



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 02:17 PM UTC

PDB ID : 3GOB / pdb_00003gob
Title : Crystal Structure of Dicamba Monooxygenase with Non-heme Cobalt and DCSA
Authors : Rydel, T.J.; Sturman, E.J.; Moshiri, F.; Brown, G.R.; Qi, Y.
Deposited on : 2009-03-18
Resolution : 2.05 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

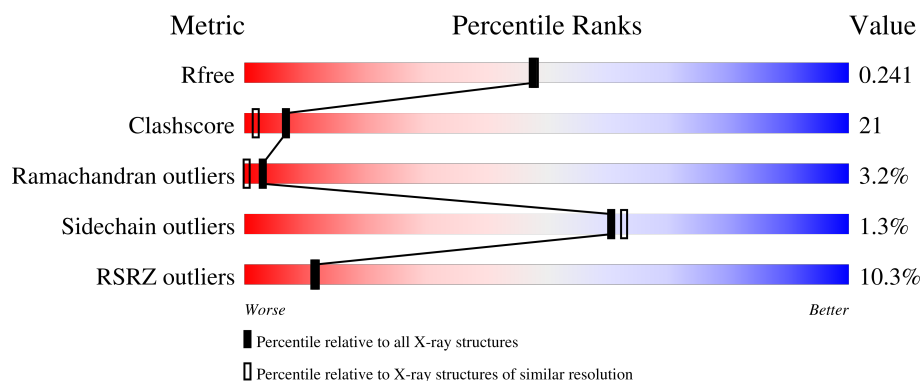
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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 $\leq 5\%$. 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	349	9% 64% 27% 7% .
1	B	349	6% 64% 30% . .
1	C	349	15% 62% 28% 7% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8517 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 DdmC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2649	1670	475	490	14			
1	B	341	Total	C	N	O	S	0	0	0
			2641	1665	474	489	13			
1	C	342	Total	C	N	O	S	0	0	0
			2649	1670	475	490	14			

There are 33 discrepancies between the modelled and reference sequences:

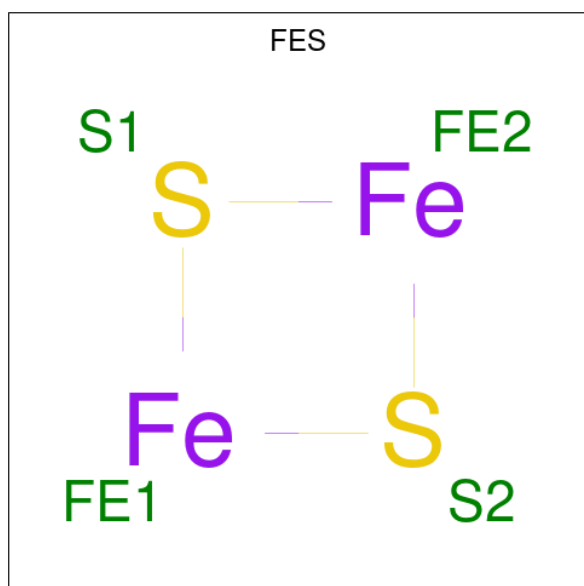
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q5S3I3
A	2	ALA	MET	engineered mutation	UNP Q5S3I3
A	341	ARG	-	expression tag	UNP Q5S3I3
A	342	LEU	-	expression tag	UNP Q5S3I3
A	343	GLU	-	expression tag	UNP Q5S3I3
A	344	HIS	-	expression tag	UNP Q5S3I3
A	345	HIS	-	expression tag	UNP Q5S3I3
A	346	HIS	-	expression tag	UNP Q5S3I3
A	347	HIS	-	expression tag	UNP Q5S3I3
A	348	HIS	-	expression tag	UNP Q5S3I3
A	349	HIS	-	expression tag	UNP Q5S3I3
B	1	MET	-	expression tag	UNP Q5S3I3
B	2	ALA	MET	engineered mutation	UNP Q5S3I3
B	341	ARG	-	expression tag	UNP Q5S3I3
B	342	LEU	-	expression tag	UNP Q5S3I3
B	343	GLU	-	expression tag	UNP Q5S3I3
B	344	HIS	-	expression tag	UNP Q5S3I3
B	345	HIS	-	expression tag	UNP Q5S3I3
B	346	HIS	-	expression tag	UNP Q5S3I3
B	347	HIS	-	expression tag	UNP Q5S3I3
B	348	HIS	-	expression tag	UNP Q5S3I3
B	349	HIS	-	expression tag	UNP Q5S3I3
C	1	MET	-	expression tag	UNP Q5S3I3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2	ALA	MET	engineered mutation	UNP Q5S3I3
C	341	ARG	-	expression tag	UNP Q5S3I3
C	342	LEU	-	expression tag	UNP Q5S3I3
C	343	GLU	-	expression tag	UNP Q5S3I3
C	344	HIS	-	expression tag	UNP Q5S3I3
C	345	HIS	-	expression tag	UNP Q5S3I3
C	346	HIS	-	expression tag	UNP Q5S3I3
C	347	HIS	-	expression tag	UNP Q5S3I3
C	348	HIS	-	expression tag	UNP Q5S3I3
C	349	HIS	-	expression tag	UNP Q5S3I3

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe S 4 2 2	0	0
2	B	1	Total Fe S 4 2 2	0	0
2	C	1	Total Fe S 4 2 2	0	0

- Molecule 3 is COBALT (II) ION (CCD ID: CO) (formula: Co).

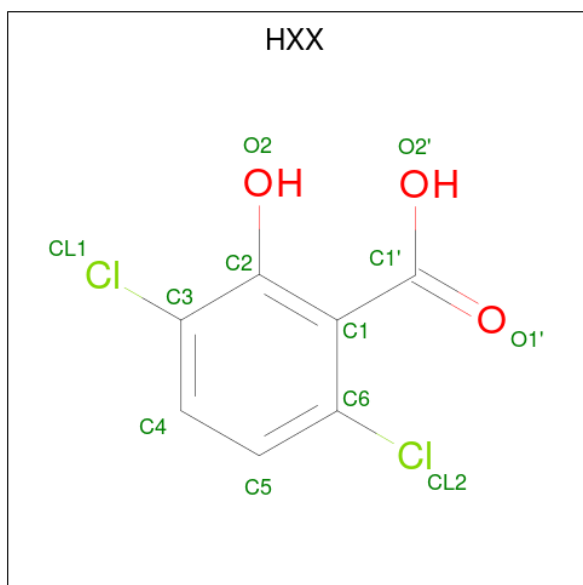
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Co 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Co	0	0
			2	2		
3	C	4	Total	Co	0	0
			4	4		

- Molecule 4 is 3,6-dichloro-2-hydroxybenzoic acid (CCD ID: HXX) (formula: $C_7H_4Cl_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	Cl	O	0	0
			12	7	2	3		
4	B	1	Total	C	Cl	O	0	0
			12	7	2	3		
4	C	1	Total	C	Cl	O	0	0
			12	7	2	3		

