



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:14 PM UTC

PDB ID : 3H9Q / pdb_00003h9q
Title : Crystal structure of E. coli MccB + SeMet MccA
Authors : Regni, C.A.; Roush, R.F.; Miller, D.; Nourse, A.; Walsh, C.T.; Schulman, B.A.
Deposited on : 2009-04-30
Resolution : 2.63 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:

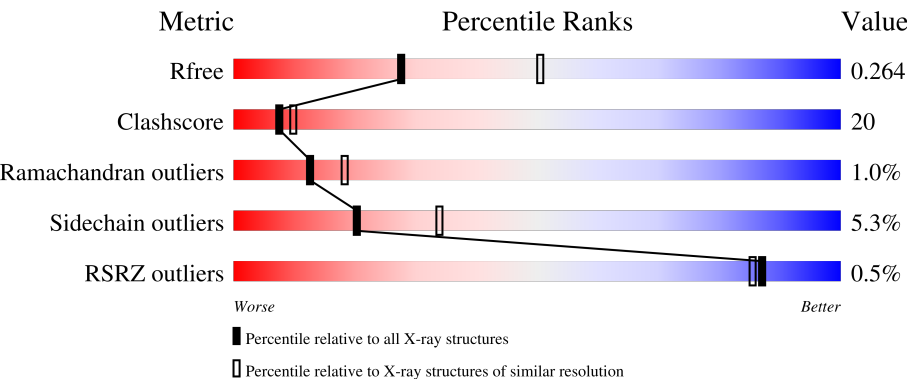
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.63 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.



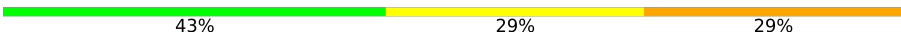
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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	353	64%29%5%
1	B	353	58%33%6%
1	C	353	66%30%. .
1	D	353	%58%31%5%6%
2	E	7	29% 14%43%14%29%

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Mol	Chain	Length	Quality of chain
2	F	7	
2	G	7	
2	H	7	

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
4	SO4	B	359	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10565 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 MccB protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2579	1649	442	477	11			
1	B	333	Total	C	N	O	S	0	0	0
			2553	1635	431	476	11			
1	C	343	Total	C	N	O	S	0	1	0
			2636	1685	446	494	11			
1	D	333	Total	C	N	O	S	0	1	0
			2526	1614	425	476	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q47506
A	-1	SER	-	expression tag	UNP Q47506
A	0	HIS	-	expression tag	UNP Q47506
B	-2	GLY	-	expression tag	UNP Q47506
B	-1	SER	-	expression tag	UNP Q47506
B	0	HIS	-	expression tag	UNP Q47506
C	-2	GLY	-	expression tag	UNP Q47506
C	-1	SER	-	expression tag	UNP Q47506
C	0	HIS	-	expression tag	UNP Q47506
D	-2	GLY	-	expression tag	UNP Q47506
D	-1	SER	-	expression tag	UNP Q47506
D	0	HIS	-	expression tag	UNP Q47506

- Molecule 2 is a protein called Microcin C7 ANALOG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	5	Total	C	N	O	Se	0	0	0
			36	20	9	6	1			
2	F	2	Total	C	N	O	Se	0	0	0
			19	11	5	2	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	7	Total	C	N	O	Se	0	0	0
			52	28	12	11	1			
2	H	2	Total	C	N	O	Se	1	0	1
			9	5	2	1	1			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

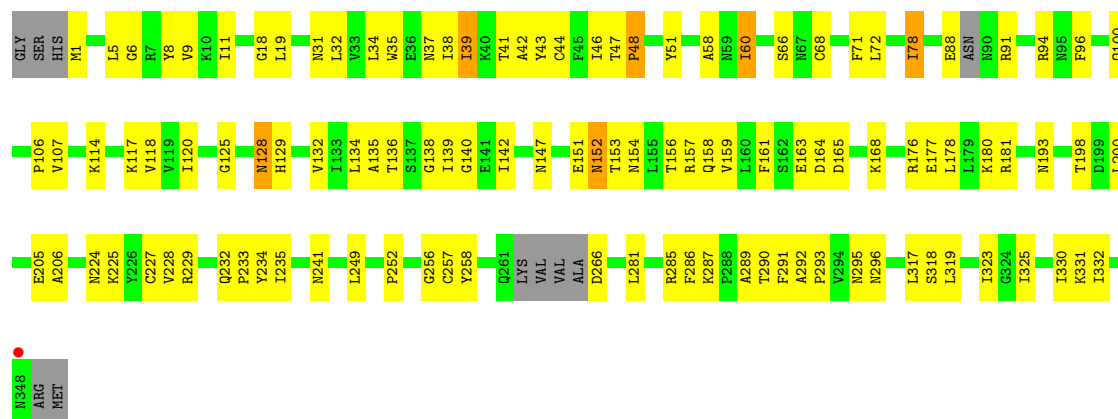
- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



