



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:44 PM GMT

PDB ID : 4U2H
Title : The crystal structure of apo CalE6, a methionine gamma lyase from *Micromonospora echinospora*
Authors : Song, H.G.; Xu, R.
Deposited on : 2014-07-17
Resolution : 1.85 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

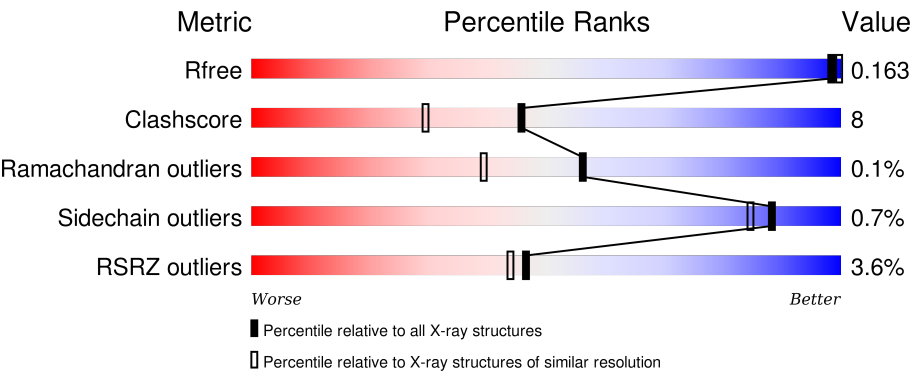
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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}	91344	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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 >=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 <=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	389	<div><div>3%</div><div>84%</div><div>9%</div><div>7%</div></div>
1	B	389	<div><div>2%</div><div>84%</div><div>10%</div><div>6%</div></div>
1	C	389	<div><div>5%</div><div>79%</div><div>13%</div><div>7%</div></div>
1	D	389	<div><div>4%</div><div>84%</div><div>10%</div><div>6%</div></div>
1	E	389	<div><div>3%</div><div>83%</div><div>12%</div><div>6%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	389	
1	G	389	
1	H	389	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	G	401	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23976 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 CalE6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	3	0
			2660	1673	478	500	9			
1	B	365	Total	C	N	O	S	0	1	0
			2674	1683	479	504	8			
1	C	360	Total	C	N	O	S	0	3	0
			2670	1679	483	500	8			
1	D	366	Total	C	N	O	S	0	0	0
			2672	1681	481	502	8			
1	E	366	Total	C	N	O	S	0	1	0
			2697	1694	486	509	8			
1	F	362	Total	C	N	O	S	0	2	0
			2651	1670	474	498	9			
1	G	361	Total	C	N	O	S	0	1	0
			2656	1670	482	495	9			
1	H	364	Total	C	N	O	S	0	1	0
			2644	1667	472	496	9			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	382	LEU	-	expression tag	UNP Q8KNG3
A	383	GLU	-	expression tag	UNP Q8KNG3
A	384	HIS	-	expression tag	UNP Q8KNG3
A	385	HIS	-	expression tag	UNP Q8KNG3
A	386	HIS	-	expression tag	UNP Q8KNG3
A	387	HIS	-	expression tag	UNP Q8KNG3
A	388	HIS	-	expression tag	UNP Q8KNG3
A	389	HIS	-	expression tag	UNP Q8KNG3
B	382	LEU	-	expression tag	UNP Q8KNG3
B	383	GLU	-	expression tag	UNP Q8KNG3
B	384	HIS	-	expression tag	UNP Q8KNG3
B	385	HIS	-	expression tag	UNP Q8KNG3
B	386	HIS	-	expression tag	UNP Q8KNG3

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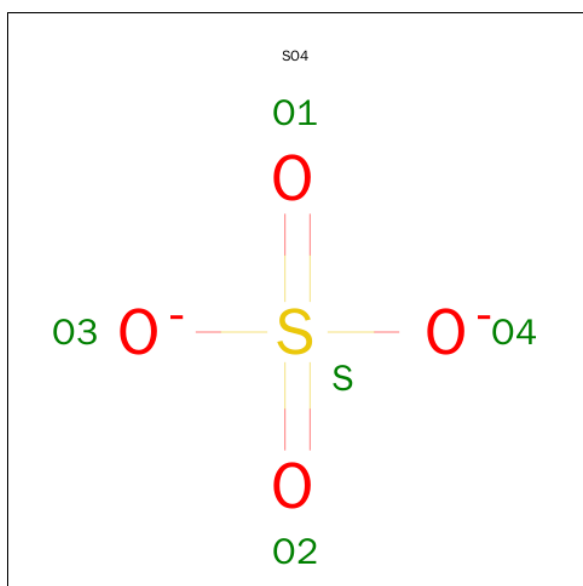
Chain	Residue	Modelled	Actual	Comment	Reference
B	387	HIS	-	expression tag	UNP Q8KNG3
B	388	HIS	-	expression tag	UNP Q8KNG3
B	389	HIS	-	expression tag	UNP Q8KNG3
C	382	LEU	-	expression tag	UNP Q8KNG3
C	383	GLU	-	expression tag	UNP Q8KNG3
C	384	HIS	-	expression tag	UNP Q8KNG3
C	385	HIS	-	expression tag	UNP Q8KNG3
C	386	HIS	-	expression tag	UNP Q8KNG3
C	387	HIS	-	expression tag	UNP Q8KNG3
C	388	HIS	-	expression tag	UNP Q8KNG3
C	389	HIS	-	expression tag	UNP Q8KNG3
D	382	LEU	-	expression tag	UNP Q8KNG3
D	383	GLU	-	expression tag	UNP Q8KNG3
D	384	HIS	-	expression tag	UNP Q8KNG3
D	385	HIS	-	expression tag	UNP Q8KNG3
D	386	HIS	-	expression tag	UNP Q8KNG3
D	387	HIS	-	expression tag	UNP Q8KNG3
D	388	HIS	-	expression tag	UNP Q8KNG3
D	389	HIS	-	expression tag	UNP Q8KNG3
E	382	LEU	-	expression tag	UNP Q8KNG3
E	383	GLU	-	expression tag	UNP Q8KNG3
E	384	HIS	-	expression tag	UNP Q8KNG3
E	385	HIS	-	expression tag	UNP Q8KNG3
E	386	HIS	-	expression tag	UNP Q8KNG3
E	387	HIS	-	expression tag	UNP Q8KNG3
E	388	HIS	-	expression tag	UNP Q8KNG3
E	389	HIS	-	expression tag	UNP Q8KNG3
F	382	LEU	-	expression tag	UNP Q8KNG3
F	383	GLU	-	expression tag	UNP Q8KNG3
F	384	HIS	-	expression tag	UNP Q8KNG3
F	385	HIS	-	expression tag	UNP Q8KNG3
F	386	HIS	-	expression tag	UNP Q8KNG3
F	387	HIS	-	expression tag	UNP Q8KNG3
F	388	HIS	-	expression tag	UNP Q8KNG3
F	389	HIS	-	expression tag	UNP Q8KNG3
G	382	LEU	-	expression tag	UNP Q8KNG3
G	383	GLU	-	expression tag	UNP Q8KNG3
G	384	HIS	-	expression tag	UNP Q8KNG3
G	385	HIS	-	expression tag	UNP Q8KNG3
G	386	HIS	-	expression tag	UNP Q8KNG3
G	387	HIS	-	expression tag	UNP Q8KNG3
G	388	HIS	-	expression tag	UNP Q8KNG3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	389	HIS	-	expression tag	UNP Q8KNG3
H	382	LEU	-	expression tag	UNP Q8KNG3
H	383	GLU	-	expression tag	UNP Q8KNG3
H	384	HIS	-	expression tag	UNP Q8KNG3
H	385	HIS	-	expression tag	UNP Q8KNG3
H	386	HIS	-	expression tag	UNP Q8KNG3
H	387	HIS	-	expression tag	UNP Q8KNG3
H	388	HIS	-	expression tag	UNP Q8KNG3
H	389	HIS	-	expression tag	UNP Q8KNG3