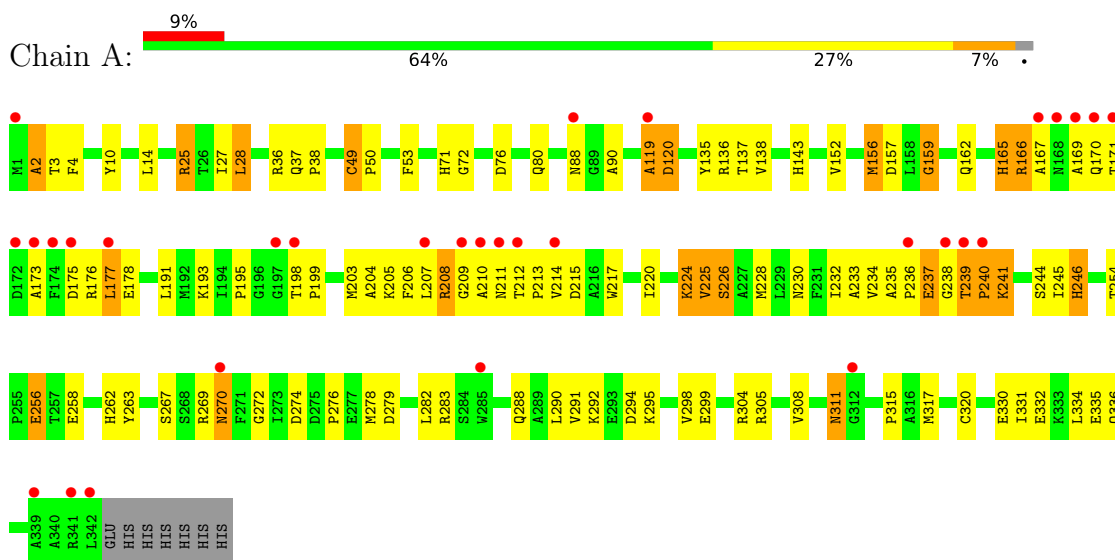
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	189	Total	O	0	0
			189	189		
5	B	173	Total	O	0	0
			173	173		
5	C	160	Total	O	0	0
			160	160		

3 Residue-property plots

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: DdmC

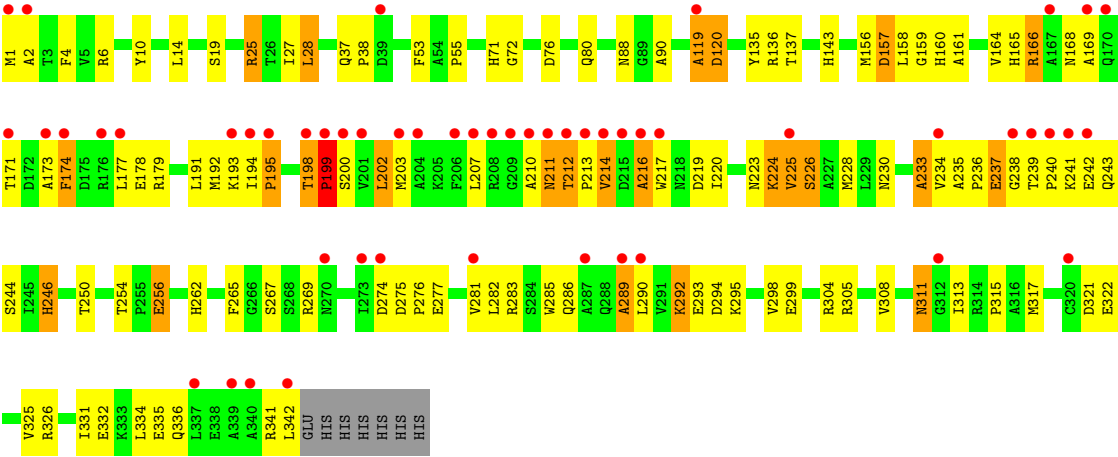


• Molecule 1: DdmC



• Molecule 1: DdmC





4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	81.01Å 81.01Å 161.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.05 20.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	81.8 (20.00-2.05) 82.1 (20.00-2.05)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.19 (at 2.05Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	0.232 , 0.267 0.211 , 0.241	Depositor DCC
R_{free} test set	6147 reflections (10.13%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.003 for -h,-k,l 0.039 for h,-h-k,-l 0.023 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8517	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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, 0.333 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: HXX, CO, FES

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	1/2714 (0.0%)	0.97	16/3695 (0.4%)
1	B	0.38	0/2706	0.94	14/3685 (0.4%)
1	C	0.37	0/2714	0.96	17/3695 (0.5%)
All	All	0.38	1/8134 (0.0%)	0.96	47/11075 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	156	MET	SD-CE	-5.49	1.65	1.79

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	VAL	N-CA-C	8.28	118.37	110.42
1	B	194	ILE	CA-C-N	7.51	127.50	119.76
1	B	194	ILE	C-N-CA	7.51	127.50	119.76
1	B	72	GLY	N-CA-C	7.17	125.62	115.30
1	C	72	GLY	N-CA-C	7.09	125.16	115.30
1	A	72	GLY	N-CA-C	6.80	124.75	115.30
1	C	256	GLU	N-CA-C	-6.66	103.01	112.13
1	C	275	ASP	CA-C-N	6.56	126.50	119.28
1	C	275	ASP	C-N-CA	6.56	126.50	119.28
1	C	198	THR	CA-C-N	6.46	127.91	119.84
1	C	198	THR	C-N-CA	6.46	127.91	119.84
1	A	165	HIS	N-CA-C	-6.36	105.39	112.57
1	A	246	HIS	N-CA-C	6.13	118.09	108.96
1	A	2	ALA	N-CA-C	-6.12	105.98	113.50
1	A	256	GLU	N-CA-C	-6.12	103.75	112.13
1	B	246	HIS	N-CA-C	6.11	118.06	108.96
1	C	246	HIS	N-CA-C	6.09	118.03	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	256	GLU	N-CA-C	-6.07	103.82	112.13
1	C	311	ASN	N-CA-C	-5.99	101.60	110.46
1	C	159	GLY	N-CA-C	5.91	119.79	112.64
1	A	14	LEU	N-CA-C	-5.89	102.19	110.31
1	A	311	ASN	N-CA-C	-5.89	101.75	110.46
1	C	14	LEU	N-CA-C	-5.83	102.26	110.31
1	B	311	ASN	N-CA-C	-5.80	101.87	110.46
1	B	14	LEU	N-CA-C	-5.67	102.49	110.31
1	A	157	ASP	N-CA-C	5.62	118.12	109.07
1	B	53	PHE	N-CA-C	5.62	120.08	113.23
1	A	159	GLY	N-CA-C	5.61	120.89	113.37
1	B	226	SER	N-CA-C	5.59	118.50	109.83
1	C	235	ALA	N-CA-C	5.53	112.99	108.07
1	C	233	ALA	N-CA-C	5.50	116.61	108.86
1	C	53	PHE	N-CA-C	5.47	119.91	113.23
1	A	226	SER	N-CA-C	5.45	118.28	109.83
1	A	53	PHE	N-CA-C	5.42	119.85	113.23
1	A	152	VAL	N-CA-C	-5.34	105.51	110.53
1	C	226	SER	N-CA-C	5.21	117.90	109.83
1	B	313	ILE	N-CA-C	5.20	115.76	108.89
1	B	270	ASN	N-CA-C	-5.17	105.86	113.61
1	A	49	CYS	CA-C-N	5.16	124.95	119.28
1	A	49	CYS	C-N-CA	5.16	124.95	119.28
1	B	46	LEU	N-CA-C	-5.06	102.56	110.10
1	C	157	ASP	N-CA-C	5.05	117.13	108.90
1	A	270	ASN	N-CA-C	-5.05	106.03	113.61
1	C	289	ALA	N-CA-C	5.04	116.46	110.97
1	B	49	CYS	CA-C-N	5.03	124.81	119.28
1	B	49	CYS	C-N-CA	5.03	124.81	119.28
1	C	313	ILE	N-CA-C	5.02	115.52	108.89