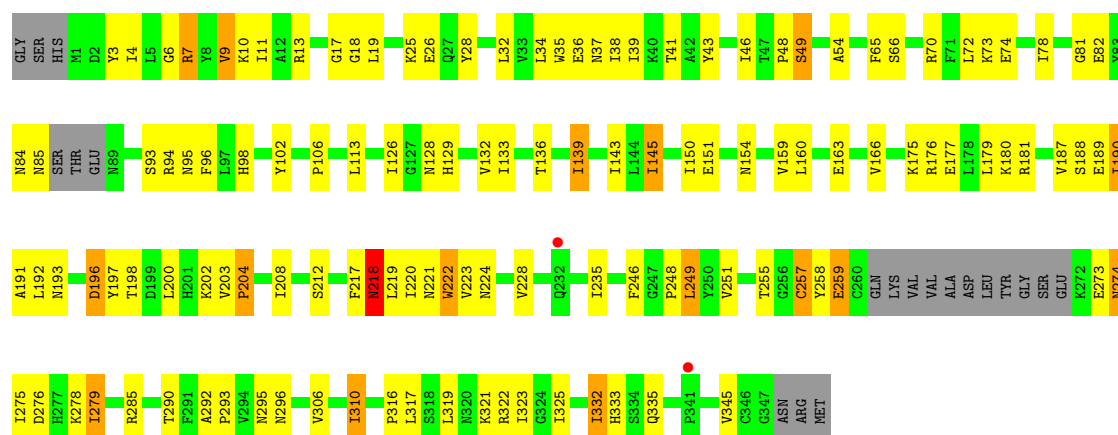
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

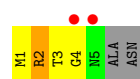
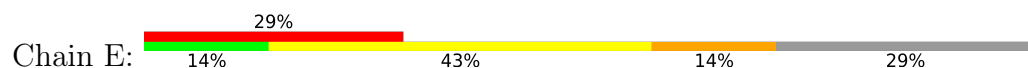
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	40	Total 40	O 40	0	0
5	B	39	Total 39	O 39	0	0
5	C	36	Total 36	O 36	0	0
5	D	23	Total 23	O 23	0	0
5	F	1	Total 1	O 1	0	0
5	G	2	Total 2	O 2	0	0



• Molecule 1: MccB protein



• Molecule 2: Microcin C7 ANALOG



• Molecule 2: Microcin C7 ANALOG



• Molecule 2: Microcin C7 ANALOG



• Molecule 2: Microcin C7 ANALOG



M1	R2	THR	GLY	ASN	ALA	ASN
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.30Å 138.60Å 81.38Å 90.00° 92.06° 90.00°	Depositor
Resolution (Å)	20.00 – 2.63 20.00 – 2.63	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.63) 99.7 (20.00-2.63)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.87 (at 2.63Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.207 , 0.273 0.199 , 0.264	Depositor DCC
R_{free} test set	1867 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	48.2	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 29.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.040 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10565	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.49	0/2632	0.94	4/3579 (0.1%)
1	B	0.50	0/2606	0.96	9/3543 (0.3%)
1	C	0.52	0/2696	0.96	7/3665 (0.2%)
1	D	0.46	0/2583	0.95	4/3519 (0.1%)
2	E	0.68	0/35	1.03	0/44
2	F	1.08	0/18	1.58	0/21
2	G	0.79	0/51	2.03	2/65 (3.1%)
2	H	2.61	1/8 (12.5%)	3.85	2/9 (22.2%)
All	All	0.50	1/10629 (0.0%)	0.96	28/14445 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	MSE	C-N	-5.92	1.25	1.33

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	6	ALA	N-CA-C	9.84	124.11	110.24
2	H	1	MSE	CB-CG-SE	-9.26	84.91	112.70
1	B	46	ILE	N-CA-C	-8.96	101.82	110.42
2	G	4	GLY	N-CA-C	-7.51	103.29	111.93
2	H	1	MSE	CG-SE-CE	6.43	113.07	98.92
1	C	256	GLY	N-CA-C	-6.18	103.13	112.89
1	C	140	GLY	N-CA-C	6.02	121.29	114.67
1	B	140	GLY	N-CA-C	6.01	119.92	112.64
1	A	77	PHE	N-CA-C	-5.88	105.59	112.89
1	B	145	ILE	N-CA-C	5.74	116.13	107.80
1	B	203	VAL	N-CA-C	5.72	114.18	107.77
1	C	200	LEU	N-CA-C	5.68	118.20	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	331	LYS	N-CA-C	5.59	116.89	108.46
1	C	78	ILE	N-CA-C	-5.58	100.45	108.48
1	D	9	VAL	N-CA-C	5.51	115.25	106.88
1	C	323	ILE	N-CA-C	5.41	116.09	108.36
1	D	321	LYS	N-CA-C	5.38	117.57	109.23
1	B	47	THR	N-CA-C	-5.27	102.36	110.32
1	A	251	VAL	CA-C-N	5.24	126.39	119.84
1	A	251	VAL	C-N-CA	5.24	126.39	119.84
1	D	296	ASN	N-CA-C	5.21	116.96	111.28
1	B	292	ALA	CA-C-N	-5.18	113.41	119.32
1	B	292	ALA	C-N-CA	-5.18	113.41	119.32
1	C	331	LYS	N-CA-C	5.15	116.89	108.55
1	C	318	SER	N-CA-C	5.12	119.16	113.02
1	A	159	VAL	N-CA-C	5.07	119.89	109.34
1	B	318	SER	N-CA-C	5.07	118.61	112.93
1	D	145	ILE	N-CA-C	5.00	113.96	106.85