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

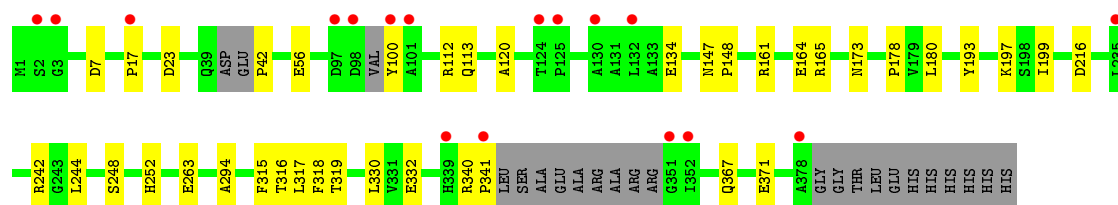
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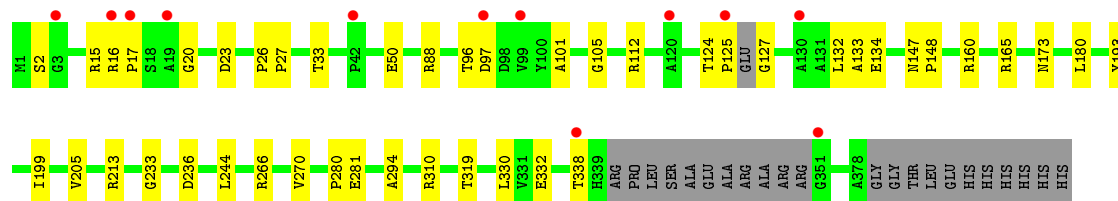
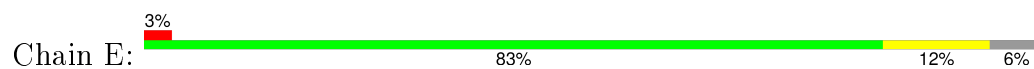
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

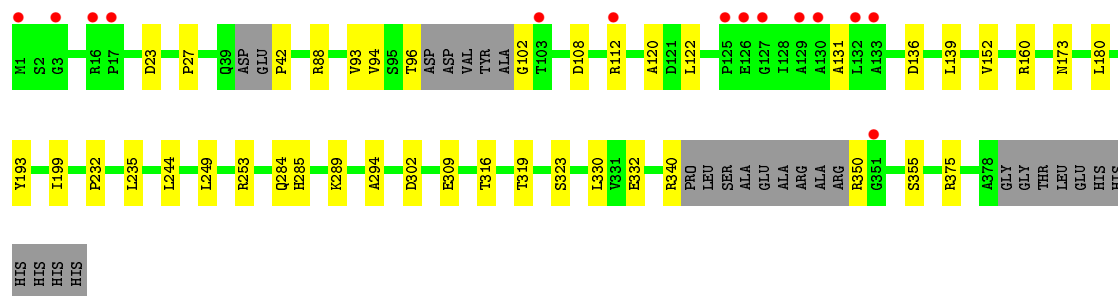
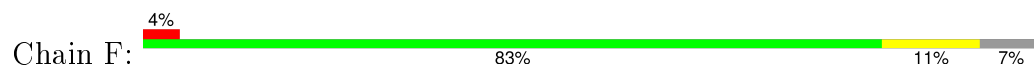
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	345	Total	O	0	0
			345	345		
3	B	331	Total	O	0	0
			331	331		
3	C	329	Total	O	0	0
			329	329		
3	D	282	Total	O	0	0
			282	282		
3	E	329	Total	O	0	0
			329	329		
3	F	300	Total	O	0	0
			300	300		
3	G	337	Total	O	0	0
			337	337		
3	H	319	Total	O	0	0
			319	319		



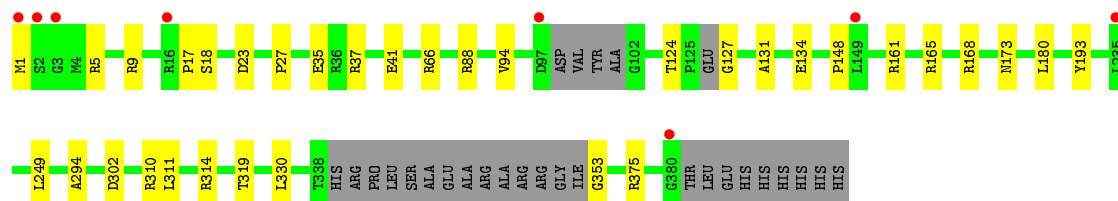
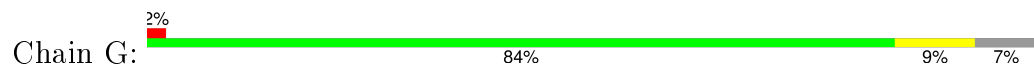
● Molecule 1: CalE6



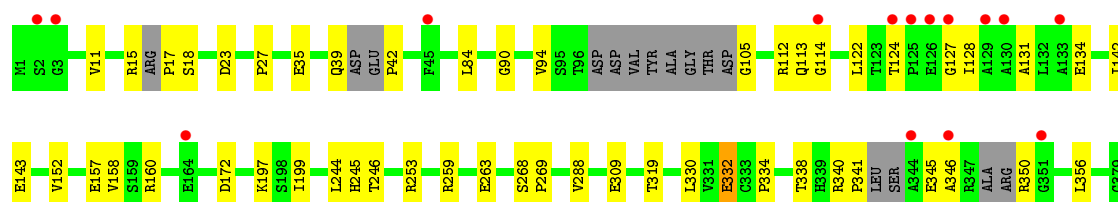
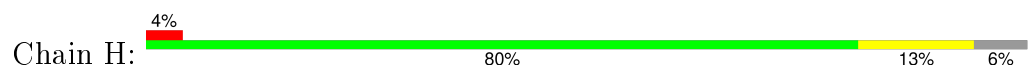
● Molecule 1: CalE6