There are no chirality outliers.

There are no planarity outliers.

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	2649	0	2589	122	0
1	B	2641	0	2577	100	0
1	C	2649	0	2589	117	0
2	A	4	0	0	1	0
2	B	4	0	0	1	0
2	C	4	0	0	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	4	0	0	0	0
4	A	12	0	3	0	0
4	B	12	0	3	0	0
4	C	12	0	3	0	0
5	A	189	0	0	16	0
5	B	173	0	0	11	0
5	C	160	0	0	8	0
All	All	8517	0	7764	336	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 21.

All (336) 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:A:156:MET:HE3	1:A:228:MET:SD	1.97	1.04
1:C:169:ALA:HB2	1:C:202:LEU:HD12	1.45	0.99
1:C:192:MET:HE3	1:C:194:ILE:HD11	1.48	0.94
1:A:166:ARG:O	1:A:170:GLN:HB2	1.67	0.93
1:B:156:MET:HE3	1:B:228:MET:SD	2.15	0.87
1:A:175:ASP:HB3	1:A:177:LEU:HD11	1.57	0.84
1:C:156:MET:HE3	1:C:228:MET:SD	2.17	0.84
1:C:203:MET:HE2	1:C:234:VAL:HB	1.58	0.84
1:C:171:THR:HG22	1:C:173:ALA:H	1.44	0.83
1:C:242:GLU:HG3	1:C:243:GLN:HE21	1.42	0.83
1:A:217:TRP:CH2	1:A:239:THR:HB	2.15	0.81
1:C:286:GLN:HA	1:C:290:LEU:HD23	1.62	0.81
1:A:206:PHE:HB2	1:A:245:ILE:HD13	1.61	0.81
1:A:215:ASP:HB2	1:A:239:THR:HG21	1.62	0.79
1:B:269:ARG:HG3	5:B:766:HOH:O	1.83	0.79
1:C:269:ARG:HD3	1:C:282:LEU:HD11	1.65	0.78
1:B:174:PHE:O	1:B:177:LEU:HG	1.82	0.78
1:A:240:PRO:O	1:A:241:LYS:HB2	1.84	0.78
1:C:194:ILE:HB	1:C:216:ALA:HB3	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:LEU:HD11	1:C:234:VAL:HG21	1.70	0.72
1:A:269:ARG:HD3	1:A:282:LEU:HD11	1.70	0.72
1:A:217:TRP:HH2	1:A:239:THR:HB	1.52	0.71
1:A:269:ARG:HG3	5:A:840:HOH:O	1.88	0.71
1:C:174:PHE:O	1:C:177:LEU:HG	1.91	0.71
1:B:162:GLN:OE1	1:B:170:GLN:HA	1.91	0.70
1:A:199:PRO:HB3	1:A:234:VAL:HG21	1.74	0.69
1:C:195:PRO:HB3	1:C:214:VAL:HA	1.74	0.68
1:C:237:GLU:C	1:C:239:THR:H	2.01	0.68
1:C:195:PRO:CB	1:C:214:VAL:HA	2.23	0.68
1:A:272:GLY:HA3	1:A:278:MET:HE1	1.76	0.68
1:A:208:ARG:HG2	1:A:209:GLY:N	2.09	0.67
1:B:171:THR:HG21	1:B:194:ILE:HG21	1.75	0.67
1:C:269:ARG:HH11	1:C:282:LEU:CD1	2.06	0.67
1:B:86:HIS:ND1	5:B:865:HOH:O	2.27	0.67
1:B:193:LYS:HE2	1:B:217:TRP:HE1	1.60	0.66
1:B:171:THR:HG22	1:B:173:ALA:H	1.59	0.66
1:A:88:ASN:HD21	1:A:90:ALA:HB2	1.61	0.66
1:C:193:LYS:HB3	5:C:1089:HOH:O	1.96	0.66
1:A:269:ARG:HD3	1:A:282:LEU:CD1	2.26	0.66
1:C:269:ARG:HH11	1:C:282:LEU:HD12	1.60	0.65
1:A:269:ARG:NE	1:A:278:MET:HE3	2.12	0.65
1:A:10:TYR:CE2	1:A:225:VAL:HG11	2.31	0.65
1:B:177:LEU:CD2	1:B:194:ILE:HG12	2.27	0.65
1:B:165:HIS:ND1	1:B:293:GLU:OE2	2.23	0.64
1:B:289:ALA:HA	1:B:293:GLU:OE2	1.98	0.64
1:B:295:LYS:O	1:B:299:GLU:HG3	1.98	0.64
1:A:233:ALA:HB2	1:A:246:HIS:HB3	1.79	0.64
1:A:270:ASN:HB3	5:A:1017:HOH:O	1.96	0.64
1:A:177:LEU:HD12	1:A:177:LEU:N	2.13	0.64
1:C:27:ILE:HD12	1:C:254:THR:HG21	1.80	0.63
1:C:1:MET:SD	1:C:6:ARG:NH1	2.71	0.63
1:C:295:LYS:O	1:C:299:GLU:HG3	1.98	0.63
1:A:143:HIS:HE1	1:A:256:GLU:OE1	1.82	0.63
1:C:88:ASN:HD21	1:C:90:ALA:HB2	1.63	0.63
1:A:315:PRO:HB2	1:A:317:MET:HE3	1.81	0.62
1:C:277:GLU:O	1:C:281:VAL:HG23	1.99	0.62
1:B:27:ILE:HD12	1:B:254:THR:HG21	1.80	0.62
1:C:160:HIS:HB2	1:C:164:VAL:HG23	1.82	0.62
1:A:4:PHE:HB3	1:A:28:LEU:HD13	1.81	0.62
1:B:4:PHE:HB3	1:B:28:LEU:HD13	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:PRO:HG2	1:B:239:THR:HG21	1.82	0.62
1:C:233:ALA:HB2	1:C:246:HIS:HB3	1.81	0.61
1:B:88:ASN:HD21	1:B:90:ALA:HB2	1.64	0.61
1:C:202:LEU:HD21	1:C:285:TRP:CE3	2.35	0.61
1:B:292:LYS:O	1:B:296:VAL:HG23	2.00	0.61
1:C:119:ALA:O	1:C:120:ASP:HB3	2.00	0.61
1:B:282:LEU:O	1:B:286:GLN:HG3	2.01	0.60
1:C:198:THR:O	1:C:199:PRO:O	2.19	0.60
1:C:289:ALA:HA	1:C:293:GLU:OE2	2.01	0.60
1:C:4:PHE:HB3	1:C:28:LEU:HD13	1.81	0.60
1:A:215:ASP:CB	1:A:239:THR:HG21	2.32	0.60
1:A:269:ARG:CD	1:A:278:MET:HE3	2.32	0.60
1:A:330:GLU:HG3	5:A:1135:HOH:O	2.00	0.60
1:A:27:ILE:HD12	1:A:254:THR:HG21	1.83	0.60
1:C:157:ASP:HB2	5:C:884:HOH:O	2.02	0.60