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	2579	0	2508	98	0
1	B	2553	0	2480	123	0
1	C	2636	0	2555	103	0
1	D	2526	0	2415	138	0
2	E	36	0	35	3	0
2	F	19	0	24	8	0
2	G	52	0	51	10	0
2	H	9	0	11	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	B	10	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	40	0	0	3	0
5	B	39	0	0	6	0
5	C	36	0	0	5	0
5	D	23	0	0	2	0
5	F	1	0	0	0	0
5	G	2	0	0	0	0
All	All	10565	0	10079	416	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 20.

All (416) 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:11:ILE:HD11	1:B:279:ILE:HG23	1.20	1.19
1:B:322:ARG:NH1	2:F:1:MSE:HB2	1.62	1.12
1:B:322:ARG:HH12	2:F:1:MSE:HB2	1.17	1.03
1:C:232[A]:GLN:CG	5:C:369:HOH:O	2.06	1.01
1:C:157:ARG:HD3	1:C:290:THR:HB	1.50	0.94
1:C:156:THR:HG21	1:D:95:ASN:HD21	1.34	0.92
1:D:113:LEU:HA	1:D:310:ILE:HD11	1.53	0.91
1:B:156:THR:HG23	1:B:157:ARG:HG3	1.57	0.87
1:D:11:ILE:HD13	1:D:39:ILE:HD13	1.56	0.87
1:B:124:GLY:HA3	4:B:359:SO4:O1	1.75	0.87
1:A:275:ILE:HD11	1:B:40:LYS:HE3	1.55	0.87
1:C:132:VAL:HG11	1:D:159:VAL:HG23	1.57	0.85
1:D:113:LEU:HD23	1:D:310:ILE:HD11	1.58	0.83
1:A:153:THR:HB	1:B:94:ARG:HD3	1.58	0.83
1:A:41:THR:HG22	1:A:65:PHE:CD1	2.13	0.83
1:B:251:VAL:HG11	1:B:254:LYS:HE3	1.59	0.83
1:C:325:ILE:HG12	1:C:332:ILE:HD12	1.61	0.82
1:B:119:VAL:HG22	1:B:143:ILE:HB	1.61	0.81
1:B:322:ARG:HH12	2:F:1:MSE:CB	1.93	0.81
1:A:189:GLU:O	1:A:190:ILE:HD12	1.81	0.81
1:D:335:GLN:HG3	2:H:1:MSE:HE3	1.63	0.81
1:B:27:GLN:HE22	1:B:75:ASN:HD21	1.30	0.79
1:A:11:ILE:CD1	1:B:279:ILE:HG23	2.08	0.79
1:C:46:ILE:HG23	1:D:285:ARG:HH11	1.49	0.78
1:C:157:ARG:HH12	1:D:94:ARG:HH11	1.33	0.77
1:C:6:GLY:O	1:C:9:VAL:HG12	1.86	0.76
1:A:211:VAL:HG21	1:A:223:VAL:HG11	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ILE:HG23	1:B:39:ILE:HD11	1.68	0.76
1:A:11:ILE:HD11	1:B:279:ILE:CG2	2.08	0.75
1:A:120:ILE:HD12	1:A:131:SER:HB3	1.68	0.75
1:B:27:GLN:HE22	1:B:75:ASN:ND2	1.85	0.75
1:A:152:ASN:H	1:A:152:ASN:HD22	1.33	0.74
1:D:11:ILE:HD13	1:D:39:ILE:CD1	2.16	0.73
1:C:134:LEU:HD22	1:C:139:ILE:HD12	1.70	0.73
1:A:189:GLU:C	1:A:190:ILE:HD12	2.13	0.72
1:C:34:LEU:O	1:C:38:ILE:HG12	1.89	0.72
1:C:94:ARG:HD2	1:D:290:THR:HG21	1.72	0.72
1:C:157:ARG:HH12	1:D:94:ARG:NH1	1.87	0.72
1:D:197:TYR:CB	1:D:222:TRP:HE1	2.03	0.71
1:C:19:LEU:HD12	1:C:19:LEU:O	1.91	0.71
1:D:18:GLY:HA3	1:D:35:TRP:CE2	2.25	0.70
1:B:206:ALA:H	1:B:232:GLN:HE22	1.38	0.69
1:C:163:GLU:HG3	1:D:180:LYS:O	1.92	0.69
