE
1	A	135	LEU
1	A	156	ARG
1	A	188	LEU
1	A	231	LEU
1	A	247	TYR
1	A	250	LEU
1	A	277	VAL
1	A	278	PRO
1	A	279	GLN
1	A	287	LEU
1	A	299	LEU
1	A	347	ARG

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Mol	Chain	Res	Type
1	A	348	ASP
1	A	354	ARG
1	A	355	LEU
1	A	357	THR
1	A	366	LEU
1	A	370	ASN
1	A	375	LYS
1	A	385[A]	ASN
1	A	385[B]	ASN
1	A	400	GLN
1	A	403	MET
1	A	412	THR
1	A	413	SER
1	A	420[A]	HIS
1	A	420[B]	HIS
1	A	428	GLU
1	A	433	VAL
1	A	438	LEU
1	A	443	ARG
1	A	452	ASN
1	A	455	SER
1	B	9	GLN
1	B	69	LEU
1	B	81	ASP
1	B	97	ARG
1	B	104[A]	ASP
1	B	104[B]	ASP
1	B	107	LYS
1	B	110	SER
1	B	120	SER
1	B	135	LEU
1	B	147	LEU
1	B	149	GLN
1	B	151	LEU
1	B	166	LYS
1	B	172	MET
1	B	176	ARG
1	B	209	SER
1	B	213	ASP
1	B	215	ARG
1	B	230	LEU
1	B	248	ASP

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Mol	Chain	Res	Type
1	B	252	SER
1	B	261	ARG
1	B	262	ASP
1	B	288	ARG
1	B	298	ARG
1	B	309	ARG
1	B	316	THR
1	B	334	SER
1	B	347	ARG
1	B	348	ASP
1	B	349	TYR
1	B	351	GLN
1	B	360	LEU
1	B	366	LEU
1	B	367	ASP
1	B	369	GLU
1	B	374	GLU
1	B	375	LYS
1	B	385	ASN
1	B	389	THR
1	B	395	ILE
1	B	423	LEU
1	B	426	LEU
1	B	431	GLN
1	B	433	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	149	GLN
1	A	150	HIS
1	A	168	GLN
1	A	190	GLN
1	A	194	ASN
1	A	237	GLN
1	A	241	GLN
1	A	279	GLN
1	A	284	GLN
1	A	346	HIS
1	A	391	GLN
1	A	400	GLN

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Mol	Chain	Res	Type
1	A	416	GLN
1	A	431	GLN
1	A	452	ASN
1	A	457	HIS
1	B	9	GLN
1	B	54	ASN
1	B	86	ASN
1	B	149	GLN
1	B	238	GLN
1	B	240	GLN
1	B	359	HIS
1	B	385	ASN
1	B	386	GLN
1	B	416	GLN
1	B	452	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	SEP	A	128	1	9,9,10	3.22	3 (33%)	9,12,14	4.91	6 (66%)
1	SEP	B	128	1	9,9,10	5.02	7 (77%)	9,12,14	5.34	4 (44%)

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	SEP	A	128	1	-	0/5/8/10	0/0/0/0
1	SEP	B	128	1	-	0/5/8/10	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	128	SEP	CA-C	-6.57	1.41	1.50
1	B	128	SEP	P-O1P	2.31	1.58	1.50
1	A	128	SEP	P-O1P	2.62	1.59	1.50
1	B	128	SEP	CA-N	3.86	1.60	1.47
1	B	128	SEP	O-C	4.07	1.37	1.19
1	B	128	SEP	CB-CA	4.85	1.66	1.52
1	B	128	SEP	P-OG	5.34	1.77	1.60
1	A	128	SEP	CB-CA	5.73	1.69	1.52
1	A	128	SEP	P-OG	6.83	1.82	1.60
1	B	128	SEP	OG-CB	9.67	1.83	1.44

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	SEP	O3P-P-OG	-4.00	96.10	106.73
1	A	128	SEP	O-C-CA	-2.21	118.91	125.02
1	B	128	SEP	O-C-CA	-2.17	119.03	125.02
1	A	128	SEP	O2P-P-OG	2.11	112.36	106.73
1	A	128	SEP	O3P-P-O2P	2.38	117.23	107.61
1	B	128	SEP	O3P-P-O2P	2.44	117.46	107.61
1	A	128	SEP	OG-CB-CA	8.93	116.97	108.17
1	B	128	SEP	P-OG-CB	10.03	145.92	118.30
1	A	128	SEP	P-OG-CB	10.20	146.40	118.30
1	B	128	SEP	OG-CB-CA	11.79	119.79	108.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	128	SEP	1	0
1	B	128	SEP	9	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