1:A:138:VAL:HG23	5:A:1152:HOH:O	2.01	0.59
1:C:290:LEU:HD22	1:C:290:LEU:H	1.66	0.59
1:A:37:GLN:HB3	1:A:38:PRO:HD2	1.84	0.59
1:C:315:PRO:HB2	1:C:317:MET:HE3	1.84	0.59
1:C:217:TRP:CH2	1:C:241:LYS:HA	2.37	0.59
1:A:119:ALA:O	1:A:120:ASP:HB3	2.02	0.59
1:C:160:HIS:HB2	1:C:164:VAL:CG2	2.33	0.58
1:A:76:ASP:OD2	1:A:80:GLN:HB3	2.03	0.58
1:C:156:MET:HE1	1:C:220:ILE:HG12	1.86	0.58
1:B:193:LYS:HG2	1:B:217:TRP:CD1	2.39	0.58
1:A:295:LYS:O	1:A:299:GLU:HG3	2.03	0.58
1:A:212:THR:HG23	1:A:213:PRO:HD2	1.86	0.57
1:C:331:ILE:O	1:C:335:GLU:HG3	2.04	0.57
1:B:269:ARG:HH11	1:B:282:LEU:HD12	1.70	0.56
1:A:162:GLN:O	1:A:166:ARG:HA	2.06	0.56
1:B:156:MET:HE1	1:B:220:ILE:HG12	1.87	0.56
5:A:820:HOH:O	1:B:320:CYS:HB3	2.05	0.56
1:C:212:THR:HG23	1:C:213:PRO:HD2	1.86	0.56
1:C:37:GLN:HB3	1:C:38:PRO:HD2	1.88	0.56
1:B:37:GLN:HB3	1:B:38:PRO:HD2	1.88	0.55
1:C:242:GLU:C	1:C:244:SER:H	2.13	0.55
1:B:225:VAL:HG12	1:B:226:SER:N	2.22	0.55
1:C:332:GLU:O	1:C:336:GLN:HG3	2.07	0.55
1:A:176:ARG:HA	5:A:771:HOH:O	2.05	0.55
1:B:143:HIS:HE1	1:B:256:GLU:OE1	1.89	0.55
1:C:283:ARG:HG2	5:C:1068:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308:VAL:O	1:C:311:ASN:O	2.25	0.55
1:C:171:THR:HG22	1:C:173:ALA:N	2.19	0.55
1:C:198:THR:O	1:C:198:THR:HG23	2.06	0.55
1:B:156:MET:HE2	1:B:156:MET:HA	1.89	0.55
1:C:202:LEU:HD11	1:C:285:TRP:CZ3	2.42	0.55
1:C:1:MET:HE1	1:C:6:ARG:CZ	2.36	0.55
1:A:237:GLU:HG3	1:A:238:GLY:N	2.22	0.54
1:C:274:ASP:O	1:C:276:PRO:HD3	2.07	0.54
1:B:315:PRO:HB2	1:B:317:MET:HE3	1.88	0.54
1:C:136:ARG:HG2	1:C:269:ARG:NH2	2.22	0.54
1:C:290:LEU:HD22	1:C:290:LEU:N	2.23	0.54
1:A:175:ASP:HB3	1:A:177:LEU:CD1	2.32	0.54
1:A:240:PRO:O	1:A:241:LYS:CB	2.56	0.54
1:C:10:TYR:CE2	1:C:225:VAL:HG11	2.42	0.54
1:A:137:THR:HA	1:A:267:SER:O	2.07	0.53
1:C:76:ASP:OD2	1:C:80:GLN:HB3	2.08	0.53
1:A:288:GLN:NE2	1:A:292:LYS:HB2	2.23	0.53
1:A:159:GLY:HA3	5:A:1121:HOH:O	2.09	0.53
1:A:245:ILE:HA	5:A:1017:HOH:O	2.09	0.53
1:A:272:GLY:HA3	1:A:278:MET:CE	2.39	0.53
1:B:55:PRO:HB3	1:C:304:ARG:CZ	2.39	0.53
1:B:190:ALA:HB2	1:B:323:ALA:CB	2.38	0.53
1:B:76:ASP:OD2	1:B:80:GLN:HB3	2.09	0.53
1:C:203:MET:HG2	1:C:207:LEU:HD12	1.90	0.52
1:A:2:ALA:O	1:A:258:GLU:OE1	2.26	0.52
1:A:214:VAL:HG12	1:A:236:PRO:HA	1.91	0.52
1:A:304:ARG:CZ	1:C:55:PRO:HB3	2.39	0.52
1:A:320:CYS:SG	5:A:1121:HOH:O	2.58	0.52
1:B:193:LYS:HE2	1:B:217:TRP:NE1	2.23	0.52
1:C:240:PRO:C	1:C:242:GLU:N	2.65	0.52
1:A:331:ILE:O	1:A:335:GLU:HG3	2.10	0.52
1:B:71:HIS:HB2	2:B:501:FES:S1	2.50	0.52
1:B:237:GLU:HA	5:B:1118:HOH:O	2.09	0.52
1:A:240:PRO:HG2	1:A:241:LYS:H	1.74	0.52
1:A:10:TYR:CZ	1:A:225:VAL:HG11	2.45	0.52
1:B:286:GLN:O	1:B:290:LEU:HB2	2.09	0.52
1:C:326:ARG:NE	5:C:1044:HOH:O	2.42	0.52
1:A:269:ARG:HH11	1:A:282:LEU:HD12	1.75	0.52
1:A:274:ASP:O	1:A:276:PRO:HD3	2.10	0.51
1:C:305:ARG:HA	1:C:308:VAL:HG22	1.92	0.51
1:B:217:TRP:CE2	1:B:241:LYS:HB3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:VAL:HG12	1:C:226:SER:N	2.25	0.51
1:B:341:ARG:HG2	1:B:342:LEU:HD22	1.93	0.51
1:B:158:LEU:HB2	1:B:192:MET:SD	2.51	0.51
1:C:237:GLU:C	1:C:239:THR:N	2.68	0.51
1:C:240:PRO:C	1:C:242:GLU:H	2.18	0.51
1:B:331:ILE:O	1:B:335:GLU:HG3	2.11	0.50
1:C:282:LEU:O	1:C:286:GLN:HG3	2.10	0.50
1:A:233:ALA:CB	1:A:246:HIS:HB3	2.41	0.50
1:C:137:THR:HA	1:C:267:SER:O	2.10	0.50
1:A:237:GLU:C	1:A:239:THR:H	2.18	0.50
1:B:305:ARG:HA	1:B:308:VAL:HG22	1.94	0.50
1:C:19:SER:HB2	5:C:1022:HOH:O	2.10	0.50
1:C:269:ARG:CD	1:C:282:LEU:HD11	2.41	0.50
1:A:235:ALA:O	1:A:239:THR:HG22	2.12	0.50
1:B:2:ALA:HB1	1:B:258:GLU:OE1	2.12	0.50
1:B:173:ALA:HB2	1:B:176:ARG:HH21	1.77	0.50
1:B:332:GLU:O	1:B:336:GLN:HG3	2.12	0.49
1:B:202:LEU:HD22	1:B:285:TRP:CE3	2.48	0.49
1:A:2:ALA:O	1:A:3:THR:OG1	2.22	0.49
1:A:193:LYS:HD3	1:A:217:TRP:HE1	1.77	0.49
1:C:191:LEU:HA	1:C:219:ASP:OD1	2.12	0.49
1:A:308:VAL:O	1:A:311:ASN:O	2.31	0.49