1:D:18:GLY:HA3	1:D:35:TRP:NE1	2.08	0.69
1:C:39:ILE:O	1:C:39:ILE:HD12	1.93	0.69
1:A:156:THR:HG21	1:B:95:ASN:HD21	1.56	0.69
1:A:41:THR:HG21	1:A:68:CYS:HB2	1.74	0.69
1:A:165:ASP:HA	1:A:168:LYS:HD2	1.76	0.68
1:B:60:ILE:HD11	1:B:65:PHE:CD1	2.29	0.68
1:D:26:GLU:OE2	2:G:2:ARG:HB3	1.94	0.67
1:A:119:VAL:HG22	1:A:143:ILE:HB	1.75	0.67
1:A:163:GLU:O	1:A:166:VAL:HG23	1.94	0.67
1:A:332:ILE:HG22	1:B:332:ILE:HG22	1.76	0.67
1:B:60:ILE:HD13	1:B:60:ILE:H	1.60	0.67
1:A:162:SER:HB3	5:B:390:HOH:O	1.94	0.67
1:A:175:LYS:HG3	1:A:187:VAL:HB	1.77	0.66
1:D:235:ILE:HB	1:D:249:LEU:HD22	1.78	0.66
1:D:9:VAL:HG23	1:D:9:VAL:O	1.94	0.66
1:D:70:ARG:O	1:D:74:GLU:HG3	1.95	0.66
1:D:13:ARG:HD2	1:D:17:GLY:O	1.95	0.66
1:D:151:GLU:H	1:D:154:ASN:HD22	1.43	0.66
1:D:335:GLN:CG	2:H:1:MSE:HE3	2.26	0.65
1:B:248:PRO:HG3	1:B:337:MET:HE2	1.78	0.65
1:A:145:ILE:CD1	1:A:203:VAL:HG13	2.27	0.65
1:D:34:LEU:O	1:D:38:ILE:HG13	1.96	0.65
1:C:292:ALA:HB3	1:C:293:PRO:HD3	1.80	0.64
1:B:107:VAL:HG23	5:B:396:HOH:O	1.97	0.64
1:C:18:GLY:HA3	1:C:35:TRP:CE2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ASN:O	1:A:132:VAL:HG23	1.97	0.64
1:D:196:ASP:HA	1:D:222:TRP:CH2	2.32	0.64
1:A:192:LEU:HD12	1:A:193:ASN:H	1.63	0.64
1:A:275:ILE:O	1:A:279:ILE:HG12	1.97	0.64
2:G:4:GLY:O	2:G:5:ASN:C	2.41	0.64
1:C:46:ILE:CG2	1:D:285:ARG:HH11	2.11	0.63
1:B:157:ARG:HG3	1:B:157:ARG:HH11	1.62	0.63
1:C:58:ALA:HB1	1:C:60:ILE:CD1	2.27	0.63
1:A:32:LEU:HG	1:A:36:GLU:OE2	1.99	0.63
1:C:128:ASN:O	1:C:132:VAL:HG23	1.98	0.63
1:D:113:LEU:HD23	1:D:310:ILE:CD1	2.27	0.63
1:C:58:ALA:HB1	1:C:60:ILE:HD12	1.78	0.63
1:C:224:ASN:ND2	1:C:258:TYR:H	1.96	0.63
1:D:10:LYS:HZ3	2:G:6:ALA:HB2	1.63	0.63
1:C:225:LYS:HE3	1:C:229:ARG:HH21	1.63	0.63
1:A:250:TYR:HA	1:A:255:THR:HG21	1.80	0.62
1:A:132:VAL:HG11	1:B:159:VAL:HG23	1.82	0.62
1:B:146:ASP:OD1	1:B:147:ASN:N	2.33	0.62
1:A:11:ILE:C	1:A:11:ILE:HD12	2.25	0.62
1:B:117:LYS:O	1:B:206:ALA:HB1	1.99	0.61
1:B:322:ARG:HD3	5:B:398:HOH:O	2.00	0.61
1:C:285:ARG:O	1:D:7:ARG:HG3	2.00	0.61
1:B:224:ASN:ND2	1:B:257:CYS:HB2	2.15	0.61
1:C:43:TYR:CG	1:D:278:LYS:HD3	2.36	0.61
1:D:335:GLN:HG3	2:H:1:MSE:CE	2.31	0.61
1:D:4:ILE:CD1	1:D:48:PRO:HG3	2.31	0.61
1:C:72:LEU:HB3	1:C:78:ILE:HG23	1.83	0.61
1:C:176:ARG:NH1	1:C:177:GLU:OE2	2.33	0.61
1:C:224:ASN:O	1:C:228:VAL:HG23	2.00	0.61
1:A:147:ASN:OD1	1:A:191:ALA:HB1	1.99	0.61
1:C:107:VAL:HG23	5:C:361:HOH:O	2.00	0.61
1:D:128:ASN:O	1:D:132:VAL:HG23	2.01	0.61