● Molecule 1: CalE6



● Molecule 1: CalE6



GLY
THR
LEU
GLU
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	145.20Å 145.40Å 346.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.30 – 1.85 49.25 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.30-1.85) 97.4 (49.25-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 1.86Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.209 , 0.232 0.149 , 0.163	Depositor DCC
R_{free} test set	15221 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	18.8	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 56.9	EDS
Estimated twinning fraction	0.285 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 308727 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	23976	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.39	0/2711	0.53	0/3702
1	B	0.39	0/2725	0.54	0/3721
1	C	0.43	0/2721	0.57	1/3712 (0.0%)
1	D	0.39	0/2724	0.53	0/3722
1	E	0.42	0/2749	0.56	0/3755
1	F	0.40	0/2701	0.55	0/3687
1	G	0.40	0/2706	0.55	0/3692
1	H	0.49	0/2693	0.57	0/3676
All	All	0.41	0/21730	0.55	1/29667 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	4	MET	CA-CB-CG	5.54	122.72	113.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2660	0	2624	38	0
1	B	2674	0	2635	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2670	0	2640	49	0
1	D	2672	0	2627	39	0
1	E	2697	0	2660	43	0
1	F	2651	0	2600	37	0
1	G	2656	0	2631	43	0
1	H	2644	0	2589	51	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	1	0
2	E	10	0	0	0	0
2	F	10	0	0	0	0
2	G	15	0	0	0	0
2	H	5	0	0	0	0
3	A	345	0	0	29	1
3	B	331	0	0	25	1
3	C	329	0	0	34	1
3	D	282	0	0	30	1
3	E	329	0	0	27	1
3	F	300	0	0	23	1
3	G	337	0	0	34	1
3	H	319	0	0	32	2
All	All	23976	0	21006	328	5

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 8.