1:C:192:MET:N	1:C:219:ASP:OD1	2.38	0.49
1:C:269:ARG:NH1	1:C:282:LEU:HD12	2.25	0.49
1:A:235:ALA:HB2	1:A:244:SER:CB	2.43	0.49
1:C:71:HIS:HB2	2:C:501:FES:S1	2.53	0.49
1:A:208:ARG:HG2	1:A:209:GLY:H	1.77	0.48
1:A:263:TYR:CD1	1:A:290:LEU:HD13	2.48	0.48
1:B:177:LEU:HD22	1:B:194:ILE:HG12	1.95	0.48
1:A:162:GLN:HG3	1:A:170:GLN:HG3	1.94	0.48
1:A:167:ALA:HA	1:A:170:GLN:HB2	1.95	0.48
1:C:158:LEU:HG	1:C:179:ARG:CZ	2.43	0.48
1:B:194:ILE:HB	1:B:216:ALA:HB3	1.94	0.48
1:B:308:VAL:O	1:B:311:ASN:O	2.30	0.48
1:A:175:ASP:CG	1:A:176:ARG:H	2.21	0.48
1:B:126:ASP:HA	5:B:762:HOH:O	2.13	0.48
1:A:225:VAL:HG12	1:A:226:SER:N	2.28	0.48
1:A:237:GLU:CG	1:A:238:GLY:H	2.26	0.48
1:B:118:LEU:O	1:B:119:ALA:C	2.57	0.48
1:B:190:ALA:HB2	1:B:323:ALA:HB2	1.96	0.48
1:C:315:PRO:HB2	1:C:317:MET:CE	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:THR:O	1:C:198:THR:CG2	2.61	0.48
1:B:156:MET:HE2	1:B:220:ILE:HD13	1.96	0.47
1:C:289:ALA:O	1:C:293:GLU:HB2	2.13	0.47
1:A:305:ARG:HA	1:A:308:VAL:HG22	1.95	0.47
1:A:332:GLU:O	1:A:336:GLN:HG3	2.14	0.47
1:C:199:PRO:HG3	1:C:203:MET:SD	2.55	0.47
1:A:25:ARG:HD2	1:A:262:HIS:CE1	2.50	0.47
1:A:88:ASN:ND2	1:A:90:ALA:HB2	2.28	0.47
1:A:165:HIS:HB2	1:A:169:ALA:HB3	1.96	0.47
1:A:294:ASP:O	1:A:298:VAL:HG22	2.14	0.47
1:C:242:GLU:C	1:C:244:SER:N	2.69	0.47
1:C:342:LEU:C	1:C:342:LEU:HD23	2.38	0.47
1:B:162:GLN:HG3	1:B:174:PHE:CD1	2.50	0.47
1:B:174:PHE:CE1	1:B:177:LEU:HD11	2.50	0.47
1:C:10:TYR:CZ	1:C:225:VAL:HG11	2.50	0.47
1:B:277:GLU:O	1:B:281:VAL:HG23	2.14	0.47
1:B:289:ALA:O	1:B:293:GLU:HB2	2.14	0.47
1:B:341:ARG:HD3	5:B:1069:HOH:O	2.14	0.47
1:C:88:ASN:ND2	1:C:90:ALA:HB2	2.29	0.47
1:A:195:PRO:HA	1:A:215:ASP:OD2	2.15	0.46
1:A:171:THR:C	1:A:173:ALA:H	2.23	0.46
1:A:237:GLU:O	1:A:239:THR:N	2.38	0.46
1:C:203:MET:CE	1:C:234:VAL:HB	2.38	0.46
1:C:237:GLU:O	1:C:239:THR:N	2.48	0.46
1:C:178:GLU:O	1:C:192:MET:HG3	2.16	0.46
1:A:135:TYR:HA	1:A:269:ARG:O	2.16	0.46
1:C:25:ARG:HD2	1:C:262:HIS:CE1	2.51	0.46
1:C:214:VAL:O	1:C:214:VAL:HG13	2.16	0.46
1:A:171:THR:C	1:A:173:ALA:N	2.72	0.46
1:C:158:LEU:HD13	1:C:192:MET:CE	2.46	0.46
1:B:294:ASP:O	1:B:298:VAL:HG22	2.16	0.45
1:C:294:ASP:O	1:C:298:VAL:HG22	2.16	0.45
1:A:234:VAL:O	1:A:244:SER:HB2	2.16	0.45
1:C:165:HIS:O	1:C:166:ARG:C	2.58	0.45
1:A:71:HIS:HB2	2:A:501:FES:S1	2.56	0.45
1:A:237:GLU:O	1:A:239:THR:HG23	2.16	0.45
1:B:196:GLY:N	1:B:215:ASP:OD2	2.49	0.45
1:B:291:VAL:O	1:B:291:VAL:HG12	2.17	0.45
1:C:220:ILE:HA	1:C:230:ASN:HA	1.98	0.45
1:B:10:TYR:CZ	1:B:225:VAL:HG11	2.51	0.45
1:B:88:ASN:ND2	1:B:90:ALA:HB2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:SD	1:C:6:ARG:HD2	2.57	0.45
1:C:143:HIS:HE1	1:C:256:GLU:OE1	2.00	0.45
1:A:171:THR:HG22	1:A:173:ALA:H	1.82	0.45
1:A:212:THR:CG2	1:A:213:PRO:HD2	2.46	0.45
1:A:224:LYS:O	1:A:225:VAL:HB	2.17	0.45
1:B:36:ARG:NH1	5:B:1213:HOH:O	2.49	0.45
1:B:305:ARG:O	1:B:308:VAL:HG22	2.17	0.45
1:A:156:MET:HE2	1:A:156:MET:HA	1.99	0.44
1:A:305:ARG:O	1:A:308:VAL:HG22	2.16	0.44
1:B:163:TYR:O	1:B:166:ARG:HB2	2.17	0.44
1:C:213:PRO:O	1:C:214:VAL:HB	2.17	0.44
1:A:171:THR:CG2	1:A:173:ALA:HB3	2.47	0.44
1:A:315:PRO:HB2	1:A:317:MET:CE	2.46	0.44
1:C:210:ALA:O	1:C:211:ASN:ND2	2.49	0.44
1:B:10:TYR:CE2	1:B:225:VAL:HG11	2.52	0.44
1:B:276:PRO:O	1:B:279:ASP:HB2	2.17	0.44
1:A:215:ASP:H	1:A:239:THR:HG21	1.82	0.44
1:C:156:MET:HE2	1:C:156:MET:HA	2.00	0.44
1:A:119:ALA:O	1:A:120:ASP:CB	2.65	0.44
1:B:212:THR:O	1:B:213:PRO:C	2.59	0.44
1:B:289:ALA:HA	1:B:293:GLU:HB2	2.00	0.44
1:C:1:MET:HE1	1:C:6:ARG:NH1	2.32	0.44
1:B:208:ARG:HG2	1:B:208:ARG:HH11	1.83	0.44
1:B:217:TRP:CZ2	1:B:241:LYS:HB3	2.52	0.44
1:C:212:THR:HG22	1:C:214:VAL:HG12	2.00	0.44
1:C:223:ASN:ND2	5:C:736:HOH:O	2.46	0.44
1:B:212:THR:HG22	1:B:213:PRO:HD2	1.99	0.43
1:C:217:TRP:CZ2	1:C:241:LYS:HA	2.52	0.43
1:B:36:ARG:NE	5:B:769:HOH:O	2.38	0.43