1:C:286:PHE:CE1	1:D:10:LYS:HG3	2.36	0.61
1:D:133:ILE:O	1:D:136:THR:HG22	2.00	0.61
1:C:286:PHE:CE2	2:G:6:ALA:HB1	2.36	0.60
1:B:255:THR:HB	1:B:320:ASN:OD1	2.02	0.60
1:C:152:ASN:N	1:C:152:ASN:HD22	1.98	0.60
1:A:152:ASN:HD22	1:A:152:ASN:N	1.99	0.60
1:C:156:THR:HG21	1:D:95:ASN:ND2	2.11	0.60
1:A:90:ASN:ND2	1:A:92:TYR:H	2.00	0.60
5:A:399:HOH:O	1:B:94:ARG:NH1	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:GLU:HA	1:D:166:VAL:HG23	1.83	0.59
1:C:120:ILE:HD13	1:C:142:ILE:HG23	1.82	0.59
1:B:117:LYS:HG2	1:B:141:GLU:OE1	2.03	0.59
1:C:281:LEU:HD23	1:D:43:TYR:CE1	2.36	0.59
1:B:37:ASN:O	1:B:41:THR:HG23	2.02	0.59
1:A:126:ILE:HB	1:A:212:SER:HB2	1.84	0.58
1:A:132:VAL:HG22	1:A:160:LEU:HD11	1.86	0.58
5:A:368:HOH:O	1:B:94:ARG:HG3	2.02	0.58
1:C:132:VAL:O	1:C:136:THR:HG23	2.04	0.58
1:C:134:LEU:HD22	1:C:139:ILE:CD1	2.32	0.58
1:D:316:PRO:HD2	1:D:319:LEU:HD11	1.85	0.58
1:D:323:ILE:CG2	1:D:332:ILE:HD11	2.34	0.58
1:A:224:ASN:HD21	1:A:257:CYS:HB2	1.69	0.57
1:B:173:VAL:HG13	1:B:176:ARG:NH2	2.18	0.57
1:D:145:ILE:CD1	1:D:203:VAL:HG13	2.35	0.57
1:A:105:ASN:HB3	1:A:108:LEU:HB2	1.87	0.57
1:B:95:ASN:N	1:B:95:ASN:HD22	2.03	0.57
1:C:286:PHE:CZ	2:G:6:ALA:HB1	2.39	0.57
1:B:224:ASN:HD21	1:B:257:CYS:CB	2.18	0.57
1:B:1:MET:HA	5:B:391:HOH:O	2.04	0.56
1:B:224:ASN:HD21	1:B:257:CYS:HB2	1.70	0.56
1:A:255:THR:HG23	1:A:256:GLY:O	2.05	0.56
1:C:151:GLU:H	1:C:154:ASN:ND2	2.02	0.56
1:D:259:GLU:HG2	1:D:345:VAL:HG21	1.87	0.56
1:B:37:ASN:HD22	1:B:64:ASP:HB3	1.70	0.56
1:C:296:ASN:HD22	1:C:296:ASN:N	2.03	0.56
1:A:7:ARG:NH2	1:B:287:LYS:HD3	2.20	0.56
1:B:235:ILE:HB	1:B:249:LEU:HD13	1.88	0.56
1:D:217:PHE:CG	1:D:218:ASN:N	2.74	0.56
1:D:143:ILE:HD12	1:D:143:ILE:N	2.20	0.55
1:D:196:ASP:HA	1:D:222:TRP:CZ2	2.41	0.55
1:A:275:ILE:HD12	1:B:36:GLU:HG2	1.88	0.55
1:B:187:VAL:HG12	1:B:188:SER:N	2.20	0.55
1:C:330:ILE:HG23	1:D:332:ILE:HD12	1.87	0.55
1:C:117:LYS:O	1:C:206:ALA:HB1	2.06	0.55
1:A:133:ILE:HD11	1:B:296:ASN:OD1	2.07	0.55
1:B:126:ILE:HD12	1:B:126:ILE:N	2.22	0.55
1:D:4:ILE:HD12	1:D:84:ASN:HB2	1.89	0.54
1:A:292:ALA:HB3	1:A:293:PRO:HD3	1.89	0.54
1:B:134:LEU:HB3	1:B:139:ILE:HG13	1.90	0.54
1:D:4:ILE:HG12	1:D:48:PRO:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ALA:H	1:A:232:GLN:HE22	1.54	0.54
1:A:122:GLY:HA3	1:A:213:ALA:HB2	1.90	0.54
1:B:154:ASN:HB3	1:B:158:GLN:NE2	2.22	0.54
1:C:96:PHE:CD2	1:C:106:PRO:HB2	2.43	0.54
1:B:126:ILE:HB	1:B:212:SER:OG	2.08	0.54
1:B:131:SER:OG	1:B:178:LEU:HD11	2.08	0.53