All (328) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:160:ARG:HD2	3:E:805:HOH:O	1.25	1.29
1:F:122:LEU:HG	3:F:797:HOH:O	1.33	1.27
1:B:281:GLU:CA	3:B:782:HOH:O	1.90	1.17
1:A:114:GLY:C	3:A:834:HOH:O	1.81	1.16
1:B:281:GLU:C	3:B:782:HOH:O	1.83	1.13
1:A:109:LEU:HB2	3:A:792:HOH:O	1.50	1.08
1:E:310:ARG:NH1	3:E:627:HOH:O	1.88	1.06
1:E:96:THR:CA	3:E:828:HOH:O	2.02	1.06
1:D:315:PHE:HB3	3:D:729:HOH:O	1.54	1.06
1:C:36:ARG:CB	3:C:821:HOH:O	2.02	1.05
1:G:37:ARG:NH2	3:G:817:HOH:O	1.87	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:GLN:NE2	3:B:823:HOH:O	1.91	1.03
1:E:96:THR:HA	3:E:828:HOH:O	1.55	1.02
1:F:102:GLY:N	3:F:696:HOH:O	1.94	1.00
1:H:269:PRO:HA	3:H:502:HOH:O	1.59	1.00
1:D:147:ASN:ND2	3:D:723:HOH:O	1.92	1.00
1:G:375:ARG:NH2	3:G:722:HOH:O	1.93	0.99
1:H:157:GLU:CD	3:H:775:HOH:O	2.01	0.99
1:A:136:ASP:CB	3:A:814:HOH:O	2.10	0.99
1:B:36:ARG:O	3:B:797:HOH:O	1.81	0.98
1:H:90:GLY:O	3:H:501:HOH:O	1.80	0.98
1:B:280:PRO:O	3:B:782:HOH:O	1.81	0.97
1:C:163:HIS:C	3:C:822:HOH:O	2.02	0.97
1:H:268:SER:O	3:H:502:HOH:O	1.83	0.96
1:H:35:GLU:O	3:H:796:HOH:O	1.83	0.96
1:D:371:GLU:OE2	3:D:782:HOH:O	1.82	0.96
1:H:309:GLU:OE1	3:H:751:HOH:O	1.82	0.96
1:H:157:GLU:CG	3:H:775:HOH:O	2.14	0.95
1:H:345:GLU:O	3:H:800:HOH:O	1.82	0.95
1:H:160:ARG:NH1	3:H:766:HOH:O	2.00	0.94
1:H:157:GLU:OE2	3:H:775:HOH:O	1.82	0.93
1:C:184:LEU:HD12	3:C:809:HOH:O	1.69	0.93
1:B:17:PRO:O	3:B:781:HOH:O	1.85	0.92
1:A:66:ARG:NH2	3:A:845:HOH:O	2.02	0.92
1:D:120:ALA:C	3:D:772:HOH:O	2.08	0.92
1:H:157:GLU:HG2	3:H:775:HOH:O	1.69	0.92
1:A:114:GLY:O	3:A:834:HOH:O	1.80	0.91
1:H:345:GLU:C	3:H:800:HOH:O	2.08	0.90
1:F:302:ASP:OD2	3:F:621:HOH:O	1.90	0.90
1:G:127:GLY:N	3:G:737:HOH:O	2.04	0.90
1:C:163:HIS:O	3:C:822:HOH:O	1.89	0.89
1:B:197[A]:LYS:NZ	3:B:825:HOH:O	2.05	0.88
1:A:105:GLY:O	3:A:792:HOH:O	1.90	0.88
1:G:41:GLU:O	3:G:789:HOH:O	1.93	0.87
1:E:88:ARG:NH2	3:E:744:HOH:O	2.07	0.87
1:D:120:ALA:O	3:D:772:HOH:O	1.93	0.86
1:B:281:GLU:HA	3:B:782:HOH:O	1.60	0.84
1:B:130:ALA:C	3:B:804:HOH:O	2.15	0.84
1:B:130:ALA:O	3:B:804:HOH:O	1.96	0.84
1:C:134:GLU:O	1:C:165:ARG:NH1	2.11	0.84
1:C:38:ALA:O	3:C:720:HOH:O	1.94	0.84
1:F:120:ALA:O	3:F:797:HOH:O	1.96	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:42:PRO:N	3:H:738:HOH:O	2.12	0.82
1:E:205:VAL:HA	3:E:811:HOH:O	1.78	0.82
1:B:42:PRO:HD3	3:B:811:HOH:O	1.80	0.82
1:F:96:THR:C	3:F:747:HOH:O	2.17	0.81
1:C:157:GLU:OE1	1:C:160:ARG:NH1	2.13	0.81
1:H:35:GLU:C	3:H:796:HOH:O	2.17	0.81
1:E:97:ASP:N	3:E:828:HOH:O	2.14	0.81
1:D:120:ALA:HB3	3:D:772:HOH:O	1.78	0.80
1:G:148:PRO:O	3:G:748:HOH:O	1.99	0.80
1:D:263:GLU:OE2	3:D:694:HOH:O	1.98	0.80
1:H:105:GLY:N	3:H:720:HOH:O	2.14	0.80
1:A:236:ASP:OD1	3:A:700:HOH:O	1.98	0.80
1:C:9:ARG:HD2	3:C:818:HOH:O	1.82	0.79
1:B:263:GLU:OE1	3:B:501:HOH:O	2.01	0.78
1:C:36:ARG:CA	3:C:821:HOH:O	2.28	0.78
1:C:9:ARG:CD	3:C:818:HOH:O	2.30	0.78
1:H:269:PRO:CA	3:H:502:HOH:O	2.22	0.78
1:H:350:ARG:N	3:H:709:HOH:O	2.16	0.77
1:A:113:GLN:O	3:A:778:HOH:O	2.02	0.77
1:E:266:ARG:NH1	1:E:281:GLU:OE2	2.18	0.76
1:G:168:ARG:NH2	3:G:823:HOH:O	2.18	0.76
1:G:311:LEU:N	3:G:502:HOH:O	2.18	0.75
1:C:103:THR:HG23	3:C:808:HOH:O	1.86	0.75
1:H:122:LEU:HD22	1:H:128:ILE:HD13	1.69	0.75
1:A:19:ALA:O	3:A:819:HOH:O	2.06	0.74
1:D:120:ALA:CA	3:D:772:HOH:O	2.35	0.74
1:E:199:ILE:HG23	1:E:244:LEU:HD13	1.68	0.74
1:D:17:PRO:HA	3:D:564:HOH:O	1.86	0.74
1:H:90:GLY:C	3:H:501:HOH:O	2.22	0.74
1:A:239:LEU:HA	3:D:776:HOH:O	1.88	0.74
1:A:114:GLY:CA	3:A:834:HOH:O	2.26	0.74
1:G:17:PRO:HA	3:G:803:HOH:O	1.88	0.73
1:C:36:ARG:O	3:C:814:HOH:O	2.06	0.73
2:D:402:SO4:O1	3:D:703:HOH:O	2.06	0.73
1:G:88:ARG:NE	3:G:501:HOH:O	1.85	0.73
1:H:263:GLU:OE2	3:H:503:HOH:O	2.07	0.73
1:G:134:GLU:CD	3:G:759:HOH:O	2.27	0.73
1:C:36:ARG:C	3:C:821:HOH:O	2.28	0.72
1:F:122:LEU:N	3:F:797:HOH:O	2.21	0.72
1:G:302:ASP:OD2	3:G:719:HOH:O	2.07	0.72
1:E:96:THR:CB	3:E:828:HOH:O	2.32	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:94:VAL:HG11	1:H:131:ALA:HB1	1.72	0.71
1:F:96:THR:O	3:F:747:HOH:O	2.09	0.71
1:E:101:ALA:O	3:E:704:HOH:O	2.08	0.70
1:G:134:GLU:O	1:G:165:ARG:NH1	2.25	0.70
1:H:124:THR:OG1	1:H:127:GLY:N	2.23	0.70
1:C:36:ARG:O	3:C:821:HOH:O	2.09	0.70
1:D:120:ALA:CB	3:D:772:HOH:O	2.37	0.69
1:D:242:ARG:NH2	3:D:776:HOH:O	2.23	0.69
1:H:17:PRO:O	3:H:642:HOH:O	2.10	0.69
1:E:125:PRO:O	1:E:127:GLY:N	2.26	0.69
1:A:136:ASP:HA	3:A:829:HOH:O	1.92	0.69
1:E:96:THR:HB	3:E:828:HOH:O	1.92	0.68
1:D:112:ARG:NH1	3:D:502:HOH:O	2.26	0.68
1:A:213:ARG:O	3:A:840:HOH:O	2.11	0.68
1:C:120:ALA:O	3:C:678:HOH:O	2.12	0.68
1:G:66:ARG:NE	3:G:720:HOH:O	2.27	0.68
1:C:379:GLY:O	3:C:792:HOH:O	2.10	0.68
1:A:259:ARG:NH1	3:A:672:HOH:O	1.99	0.67
1:B:100:TYR:CB	3:B:774:HOH:O	2.41	0.67