1:B:121:PRO:C	1:B:123:ALA:N	2.75	0.43
1:B:179:ARG:HA	1:B:191:LEU:O	2.17	0.43
1:B:212:THR:CG2	1:B:213:PRO:HD2	2.47	0.43
1:B:224:LYS:O	1:B:225:VAL:HB	2.18	0.43
1:C:160:HIS:O	1:C:161:ALA:C	2.60	0.43
1:A:191:LEU:HB3	5:A:1099:HOH:O	2.17	0.43
1:A:330:GLU:CD	5:A:1135:HOH:O	2.61	0.43
1:C:156:MET:HE2	1:C:220:ILE:HD13	2.00	0.43
1:A:203:MET:HE1	1:A:232:ILE:HG22	2.01	0.43
1:C:211:ASN:HD22	1:C:211:ASN:HA	1.62	0.43
1:C:250:THR:O	1:C:265:PHE:HA	2.18	0.43
1:C:286:GLN:HA	1:C:290:LEU:CD2	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ALA:O	1:A:170:GLN:N	2.52	0.43
1:A:220:ILE:HA	1:A:230:ASN:HA	2.01	0.43
1:A:167:ALA:HA	1:A:170:GLN:CB	2.49	0.43
1:A:213:PRO:O	1:A:236:PRO:HA	2.19	0.43
1:B:195:PRO:O	1:B:196:GLY:C	2.61	0.43
1:A:175:ASP:CG	1:A:176:ARG:N	2.75	0.43
1:B:49:CYS:HA	1:B:50:PRO:HD3	1.86	0.43
1:B:220:ILE:HA	1:B:230:ASN:HA	2.01	0.43
1:C:135:TYR:HA	1:C:269:ARG:O	2.19	0.43
1:A:49:CYS:HA	1:A:50:PRO:HD3	1.85	0.43
1:A:214:VAL:HG12	1:A:236:PRO:CA	2.49	0.43
1:B:326:ARG:NE	5:B:890:HOH:O	2.51	0.43
1:B:223:ASN:ND2	5:B:721:HOH:O	2.51	0.42
1:C:292:LYS:HD2	5:C:1205:HOH:O	2.19	0.42
1:A:176:ARG:N	1:A:177:LEU:HD12	2.34	0.42
1:B:27:ILE:HD12	1:B:254:THR:CG2	2.48	0.42
1:A:235:ALA:HB2	1:A:244:SER:HB3	2.02	0.42
1:A:263:TYR:HD1	1:A:290:LEU:HD13	1.83	0.42
1:B:36:ARG:NH2	5:B:769:HOH:O	2.50	0.42
1:C:224:LYS:O	1:C:225:VAL:HB	2.19	0.42
1:B:214:VAL:HG21	1:B:234:VAL:HG22	2.02	0.42
1:A:166:ARG:NE	5:A:1085:HOH:O	2.53	0.42
1:A:171:THR:HG22	1:A:173:ALA:N	2.35	0.42
1:B:25:ARG:HD2	1:B:262:HIS:CE1	2.55	0.42
1:B:322:GLU:OE2	1:B:326:ARG:CZ	2.68	0.42
1:C:341:ARG:HD3	5:C:1144:HOH:O	2.19	0.42
1:A:207:LEU:O	1:A:208:ARG:C	2.62	0.42
1:A:225:VAL:HB	5:A:925:HOH:O	2.19	0.42
1:C:233:ALA:CB	1:C:246:HIS:HB3	2.47	0.42
1:B:36:ARG:NH1	1:B:36:ARG:HB2	2.35	0.42
1:A:205:LYS:O	1:A:205:LYS:HG3	2.19	0.42
1:A:276:PRO:O	1:A:279:ASP:HB2	2.20	0.42
1:A:330:GLU:CG	5:A:1135:HOH:O	2.65	0.42
1:A:28:LEU:HD23	1:A:28:LEU:N	2.34	0.41
1:B:151:LEU:HD23	1:B:151:LEU:HA	1.87	0.41
1:B:236:PRO:O	1:B:239:THR:HG23	2.20	0.41
1:B:282:LEU:HD13	5:B:766:HOH:O	2.20	0.41
1:C:321:ASP:O	1:C:325:VAL:HG23	2.20	0.41
1:A:36:ARG:NH1	5:A:832:HOH:O	2.53	0.41
1:B:112:TRP:CD2	1:B:119:ALA:HA	2.56	0.41
1:B:166:ARG:HB2	1:B:166:ARG:HE	1.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:LEU:HG	1:C:234:VAL:HG11	2.02	0.41
1:A:204:ALA:C	1:A:206:PHE:H	2.29	0.41
1:A:224:LYS:HE3	1:A:334:LEU:HD22	2.03	0.41
1:B:342:LEU:H	1:B:342:LEU:HD23	1.83	0.41
1:B:342:LEU:HD23	1:B:342:LEU:N	2.35	0.41
1:A:237:GLU:HG3	1:A:238:GLY:H	1.81	0.41
1:A:283:ARG:HG2	1:A:283:ARG:HH11	1.86	0.41
1:A:304:ARG:NH2	1:C:55:PRO:HB3	2.36	0.41
1:A:136:ARG:NH2	1:A:279:ASP:OD1	2.50	0.41
1:A:166:ARG:O	1:A:170:GLN:CB	2.55	0.41
1:A:198:THR:O	1:A:198:THR:HG22	2.21	0.41
1:B:137:THR:HA	1:B:267:SER:O	2.21	0.41
1:B:156:MET:CE	1:B:220:ILE:HD13	2.51	0.41
1:B:214:VAL:HG23	1:B:235:ALA:C	2.46	0.41
1:C:223:ASN:O	1:C:224:LYS:C	2.64	0.41
1:C:305:ARG:O	1:C:308:VAL:HG22	2.19	0.41
1:A:283:ARG:NH2	5:A:806:HOH:O	2.54	0.41
1:C:28:LEU:N	1:C:28:LEU:HD23	2.36	0.41
1:C:224:LYS:HE3	1:C:334:LEU:HD22	2.03	0.40
1:C:242:GLU:HG3	1:C:243:GLN:NE2	2.22	0.40
1:A:176:ARG:C	1:A:177:LEU:HD12	2.45	0.40
1:C:285:TRP:CZ3	1:C:289:ALA:HB2	2.57	0.40
1:A:237:GLU:C	1:A:239:THR:N	2.78	0.40
1:B:315:PRO:HB2	1:B:317:MET:CE	2.51	0.40
1:B:329:ARG:O	1:B:333:LYS:HG3	2.21	0.40
1:C:194:ILE:HB	1:C:216:ALA:CB	2.46	0.40
1:C:304:ARG:HH11	1:C:304:ARG:HG3	1.86	0.40
1:C:322:GLU:OE2	1:C:326:ARG:CZ	2.70	0.40
1:B:214:VAL:CG2	1:B:235:ALA:C	2.95	0.40
1:B:239:THR:HA	1:B:240:PRO:HD3	1.92	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	340/349 (97%)	308 (91%)	19 (6%)	13 (4%)	2	0
1	B	339/349 (97%)	314 (93%)	21 (6%)	4 (1%)	10	4
1	C	340/349 (97%)	298 (88%)	26 (8%)	16 (5%)	2	0
All	All	1019/1047 (97%)	920 (90%)	66 (6%)	33 (3%)	3	0