1:D:306:VAL:O	1:D:310:ILE:HG23	2.08	0.53
1:C:281:LEU:HD23	1:D:43:TYR:HE1	1.73	0.53
1:D:197:TYR:N	1:D:222:TRP:CZ2	2.77	0.53
1:A:129:HIS:O	1:A:133:ILE:HG12	2.09	0.53
1:B:44:CYS:SG	1:B:58:ALA:HB2	2.49	0.53
1:D:275:ILE:O	1:D:279:ILE:HG23	2.09	0.53
1:C:37:ASN:O	1:C:41:THR:HG23	2.09	0.53
1:D:292:ALA:HB3	1:D:293:PRO:HD3	1.89	0.53
1:B:322:ARG:HH12	2:F:1:MSE:C	2.16	0.53
1:C:164:ASP:O	1:C:168:LYS:HE3	2.08	0.53
1:D:93:SER:O	1:D:96:PHE:HB2	2.08	0.53
1:B:27:GLN:NE2	1:B:75:ASN:ND2	2.56	0.53
1:B:335:GLN:HG2	2:F:1:MSE:HE3	1.91	0.53
1:C:147:ASN:H	1:C:193:ASN:ND2	2.07	0.53
1:A:94:ARG:HG2	1:B:153:THR:OG1	2.08	0.52
1:A:275:ILE:HG23	1:B:39:ILE:CD1	2.37	0.52
1:C:31:ASN:HD22	1:C:34:LEU:HB2	1.73	0.52
1:A:251:VAL:H	1:A:255:THR:CG2	2.23	0.52
1:B:119:VAL:CG2	1:B:143:ILE:HB	2.38	0.52
1:B:141:GLU:HA	1:B:186:SER:O	2.10	0.52
1:C:43:TYR:CD1	1:D:278:LYS:HD3	2.45	0.52
1:D:26:GLU:CD	2:G:2:ARG:HB3	2.35	0.52
1:D:49:SER:OG	1:D:54:ALA:HB2	2.09	0.52
1:D:332:ILE:HD13	1:D:333:HIS:N	2.24	0.52
1:B:60:ILE:H	1:B:60:ILE:CD1	2.22	0.52
1:C:235:ILE:HB	1:C:249:LEU:HD13	1.92	0.52
1:D:175:LYS:HG3	1:D:187:VAL:HB	1.92	0.52
1:C:11:ILE:HD13	1:C:39:ILE:HB	1.92	0.52
1:D:159:VAL:HG22	1:D:159:VAL:O	2.09	0.52
1:C:38:ILE:HD12	1:C:71:PHE:CD2	2.44	0.52
1:D:126:ILE:HB	1:D:212:SER:HB2	1.91	0.52
1:D:25:LYS:NZ	5:D:376:HOH:O	2.41	0.52
1:D:72:LEU:HB3	1:D:78:ILE:HG12	1.92	0.52
1:A:145:ILE:HG12	1:A:190:ILE:HB	1.91	0.52
1:A:36:GLU:O	1:A:40:LYS:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:TYR:CE2	1:D:73:LYS:HE2	2.46	0.51
1:A:105:ASN:CB	1:A:108:LEU:HD12	2.41	0.51
1:A:228:VAL:HG11	1:A:346:CYS:HB3	1.92	0.51
1:D:224:ASN:C	1:D:224:ASN:ND2	2.69	0.51
1:A:35:TRP:CZ2	1:A:39:ILE:HD11	2.45	0.51
1:B:60:ILE:HD11	1:B:65:PHE:HD1	1.71	0.51
1:B:217:PHE:CG	1:B:218:ASN:N	2.79	0.51
1:C:94:ARG:HD2	1:D:290:THR:CG2	2.39	0.51
1:D:96:PHE:CD2	1:D:106:PRO:HB2	2.46	0.51
1:D:166:VAL:HG13	1:D:166:VAL:O	2.10	0.51
1:A:322:ARG:NH2	2:E:3:THR:O	2.44	0.51
1:C:290:THR:HG21	1:D:94:ARG:HD3	1.92	0.51
1:C:18:GLY:HA3	1:C:35:TRP:NE1	2.26	0.51
1:B:58:ALA:CB	1:B:60:ILE:HD12	2.42	0.50
1:B:240:VAL:HG21	2:F:1:MSE:HA	1.93	0.50
1:C:287:LYS:HB2	1:D:7:ARG:HG2	1.92	0.50
1:B:4:ILE:HD12	1:B:48:PRO:HD3	1.93	0.50
1:B:39:ILE:HG13	1:B:40:LYS:N	2.23	0.50
1:C:60:ILE:HD13	1:C:60:ILE:H	1.75	0.50
1:D:181:ARG:HG3	1:D:181:ARG:HH11	1.75	0.50
1:D:132:VAL:HG22	1:D:160:LEU:HD11	1.93	0.50
1:D:176:ARG:HG3	1:D:176:ARG:HH11	1.77	0.49