1:G:37:ARG:CZ	3:G:817:HOH:O	2.33	0.67
1:G:134:GLU:OE2	3:G:759:HOH:O	2.13	0.66
1:H:259:ARG:NH1	3:H:572:HOH:O	2.19	0.66
1:G:161:ARG:NH1	3:G:763:HOH:O	2.25	0.66
1:D:113:GLN:NE2	3:D:501:HOH:O	2.28	0.66
1:H:39:GLN:NE2	3:H:796:HOH:O	2.28	0.65
1:F:309:GLU:O	3:F:740:HOH:O	2.15	0.65
1:F:253:ARG:HD2	1:G:249:LEU:HD21	1.78	0.65
1:H:114:GLY:O	3:H:504:HOH:O	2.15	0.65
1:A:106:LEU:HA	3:A:792:HOH:O	1.97	0.65
1:E:97:ASP:OD1	3:E:812:HOH:O	2.14	0.65
1:E:213:ARG:NH1	3:E:795:HOH:O	2.27	0.64
1:H:332:GLU:OE1	1:H:338:THR:HG23	1.98	0.64
1:C:9:ARG:NE	3:C:818:HOH:O	2.30	0.64
1:C:310:ARG:NH1	3:C:502:HOH:O	2.24	0.64
3:A:710:HOH:O	1:D:367:GLN:HG3	1.98	0.64
1:H:346:ALA:C	3:H:800:HOH:O	2.35	0.64
1:A:114:GLY:HA3	3:A:834:HOH:O	1.93	0.64
1:C:338:THR:O	3:C:787:HOH:O	2.15	0.63
1:F:249:LEU:HD23	3:F:769:HOH:O	1.98	0.63
1:F:289:LYS:O	3:F:669:HOH:O	2.15	0.63
1:D:248:SER:O	1:D:252:HIS:ND1	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:263:GLU:HG3	3:D:761:HOH:O	1.98	0.62
1:E:133:ALA:O	3:E:721:HOH:O	2.15	0.62
1:A:239:LEU:HD23	3:D:776:HOH:O	2.00	0.62
1:E:134:GLU:O	1:E:165:ARG:NH1	2.32	0.62
1:E:15:ARG:O	1:E:17:PRO:HD3	2.00	0.62
1:G:41:GLU:CB	3:G:789:HOH:O	2.46	0.62
1:E:132:LEU:O	1:E:165:ARG:NE	2.24	0.62
1:C:89:PRO:O	3:C:501:HOH:O	2.16	0.61
1:D:113:GLN:OE1	3:D:501:HOH:O	2.16	0.61
1:D:317:LEU:N	3:D:729:HOH:O	2.28	0.60
1:E:112:ARG:O	1:F:88:ARG:NH1	2.35	0.60
1:D:56:GLU:OE2	3:D:628:HOH:O	2.16	0.60
1:F:94:VAL:HG11	1:F:131:ALA:HB1	1.83	0.59
1:E:26:PRO:HD2	3:E:738:HOH:O	2.02	0.59
1:B:199:ILE:HG23	1:B:244:LEU:HD13	1.83	0.59
1:F:102:GLY:N	3:F:695:HOH:O	2.36	0.59
1:B:131:ALA:HA	3:B:804:HOH:O	2.00	0.59
1:G:18:SER:N	3:G:803:HOH:O	2.29	0.59
1:A:319:THR:HB	1:A:330:LEU:HD23	1.84	0.59
1:E:33:THR:HG21	1:F:323:SER:HB3	1.85	0.59
1:E:2:SER:O	3:E:612:HOH:O	2.17	0.59
1:F:120:ALA:C	3:F:797:HOH:O	2.37	0.58
1:G:165:ARG:HD2	3:G:830:HOH:O	2.04	0.58
1:H:143:GLU:HG3	1:H:172:ASP:HB3	1.85	0.58
1:E:16:ARG:O	3:E:656:HOH:O	2.16	0.58
1:E:160:ARG:CD	3:E:805:HOH:O	2.04	0.58
1:F:285:HIS:CD2	3:F:501:HOH:O	2.56	0.58
1:A:89:PRO:HA	3:A:834:HOH:O	2.04	0.57
1:A:266:ARG:NH1	3:A:502:HOH:O	2.38	0.57
1:A:375:ARG:NH1	3:A:606:HOH:O	2.36	0.57
1:C:310:ARG:NE	3:C:502:HOH:O	2.27	0.57
1:A:199:ILE:HG23	1:A:244:LEU:HD13	1.87	0.57
1:G:37:ARG:NE	3:G:817:HOH:O	2.36	0.56
1:G:353:GLY:N	3:G:745:HOH:O	2.38	0.56
1:G:310:ARG:C	3:G:502:HOH:O	2.44	0.56
1:D:134:GLU:O	1:D:165:ARG:NH2	2.38	0.56
1:A:77:GLN:OE1	3:A:613:HOH:O	2.17	0.56
1:G:1:MET:HG2	1:G:9:ARG:HG2	1.86	0.56
1:G:5:ARG:HG2	3:G:813:HOH:O	2.05	0.56
1:D:113:GLN:CD	3:D:501:HOH:O	2.44	0.56
1:E:160:ARG:CB	3:E:805:HOH:O	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:108:ASP:O	1:F:112:ARG:HG3	2.06	0.55
1:C:161:ARG:NH1	1:C:164:GLU:OE2	2.30	0.55
1:G:88:ARG:NH2	3:G:501:HOH:O	2.39	0.55
1:G:302:ASP:HB3	3:G:701:HOH:O	2.07	0.54
1:C:199:ILE:HG23	1:C:244:LEU:HD13	1.88	0.54
1:C:124:THR:HG1	1:C:127:GLY:N	2.05	0.54
1:G:35:GLU:OE2	3:G:817:HOH:O	2.18	0.54
1:C:135:PRO:O	3:C:786:HOH:O	2.18	0.54
1:C:127:GLY:N	3:C:674:HOH:O	2.40	0.54
1:G:66:ARG:CZ	3:G:720:HOH:O	2.56	0.54
1:F:160:ARG:NH1	3:F:722:HOH:O	2.15	0.54
1:D:216:ASP:OD2	3:D:778:HOH:O	2.18	0.53
1:A:242:ARG:HB3	3:D:776:HOH:O	2.08	0.53
1:H:199:ILE:HG23	1:H:244:LEU:HD13	1.91	0.53
1:D:17:PRO:HA	3:D:745:HOH:O	2.07	0.53
1:C:270:VAL:HG11	3:C:734:HOH:O	2.09	0.53
1:F:173:ASN:HB3	1:F:193:TYR:CE1	2.43	0.53
1:A:136:ASP:CB	3:A:809:HOH:O	2.56	0.53
1:C:94:VAL:HG11	1:C:131:ALA:HB1	1.91	0.52
1:H:263:GLU:HB3	3:H:518:HOH:O	2.09	0.52
1:B:17:PRO:N	3:B:781:HOH:O	2.42	0.52
1:B:355:SER:HB2	3:B:674:HOH:O	2.08	0.52
1:C:253:ARG:NH1	3:C:607:HOH:O	2.38	0.52
1:H:15:ARG:HG2	1:H:15:ARG:HH11	1.74	0.52
1:B:319:THR:HB	1:B:330:LEU:HD23	1.92	0.52
1:E:213:ARG:NE	3:E:795:HOH:O	2.43	0.51
1:G:124:THR:HG1	1:G:127:GLY:N	2.08	0.51
1:D:180:LEU:HD22	1:D:294:ALA:HB3	1.92	0.51
1:C:281:GLU:HG3	3:C:511:HOH:O	2.10	0.51
1:H:112:ARG:O	3:H:678:HOH:O	2.19	0.51
1:F:93:VAL:HG22	1:F:139:LEU:HB3	1.91	0.51
1:E:20:GLY:N	3:E:764:HOH:O	1.92	0.51
1:G:319:THR:HB	1:G:330:LEU:HD23	1.93	0.51
1:D:340:ARG:N	1:D:341:PRO:HD2	2.25	0.51
1:F:355[B]:SER:OG	3:F:686:HOH:O	2.00	0.51
1:E:27:PRO:HB2	1:G:27:PRO:HB2	1.92	0.50
1:A:161:ARG:NH2	1:A:164:GLU:OE2	2.44	0.50
1:B:108:ASP:O	1:B:112:ARG:HG3	2.11	0.50
1:B:131:ALA:N	3:B:804:HOH:O	2.43	0.50
1:B:178:PRO:HD3	1:B:193:TYR:CE1	2.46	0.50
1:F:350:ARG:N	3:F:718:HOH:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:316:THR:N	3:D:729:HOH:O	2.44	0.50
1:H:253:ARG:NH2	3:H:804:HOH:O	2.43	0.50
1:F:319:THR:HB	1:F:330:LEU:HD23	1.94	0.50
1:A:89:PRO:HG3	3:A:778:HOH:O	2.12	0.50
1:H:15:ARG:HG2	1:H:15:ARG:NH1	2.27	0.49
1:E:124:THR:HG1	1:E:127:GLY:N	2.09	0.49
1:A:7:ASP:OD2	3:A:837:HOH:O	2.20	0.49
1:F:253:ARG:NH2	3:F:796:HOH:O	2.24	0.49