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	ALA
1	A	166	ARG
1	A	225	VAL
1	B	196	GLY
1	B	225	VAL
1	C	119	ALA
1	C	199	PRO
1	C	214	VAL
1	C	225	VAL
1	C	237	GLU
1	A	210	ALA
1	A	240	PRO
1	A	241	LYS
1	C	236	PRO
1	A	224	LYS
1	A	237	GLU
1	B	224	LYS
1	B	237	GLU
1	C	2	ALA
1	C	195	PRO
1	C	200	SER
1	C	216	ALA
1	C	224	LYS
1	A	120	ASP
1	A	211	ASN
1	C	120	ASP
1	C	166	ARG
1	C	202	LEU
1	A	178	GLU
1	A	208	ARG
1	C	168	ASN

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Mol	Chain	Res	Type
1	A	239	THR
1	C	238	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	277/284 (98%)	274 (99%)	3 (1%)	65	68
1	B	276/284 (97%)	275 (100%)	1 (0%)	84	88
1	C	277/284 (98%)	270 (98%)	7 (2%)	42	39
All	All	830/852 (97%)	819 (99%)	11 (1%)	61	63

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ARG
1	A	28	LEU
1	A	177	LEU
1	B	28	LEU
1	C	25	ARG
1	C	28	LEU
1	C	174	PHE
1	C	199	PRO
1	C	211	ASN
1	C	212	THR
1	C	292	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	88	ASN
1	A	143	HIS
1	A	154	ASN

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Mol	Chain	Res	Type
1	A	168	ASN
1	A	170	GLN
1	A	211	ASN
1	A	336	GLN
1	B	80	GLN
1	B	88	ASN
1	B	143	HIS
1	B	168	ASN
1	B	211	ASN
1	B	223	ASN
1	B	336	GLN
1	C	80	GLN
1	C	143	HIS
1	C	170	GLN
1	C	211	ASN
1	C	223	ASN
1	C	243	GLN
1	C	336	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 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	FES	B	501	1	0,4,4	-	-	-		
2	FES	A	501	1	0,4,4	-	-	-		
4	HXX	A	601	-	12,12,12	3.14	7 (58%)	17,17,17	1.41	3 (17%)
4	HXX	C	601	-	12,12,12	3.04	7 (58%)	17,17,17	1.43	3 (17%)
4	HXX	B	601	-	12,12,12	3.08	7 (58%)	17,17,17	1.42	3 (17%)
2	FES	C	501	1	0,4,4	-	-	-		