1:A:152:ASN:ND2	1:A:153:THR:H	2.10	0.49
1:D:197:TYR:CB	1:D:222:TRP:NE1	2.73	0.49
1:D:224:ASN:C	1:D:224:ASN:HD22	2.20	0.49
1:D:113:LEU:HD22	1:D:139:ILE:CD1	2.42	0.49
1:C:241:ASN:ND2	1:C:289:ALA:H	2.11	0.49
1:A:156:THR:HG22	1:A:157:ARG:HG3	1.94	0.49
1:A:293:PRO:O	1:A:297:VAL:HG23	2.13	0.49
1:B:58:ALA:HB1	1:B:60:ILE:HD12	1.95	0.49
1:B:106:PRO:HG2	5:B:396:HOH:O	2.13	0.49
1:C:94:ARG:HB3	1:D:290:THR:OG1	2.13	0.49
1:C:176:ARG:NH1	1:C:177:GLU:HG2	2.28	0.49
1:D:73:LYS:HD3	5:D:371:HOH:O	2.12	0.49
1:A:120:ILE:CD1	1:A:131:SER:HB3	2.43	0.48
1:A:125:GLY:C	1:A:295:ASN:HD21	2.21	0.48
1:B:158:GLN:H	1:B:158:GLN:HE21	1.60	0.48
1:C:120:ILE:N	1:C:120:ILE:HD12	2.28	0.48
1:C:227:CYS:SG	1:C:232[B]:GLN:CG	3.01	0.48
1:D:32:LEU:O	1:D:36:GLU:HG3	2.14	0.48
1:D:246:PHE:CE1	1:D:323:ILE:HB	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:VAL:HG21	1:C:139:ILE:HD13	1.94	0.48
1:B:94:ARG:HH11	1:B:94:ARG:HG2	1.78	0.48
1:D:200:LEU:C	1:D:202:LYS:H	2.21	0.48
1:A:320:ASN:C	1:A:321:LYS:HG3	2.39	0.48
1:C:330:ILE:HG12	1:D:317:LEU:HD22	1.95	0.48
1:D:41:THR:HG22	1:D:65:PHE:CE1	2.49	0.48
1:D:192:LEU:HD22	1:D:193:ASN:O	2.14	0.48
1:A:5:LEU:HD13	1:A:42:ALA:HB1	1.95	0.48
1:C:114:LYS:HE3	1:C:114:LYS:HB2	1.58	0.48
1:C:224:ASN:HD21	1:C:257:CYS:HB2	1.78	0.48
1:A:255:THR:HG23	1:A:256:GLY:N	2.28	0.48
1:B:156:THR:CG2	1:B:157:ARG:HH11	2.27	0.48
1:B:220:ILE:HD11	1:B:236:ASN:HB2	1.95	0.48
1:B:292:ALA:O	1:B:293:PRO:C	2.55	0.47
1:D:189:GLU:O	1:D:190:ILE:HG13	2.14	0.47
1:A:249:LEU:O	5:A:371:HOH:O	2.19	0.47
1:A:240:VAL:HG22	2:E:4:GLY:O	2.14	0.47
1:B:26:GLU:OE1	2:E:2:ARG:HD3	2.15	0.47
1:A:8:TYR:HE2	1:A:100:GLN:HE21	1.63	0.47
1:C:285:ARG:HD3	1:D:46:ILE:HG23	1.96	0.47
1:D:224:ASN:ND2	1:D:228:VAL:HG23	2.29	0.47
1:B:43:TYR:O	1:B:46:ILE:HG12	2.15	0.47
1:B:241:ASN:ND2	1:B:289:ALA:H	2.12	0.47
1:B:27:GLN:HE22	1:B:75:ASN:CG	2.23	0.47
1:C:224:ASN:HD21	1:C:258:TYR:H	1.62	0.47
1:B:322:ARG:NH1	2:F:1:MSE:CB	2.52	0.46
1:C:91:ARG:NH2	1:C:181:ARG:O	2.48	0.46
1:C:134:LEU:HB3	1:C:139:ILE:HD12	1.97	0.46
1:B:54:ALA:O	1:B:57:THR:HB	2.15	0.46
1:B:154:ASN:C	1:B:156:THR:H	2.24	0.46
1:D:139:ILE:O	1:D:139:ILE:HG22	2.14	0.46
1:A:151:GLU:H	1:A:154:ASN:HD22	1.63	0.46
1:C:37:ASN:HB3	1:C:68:CYS:SG	2.56	0.46
1:A:234:TYR:CD1	1:A:234:TYR:C	2.92	0.46
1:B:146:ASP:O	1:B:191:ALA:HA	2.15	0.46
1:B:196:ASP:HA	1:B:222:TRP:CH2	2.51	0.46
1:D:4:ILE:HG13	1:D:81:GLY:HA2	1.97	0.46
1:B:220:ILE:HD13	1:B:236:ASN:ND2	2.31	0.46