1:G:94:VAL:HG11	1:G:131:ALA:HB1	1.94	0.49
1:H:142:ILE:HD11	1:H:158:VAL:HG11	1.95	0.49
1:E:50:GLU:OE2	3:E:702:HOH:O	2.20	0.49
1:A:27:PRO:HB2	1:C:27:PRO:HB2	1.95	0.49
1:D:263:GLU:CB	3:D:761:HOH:O	2.60	0.48
1:C:159:SER:HA	1:C:169:VAL:HG21	1.94	0.48
1:G:314:ARG:HD2	3:G:518:HOH:O	2.12	0.48
1:F:232:PRO:HB3	3:F:693:HOH:O	2.13	0.48
1:H:42:PRO:HG3	3:H:637:HOH:O	2.12	0.48
1:H:246:THR:HG21	3:H:694:HOH:O	2.13	0.48
1:H:128:ILE:HD12	1:H:158:VAL:HG22	1.95	0.48
1:C:143:GLU:HG2	1:C:172:ASP:HB3	1.96	0.48
1:E:319:THR:HB	1:E:330:LEU:HD23	1.96	0.48
1:B:282:HIS:N	3:B:782:HOH:O	2.29	0.48
1:A:109:LEU:CD1	3:A:772:HOH:O	2.61	0.48
1:E:236:ASP:OD1	3:E:739:HOH:O	2.20	0.47
1:G:375:ARG:NH1	3:G:619:HOH:O	2.46	0.47
1:E:173:ASN:HB3	1:E:193:TYR:CE1	2.49	0.47
1:C:180:LEU:HD22	1:C:294:ALA:HB3	1.95	0.47
1:C:184:LEU:CD1	3:C:809:HOH:O	2.44	0.47
1:C:96:THR:HG23	3:C:772:HOH:O	2.14	0.47
1:E:233:GLY:CA	3:F:776:HOH:O	2.62	0.47
1:D:161:ARG:NH1	1:D:164:GLU:OE2	2.20	0.47
1:E:180:LEU:HD22	1:E:294:ALA:HB3	1.96	0.47
1:H:269:PRO:C	3:H:502:HOH:O	2.48	0.47
1:B:131:ALA:CA	3:B:804:HOH:O	2.62	0.47
1:A:109:LEU:HD13	3:A:772:HOH:O	2.13	0.47
1:F:122:LEU:CG	3:F:797:HOH:O	2.18	0.47
3:B:717:HOH:O	1:F:88:ARG:HG3	2.15	0.47
1:F:180:LEU:HD22	1:F:294:ALA:HB3	1.97	0.47
1:C:319:THR:HB	1:C:330:LEU:HD23	1.97	0.47
1:F:199:ILE:HG23	1:F:244:LEU:HD13	1.97	0.46
1:H:340:ARG:N	1:H:341:PRO:HD2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:346:ALA:CA	3:H:800:HOH:O	2.62	0.46
1:G:314:ARG:NH1	3:G:502:HOH:O	2.48	0.46
1:G:302:ASP:CB	3:G:701:HOH:O	2.63	0.46
1:G:180:LEU:HD22	1:G:294:ALA:HB3	1.98	0.46
1:F:42:PRO:HB3	3:F:594:HOH:O	2.15	0.45
1:H:128:ILE:CD1	1:H:158:VAL:HG22	2.45	0.45
1:D:199:ILE:HG23	1:D:244:LEU:HD13	1.97	0.45
1:B:36:ARG:C	3:B:797:HOH:O	2.43	0.45
1:G:165:ARG:HG2	3:G:836:HOH:O	2.17	0.45
1:H:334:PRO:HD2	1:H:356:LEU:O	2.16	0.45
1:D:319:THR:HB	1:D:330:LEU:HD23	1.99	0.45
1:F:340:ARG:NE	3:F:655:HOH:O	2.50	0.45
1:C:160:ARG:NE	3:C:694:HOH:O	2.40	0.44
1:F:235:LEU:HB2	3:F:742:HOH:O	2.16	0.44
1:H:113:GLN:HA	1:H:113:GLN:OE1	2.17	0.44
1:C:9:ARG:HB3	3:C:575:HOH:O	2.18	0.43
1:B:351:GLY:N	3:B:696:HOH:O	2.51	0.43
1:A:180:LEU:HD22	1:A:294:ALA:HB3	2.00	0.43
1:A:159:SER:HA	1:A:169:VAL:HG21	2.00	0.43
1:B:9:ARG:HD2	3:B:686:HOH:O	2.18	0.43
1:C:147:ASN:HA	1:C:148:PRO:HA	1.85	0.43
1:D:100:TYR:N	3:D:666:HOH:O	2.51	0.43
1:B:18:SER:HA	3:B:560:HOH:O	2.18	0.43
1:E:270:VAL:HG11	3:E:677:HOH:O	2.17	0.43
1:G:353:GLY:HA2	3:G:666:HOH:O	2.19	0.43
1:E:147:ASN:HA	1:E:148:PRO:HA	1.86	0.43
1:D:147:ASN:HA	1:D:148:PRO:HA	1.82	0.43
1:G:314:ARG:CZ	3:G:502:HOH:O	2.67	0.43
1:D:178:PRO:HD3	1:D:193:TYR:CE1	2.54	0.43
1:E:213:ARG:CZ	3:E:795:HOH:O	2.66	0.43
1:C:367:GLN:NE2	3:C:750:HOH:O	2.17	0.42
1:B:94:VAL:HG11	1:B:131:ALA:HB1	2.01	0.42
1:B:259:ARG:NH2	3:B:770:HOH:O	2.51	0.42
1:G:17:PRO:CA	3:G:803:HOH:O	2.57	0.42
1:F:316:THR:OG1	1:F:375:ARG:NH1	2.51	0.42
1:B:152:VAL:HG22	1:B:284:GLN:HB2	2.00	0.42
1:E:280:PRO:HD2	3:E:501:HOH:O	2.18	0.42
1:C:67:ALA:HB2	3:C:809:HOH:O	2.19	0.42
1:C:5:ARG:NE	3:C:770:HOH:O	2.41	0.42
1:H:134:GLU:O	3:H:762:HOH:O	2.22	0.42
3:A:605:HOH:O	1:D:7:ASP:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:205:VAL:CA	3:E:811:HOH:O	2.52	0.42
1:F:152:VAL:HG22	1:F:284:GLN:HB2	2.02	0.42
1:F:27:PRO:HB2	1:H:27:PRO:HB2	2.01	0.42
1:H:11:VAL:HA	1:H:245:HIS:ND1	2.35	0.42
1:D:42:PRO:HB3	3:D:616:HOH:O	2.20	0.42
1:G:173:ASN:HB3	1:G:193:TYR:CE1	2.54	0.41
1:D:248:SER:HB2	1:D:252:HIS:CE1	2.55	0.41
1:H:152:VAL:HG11	1:H:288:VAL:HG22	2.01	0.41
1:D:173:ASN:HB3	1:D:193:TYR:CE1	2.54	0.41
1:C:259:ARG:NH1	3:C:652:HOH:O	2.43	0.41
1:C:109:LEU:HD11	3:D:675:HOH:O	2.20	0.41
1:C:88:ARG:NH1	3:C:505:HOH:O	2.50	0.41
1:D:318:PHE:N	3:D:729:HOH:O	2.54	0.41
1:E:105:GLY:N	3:E:704:HOH:O	2.53	0.41
1:B:159:SER:HA	1:B:169:VAL:HG21	2.03	0.41
1:A:213:ARG:NE	3:A:765:HOH:O	2.18	0.41
1:C:340:ARG:N	1:C:341:PRO:HD2	2.36	0.41
1:A:334:PRO:HD2	1:A:356:LEU:O	2.21	0.41
1:D:340:ARG:N	1:D:341:PRO:CD	2.83	0.40
1:B:68:PRO:HG2	1:B:213:ARG:HA	2.03	0.40
1:E:332:GLU:OE1	1:E:338:THR:HG23	2.20	0.40
1:H:319:THR:HB	1:H:330:LEU:HD23	2.03	0.40
1:B:147:ASN:HA	1:B:148:PRO:HA	1.82	0.40
1:C:152:VAL:HG21	1:C:288:VAL:HG22	2.03	0.40
1:C:340:ARG:NE	3:C:506:HOH:O	2.53	0.40
1:A:353:GLY:N	3:A:667:HOH:O	2.54	0.40
1:A:147:ASN:HA	1:A:148:PRO:HA	1.81	0.40
1:A:109:LEU:HD13	3:A:792:HOH:O	2.21	0.40
1:H:84:LEU:HD12	1:H:84:LEU:HA	1.89	0.40
1:F:136:ASP:N	1:F:136:ASP:OD1	2.52	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:522:HOH:O	3:H:517:HOH:O[6_445]	1.82	0.38
3:H:776:HOH:O	3:H:776:HOH:O[2_455]	1.83	0.37
3:B:504:HOH:O	3:F:507:HOH:O[8_444]	1.90	0.30
3:A:523:HOH:O	3:E:509:HOH:O[8_544]	2.03	0.17
3:D:515:HOH:O	3:G:527:HOH:O[7_454]	2.10	0.10