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
2	FES	B	501	1	-	-	0/1/1/1
2	FES	A	501	1	-	-	0/1/1/1
4	HXX	A	601	-	-	0/4/4/4	0/1/1/1
4	HXX	C	601	-	-	0/4/4/4	0/1/1/1
4	HXX	B	601	-	-	0/4/4/4	0/1/1/1
2	FES	C	501	1	-	-	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	HXX	C1-C6	6.20	1.49	1.39
4	C	601	HXX	C1-C6	6.07	1.48	1.39
4	B	601	HXX	C1-C6	5.63	1.48	1.39
4	B	601	HXX	C2-C3	5.59	1.48	1.39
4	A	601	HXX	C2-C3	5.42	1.47	1.39
4	C	601	HXX	C2-C3	5.10	1.47	1.39
4	B	601	HXX	C1-C2	3.71	1.48	1.41
4	A	601	HXX	C1-C2	3.65	1.48	1.41
4	C	601	HXX	C1-C2	3.64	1.48	1.41
4	B	601	HXX	O2-C2	3.06	1.43	1.36
4	A	601	HXX	C4-C3	3.03	1.45	1.38
4	B	601	HXX	C4-C3	3.02	1.45	1.38
4	C	601	HXX	C4-C3	2.98	1.44	1.38
4	A	601	HXX	O2-C2	2.89	1.43	1.36
4	C	601	HXX	O2-C2	2.72	1.43	1.36
4	C	601	HXX	C5-C4	2.70	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	HXX	C5-C6	2.65	1.44	1.38
4	A	601	HXX	C5-C4	2.65	1.43	1.38
4	A	601	HXX	C5-C6	2.62	1.44	1.38
4	B	601	HXX	C5-C4	2.59	1.43	1.38
4	C	601	HXX	C5-C6	2.48	1.43	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	601	HXX	C1-C6-CL2	3.01	123.50	119.62
4	B	601	HXX	C2-C3-CL1	2.96	122.48	118.81
4	A	601	HXX	C1-C6-CL2	2.93	123.40	119.62
4	A	601	HXX	C2-C3-CL1	2.87	122.38	118.81
4	C	601	HXX	C2-C3-CL1	2.86	122.36	118.81
4	B	601	HXX	C1-C6-CL2	2.71	123.11	119.62
4	A	601	HXX	C4-C3-C2	-2.41	119.62	121.82
4	C	601	HXX	C4-C3-C2	-2.40	119.63	121.82
4	B	601	HXX	C4-C3-C2	-2.39	119.64	121.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	FES	1	0
2	A	501	FES	1	0
2	C	501	FES	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	342/349 (97%)	0.54	31 (9%)	15 15	25, 39, 80, 90	0
1	B	341/349 (97%)	0.49	22 (6%)	25 24	26, 40, 74, 86	0
1	C	342/349 (97%)	0.73	53 (15%)	5 4	26, 43, 85, 90	0
All	All	1025/1047 (97%)	0.59	106 (10%)	12 11	25, 41, 81, 90	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	239	THR	7.8
1	C	213	PRO	5.9
1	C	214	VAL	5.8
1	A	210	ALA	5.7
1	C	210	ALA	5.7
1	C	342	LEU	5.3
1	C	174	PHE	5.2
1	C	240	PRO	5.1
1	A	172	ASP	5.0
1	A	169	ALA	4.9
1	A	238	GLY	4.8
1	C	198	THR	4.6
1	B	240	PRO	4.4
1	A	211	ASN	4.4
1	A	173	ALA	4.4
1	A	174	PHE	4.3
1	A	342	LEU	4.3
1	B	2	ALA	4.2
1	A	177	LEU	4.2
1	B	342	LEU	4.1
1	A	212	THR	4.0
1	A	170	GLN	4.0
1	C	167	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	212	THR	3.7
1	C	199	PRO	3.7
1	A	312	GLY	3.7
1	C	238	GLY	3.6
1	C	169	ALA	3.6
1	C	225	VAL	3.6
1	A	1	MET	3.5
1	C	1	MET	3.5
1	B	180	GLU	3.5
1	B	270	ASN	3.5
1	B	204	ALA	3.4
1	C	241	LYS	3.4
1	A	197	GLY	3.4
1	A	119	ALA	3.4
1	C	209	GLY	3.4
1	B	200	SER	3.3
1	A	240	PRO	3.3
1	C	2	ALA	3.3
1	B	239	THR	3.3
1	A	214	VAL	3.2
1	C	239	THR	3.2
1	B	225	VAL	3.2
1	C	216	ALA	3.2
1	A	167	ALA	3.1
1	C	206	PHE	3.1
1	C	207	LEU	3.0
1	C	176	ARG	3.0
1	B	177	LEU	3.0
1	A	209	GLY	2.9
1	C	234	VAL	2.9
1	C	193	LYS	2.9
1	C	203	MET	2.8
1	A	341	ARG	2.8
1	A	339	ALA	2.8
1	B	245	ILE	2.8
1	B	192	MET	2.6
1	B	211	ASN	2.6
1	C	217	TRP	2.6
1	C	194	ILE	2.6
1	C	242	GLU	2.5
1	B	210	ALA	2.5
1	C	173	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	289	ALA	2.5
1	C	281	VAL	2.5
1	C	337	LEU	2.5
1	A	168	ASN	2.5
1	A	285	TRP	2.5
1	C	211	ASN	2.5
1	C	273	ILE	2.5
1	C	195	PRO	2.4
1	C	200	SER	2.4
1	B	195	PRO	2.4
1	A	175	ASP	2.4
1	A	236	PRO	2.4
1	C	177	LEU	2.4
1	B	291	VAL	2.4
1	C	208	ARG	2.4
1	C	340	ALA	2.3
1	A	88	ASN	2.3
1	B	157	ASP	2.3
1	C	320	CYS	2.3
1	C	287	ALA	2.3
1	A	207	LEU	2.3
1	C	274	ASP	2.3
1	B	273	ILE	2.3
1	C	171	THR	2.2
1	C	270	ASN	2.2
1	C	39	ASP	2.2
1	C	201	VAL	2.1
1	B	272	GLY	2.1
1	B	191	LEU	2.1
1	C	290	LEU	2.1
1	C	215	ASP	2.1
1	B	340	ALA	2.1
1	C	119	ALA	2.1
1	A	270	ASN	2.1
1	A	171	THR	2.1
1	C	204	ALA	2.1
1	C	339	ALA	2.1
1	B	213	PRO	2.0
1	C	312	GLY	2.0
1	C	170	GLN	2.0
1	A	198	THR	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
4	HXX	A	601	12/12	0.47	0.20	87,89,89,89	0
4	HXX	C	601	12/12	0.72	0.13	73,75,76,77	0
4	HXX	B	601	12/12	0.74	0.13	47,52,53,54	0
3	CO	B	602	1/1	0.90	0.08	64,64,64,64	0
3	CO	C	603	1/1	0.94	0.07	70,70,70,70	0
3	CO	A	602	1/1	0.95	0.09	55,55,55,55	0
3	CO	C	604	1/1	0.96	0.10	76,76,76,76	0
3	CO	C	502	1/1	0.96	0.08	54,54,54,54	0
2	FES	B	501	4/4	0.98	0.04	33,35,35,37	0
2	FES	A	501	4/4	0.99	0.03	28,29,30,31	0
3	CO	B	502	1/1	0.99	0.04	41,41,41,41	0
2	FES	C	501	4/4	0.99	0.03	28,28,29,29	0
3	CO	A	502	1/1	0.99	0.02	36,36,36,36	0
3	CO	C	602	1/1	0.99	0.06	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.