5 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
3	PGE	A	502	-	9,9,9	2.07	2 (22%)	8,8,8	1.49	3 (37%)
2	ACT	A	504	-	1,3,3	3.55	1 (100%)	0,3,3	0.00	-
2	ACT	A	505	-	1,3,3	2.69	1 (100%)	0,3,3	0.00	-
4	SAH	B	501	-	20,28,28	2.11	2 (10%)	20,40,40	2.67	2 (10%)
2	ACT	B	503	-	1,3,3	3.76	1 (100%)	0,3,3	0.00	-

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
3	PGE	A	502	-	-	0/7/7/7	0/0/0/0
2	ACT	A	504	-	-	0/0/0/0	0/0/0/0
2	ACT	A	505	-	-	0/0/0/0	0/0/0/0
4	SAH	B	501	-	-	0/7/31/31	0/3/3/3
2	ACT	B	503	-	-	0/0/0/0	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	PGE	O3-C4	-4.26	1.23	1.42
3	A	502	PGE	O4-C6	-3.51	1.23	1.42
2	A	505	ACT	CH3-C	2.69	1.52	1.48
2	A	504	ACT	CH3-C	3.55	1.53	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	503	ACT	CH3-C	3.76	1.53	1.48
4	B	501	SAH	O4'-C1'	5.56	1.48	1.41
4	B	501	SAH	C2-N1	7.03	1.47	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501	SAH	N3-C2-N1	-11.38	118.95	128.86
4	B	501	SAH	C4-C5-N7	-2.11	107.38	109.41
3	A	502	PGE	O3-C4-C3	2.15	120.29	110.41
3	A	502	PGE	O2-C3-C4	2.16	120.34	110.41
3	A	502	PGE	O3-C5-C6	2.25	120.52	110.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	PGE	8	0
2	A	504	ACT	2	0
2	A	505	ACT	12	0
2	B	503	ACT	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	447/457 (97%)	0.16	21 (4%) 32 30	18, 39, 67, 99	0
1	B	454/457 (99%)	0.09	23 (5%) 29 27	15, 34, 65, 95	0
All	All	901/914 (98%)	0.12	44 (4%) 30 28	15, 36, 66, 99	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	360	LEU	10.1
1	B	362	THR	8.1
1	A	276	CYS	7.8
1	B	272	ALA	6.9
1	B	359	HIS	6.5
1	B	275	HIS	5.3
1	B	361	LYS	4.9
1	A	277	VAL	4.8
1	A	270	LYS	4.8
1	B	369	GLU	4.7
1	B	364	GLY	4.7
1	A	364	GLY	4.5
1	A	271	ARG	4.5
1	A	249	ARG	4.3
1	A	275	HIS	4.2
1	B	374	GLU	3.8
1	B	319	HIS	3.8
1	A	348	ASP	3.7
1	B	363	GLY	3.7
1	B	318	CYS	3.6
1	B	261	ARG	3.6
1	B	276	CYS	3.5
1	A	357	THR	3.5
1	B	348	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	420[A]	HIS	3.0
1	B	172	MET	3.0
1	A	307	PHE	2.9
1	A	457	HIS	2.7
1	A	401	ALA	2.5
1	B	365	GLU	2.5
1	B	270	LYS	2.5
1	A	384[A]	LEU	2.4
1	B	262	ASP	2.4
1	A	385[A]	ASN	2.4
1	B	249	ARG	2.3
1	A	280	GLU	2.3
1	A	347	ARG	2.2
1	A	456	ASN	2.2
1	A	406	ALA	2.1
1	B	198	LYS	2.1
1	A	440	ILE	2.1
1	B	396	ALA	2.1
1	A	47	PRO	2.1
1	B	351	GLN	2.1

## 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. 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
1	SEP	B	128	10/11	0.89	0.19	-	30,38,52,53	0
1	SEP	A	128	10/11	0.76	0.27	-	31,38,53,54	0

## 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	ACT	A	504	4/4	0.64	0.30	3.59	57,59,60,61	0
3	PGE	A	502	10/10	0.89	0.16	3.55	49,54,57,58	0
2	ACT	A	505	4/4	0.96	0.17	0.65	36,39,42,42	0
4	SAH	B	501	26/26	0.95	0.10	-0.59	27,32,35,37	0
2	ACT	B	503	4/4	0.91	0.20	-	57,58,58,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.