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	359/389 (92%)	350 (98%)	9 (2%)	0	100	100
1	B	358/389 (92%)	349 (98%)	9 (2%)	0	100	100
1	C	353/389 (91%)	346 (98%)	7 (2%)	0	100	100
1	D	358/389 (92%)	352 (98%)	5 (1%)	1 (0%)	46	29
1	E	361/389 (93%)	352 (98%)	9 (2%)	0	100	100
1	F	356/389 (92%)	349 (98%)	7 (2%)	0	100	100
1	G	354/389 (91%)	346 (98%)	8 (2%)	0	100	100
1	H	353/389 (91%)	345 (98%)	6 (2%)	2 (1%)	30	13
All	All	2852/3112 (92%)	2789 (98%)	60 (2%)	3 (0%)	56	39

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	197[A]	LYS
1	H	197[B]	LYS
1	D	197	LYS

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	270/305 (88%)	268 (99%)	2 (1%)	88	84
1	B	272/305 (89%)	268 (98%)	4 (2%)	72	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	274/305 (90%)	273 (100%)	1 (0%)	93	92
1	D	271/305 (89%)	269 (99%)	2 (1%)	88	84
1	E	276/305 (90%)	275 (100%)	1 (0%)	93	92
1	F	267/305 (88%)	265 (99%)	2 (1%)	88	84
1	G	270/305 (88%)	269 (100%)	1 (0%)	93	92
1	H	265/305 (87%)	262 (99%)	3 (1%)	80	72
All	All	2165/2440 (89%)	2149 (99%)	16 (1%)	88	84

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASP
1	A	332	GLU
1	B	23	ASP
1	B	99	VAL
1	B	328	HIS
1	B	332	GLU
1	C	23	ASP
1	D	23	ASP
1	D	332	GLU
1	E	23	ASP
1	F	23	ASP
1	F	332	GLU
1	G	23	ASP
1	H	18	SER
1	H	23	ASP
1	H	332	GLU

Some 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 ⓘ

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	401	-	4,4,4	0.29	0	6,6,6	0.11	0
2	SO4	A	402	-	4,4,4	0.50	0	6,6,6	0.23	0
2	SO4	B	401	-	4,4,4	0.35	0	6,6,6	0.29	0
2	SO4	B	402	-	4,4,4	0.27	0	6,6,6	0.12	0
2	SO4	C	401	-	4,4,4	0.34	0	6,6,6	0.14	0
2	SO4	C	402	-	4,4,4	0.55	0	6,6,6	0.11	0
2	SO4	D	401	-	4,4,4	0.63	0	6,6,6	0.13	0
2	SO4	D	402	-	4,4,4	0.33	0	6,6,6	0.17	0
2	SO4	E	401	-	4,4,4	0.28	0	6,6,6	0.09	0
2	SO4	E	402	-	4,4,4	0.46	0	6,6,6	0.17	0
2	SO4	F	401	-	4,4,4	0.57	0	6,6,6	0.18	0
2	SO4	F	402	-	4,4,4	0.30	0	6,6,6	0.07	0
2	SO4	G	401	-	4,4,4	0.26	0	6,6,6	0.11	0
2	SO4	G	402	-	4,4,4	0.48	0	6,6,6	0.47	0
2	SO4	G	403	-	4,4,4	0.52	0	6,6,6	0.16	0
2	SO4	H	401	-	4,4,4	0.32	0	6,6,6	0.15	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	SO4	A	401	-	-	0/0/0/0	0/0/0/0
2	SO4	A	402	-	-	0/0/0/0	0/0/0/0
2	SO4	B	401	-	-	0/0/0/0	0/0/0/0
2	SO4	B	402	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	C	401	-	-	0/0/0/0	0/0/0/0
2	SO4	C	402	-	-	0/0/0/0	0/0/0/0
2	SO4	D	401	-	-	0/0/0/0	0/0/0/0
2	SO4	D	402	-	-	0/0/0/0	0/0/0/0
2	SO4	E	401	-	-	0/0/0/0	0/0/0/0
2	SO4	E	402	-	-	0/0/0/0	0/0/0/0
2	SO4	F	401	-	-	0/0/0/0	0/0/0/0
2	SO4	F	402	-	-	0/0/0/0	0/0/0/0
2	SO4	G	401	-	-	0/0/0/0	0/0/0/0
2	SO4	G	402	-	-	0/0/0/0	0/0/0/0
2	SO4	G	403	-	-	0/0/0/0	0/0/0/0
2	SO4	H	401	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	402	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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, 95th 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	362/389 (93%)	0.14	13 (3%) 46 44	10, 18, 46, 59	0
1	B	365/389 (93%)	0.09	8 (2%) 65 63	9, 19, 42, 56	0
1	C	360/389 (92%)	0.14	19 (5%) 30 28	9, 18, 47, 71	0
1	D	366/389 (94%)	0.12	17 (4%) 36 34	10, 21, 42, 70	0
1	E	366/389 (94%)	0.07	12 (3%) 50 47	9, 18, 41, 62	0
1	F	362/389 (93%)	0.16	14 (3%) 43 40	9, 19, 45, 65	0
1	G	361/389 (92%)	0.07	8 (2%) 65 63	9, 19, 39, 63	0
1	H	364/389 (93%)	0.11	15 (4%) 41 38	9, 18, 48, 66	0
All	All	2906/3112 (93%)	0.11	106 (3%) 46 44	9, 19, 44, 71	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	17	PRO	6.2
1	H	130	ALA	5.0
1	A	133	ALA	4.9
1	H	346	ALA	4.7
1	A	130	ALA	4.5
1	C	129	ALA	4.4
1	D	378	ALA	4.3
1	H	129	ALA	4.2
1	F	129	ALA	4.1
1	H	3	GLY	4.0
1	C	341	PRO	4.0
1	H	344	ALA	4.0
1	C	125	PRO	3.9
1	C	124	THR	3.9
1	H	124	THR	3.9
1	H	126	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	133	ALA	3.7
1	C	130	ALA	3.7
1	F	132	LEU	3.6
1	D	17	PRO	3.5
1	C	131	ALA	3.5
1	F	126	GLU	3.4
1	H	133	ALA	3.4
1	G	3	GLY	3.4
1	A	125	PRO	3.3
1	H	125	PRO	3.3
1	G	380	GLY	3.3
1	F	351	GLY	3.3
1	C	103	THR	3.3
1	D	3	GLY	3.2
1	B	2	SER	3.2
1	C	351	GLY	3.1
1	G	1	MET	3.1
1	H	127	GLY	3.0
1	B	17	PRO	3.0
1	B	351	GLY	2.9
1	E	42	PRO	2.9
1	E	338	THR	2.9
1	D	2	SER	2.9
1	B	121	ASP	2.9
1	C	132	LEU	2.9
1	G	235	LEU	2.9
1	G	149	LEU	2.9
1	E	99	VAL	2.9
1	D	341	PRO	2.8
1	D	125	PRO	2.8
1	C	104	ASP	2.8
1	E	120	ALA	2.8
1	E	130	ALA	2.8
1	D	101	ALA	2.7
1	A	380	GLY	2.7
1	H	351	GLY	2.7
1	D	339	HIS	2.7
1	F	130	ALA	2.7
1	E	97	ASP	2.7
1	G	2	SER	2.7
1	F	127	GLY	2.7
1	D	235	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	104	ASP	2.6
1	A	126	GLU	2.6
1	A	111	ALA	2.6
1	D	132	LEU	2.6
1	C	379	GLY	2.5
1	E	125	PRO	2.5
1	H	45	PHE	2.5
1	E	351	GLY	2.5
1	F	125	PRO	2.5
1	F	133	ALA	2.5
1	A	129	ALA	2.5
1	A	124	THR	2.5
1	C	135	PRO	2.5
1	F	16	ARG	2.4
1	G	97	ASP	2.4
1	E	3	GLY	2.4
1	E	19	ALA	2.4
1	D	100	TYR	2.3
1	A	103	THR	2.3
1	E	16	ARG	2.3
1	D	351	GLY	2.3
1	B	339	HIS	2.2
1	C	137	LEU	2.2
1	B	352	ILE	2.2
1	D	352	ILE	2.2
1	F	112	ARG	2.2
1	F	103	THR	2.2
1	H	164	GLU	2.2
1	C	339	HIS	2.2
1	C	38	ALA	2.2
1	C	113	GLN	2.2
1	G	16	ARG	2.2
1	F	3	GLY	2.2
1	H	2	SER	2.2
1	H	114	GLY	2.1
1	D	130	ALA	2.1
1	A	2	SER	2.1
1	D	98	ASP	2.1
1	A	101	ALA	2.1
1	C	238	PHE	2.1
1	B	101	ALA	2.1
1	C	120	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	17	PRO	2.1
1	D	97	ASP	2.0
1	F	1	MET	2.0
1	A	96	THR	2.0
1	D	124	THR	2.0
1	A	40	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	G	401	5/5	0.94	0.21	2.67	48,48,50,59	0
2	SO4	B	402	5/5	0.96	0.11	0.28	44,44,46,46	0
2	SO4	D	402	5/5	0.98	0.11	0.07	26,28,35,44	0
2	SO4	A	401	5/5	0.97	0.11	0.05	27,29,36,38	0
2	SO4	E	401	5/5	0.95	0.12	-0.25	24,34,37,39	0
2	SO4	C	402	5/5	0.98	0.10	-0.94	17,20,22,29	0
2	SO4	B	401	5/5	0.98	0.10	-1.03	15,16,21,24	0
2	SO4	F	402	5/5	0.96	0.09	-1.03	28,37,44,45	0
2	SO4	D	401	5/5	0.99	0.09	-1.19	15,17,20,26	0
2	SO4	F	401	5/5	0.99	0.09	-1.40	17,18,21,27	0
2	SO4	H	401	5/5	0.98	0.07	-1.43	29,32,38,40	0
2	SO4	A	402	5/5	0.99	0.09	-1.47	16,17,21,24	0
2	SO4	C	401	5/5	0.98	0.06	-1.77	26,34,35,38	0
2	SO4	E	402	5/5	0.99	0.07	-1.84	18,19,22,27	0
2	SO4	G	403	5/5	0.99	0.09	-2.20	18,18,20,28	0
2	SO4	G	402	5/5	0.99	0.07	-3.05	16,19,19,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.