1:C:234:TYR:CD1	1:C:234:TYR:C	2.93	0.46
1:A:286:PHE:CE2	1:A:288:PRO:HG3	2.51	0.46
1:A:279:ILE:CD1	1:B:39:ILE:HD13	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:ILE:HG22	1:B:81:GLY:HA2	1.98	0.45
1:A:220:ILE:HD13	1:A:236:ASN:OD1	2.16	0.45
1:D:10:LYS:NZ	2:G:6:ALA:HB2	2.29	0.45
1:D:113:LEU:HD23	1:D:310:ILE:CG1	2.47	0.45
1:C:47:THR:HG23	1:C:48:PRO:HD2	1.99	0.45
1:C:332:ILE:CG1	1:D:332:ILE:HB	2.47	0.45
1:D:163:GLU:O	1:D:166:VAL:HG12	2.16	0.45
1:B:341:PRO:HG2	1:B:342:VAL:H	1.82	0.45
1:B:158:GLN:HG2	1:B:161:PHE:CE2	2.52	0.45
1:C:1:MET:N	5:C:387:HOH:O	2.49	0.45
1:D:217:PHE:C	1:D:219:LEU:H	2.25	0.45
1:A:163:GLU:H	1:A:163:GLU:HG2	1.36	0.45
1:A:286:PHE:HE2	1:A:288:PRO:HG3	1.81	0.45
1:B:123:CYS:HB3	1:B:174:ILE:HD12	1.98	0.45
1:D:208:ILE:HD13	1:D:306:VAL:HG22	1.98	0.45
1:B:157:ARG:HG3	1:B:157:ARG:NH1	2.31	0.45
1:A:105:ASN:HB3	1:A:108:LEU:HD12	1.98	0.45
1:B:60:ILE:HD13	1:B:60:ILE:N	2.29	0.45
1:D:66:SER:O	1:D:70:ARG:HG3	2.17	0.45
1:D:218:ASN:HA	1:D:221:ASN:HD22	1.81	0.45
1:A:102:TYR:OH	1:B:328:ASP:HB3	2.17	0.45
1:D:72:LEU:C	1:D:78:ILE:HG12	2.42	0.45
1:D:143:ILE:HG13	1:D:188:SER:OG	2.17	0.45
1:D:235:ILE:HA	1:D:248:PRO:O	2.17	0.45
1:B:224:ASN:OD1	1:B:259:GLU:HG2	2.17	0.44
1:D:150:ILE:C	1:D:151:GLU:HG3	2.42	0.44
1:D:160:LEU:HD22	1:D:177:GLU:HB3	1.99	0.44
1:A:194:ILE:HG12	1:A:200:LEU:HD23	1.99	0.44
1:A:220:ILE:HD13	1:A:236:ASN:CG	2.43	0.44
1:D:3:TYR:HE2	1:D:73:LYS:HE2	1.82	0.44
1:D:200:LEU:C	1:D:202:LYS:N	2.74	0.44
1:C:165:ASP:HA	1:C:168:LYS:HE3	2.00	0.44
1:D:192:LEU:O	1:D:192:LEU:HD13	2.17	0.44
1:B:171:THR:HB	1:B:189:GLU:HB3	1.99	0.44
1:C:9:VAL:HG13	1:C:9:VAL:O	2.17	0.44
1:D:4:ILE:CG1	1:D:48:PRO:HG3	2.47	0.44
1:B:138:GLY:O	1:B:139:ILE:C	2.61	0.44
1:C:176:ARG:O	1:C:180:LYS:HG3	2.17	0.44
1:C:330:ILE:O	1:C:330:ILE:HG22	2.18	0.44
1:D:41:THR:HG22	1:D:65:PHE:CD1	2.53	0.44
1:D:332:ILE:O	1:D:332:ILE:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:ARG:HH12	2:F:1:MSE:CA	2.31	0.44
1:D:273:GLU:O	1:D:276:ASP:HB2	2.18	0.44
1:A:41:THR:HG22	1:A:65:PHE:HD1	1.76	0.43
1:C:47:THR:CG2	1:C:48:PRO:HD2	2.48	0.43
1:B:150:ILE:CD1	1:B:173:VAL:HG21	2.47	0.43
1:C:125:GLY:HA3	1:C:295:ASN:HD21	1.83	0.43
1:C:332:ILE:HG12	1:D:332:ILE:HB	2.00	0.43
1:A:196:ASP:HB2	1:A:198:THR:HG22	1.99	0.43
1:A:332:ILE:CG2	1:B:332:ILE:HG22	2.47	0.43
1:C:60:ILE:HD13	1:C:60:ILE:N	2.33	0.43
1:C:147:ASN:H	1:C:193:ASN:HD21	1.66	0.43
1:A:67:ASN:OD1	1:A:70:ARG:NH1	2.51	0.43
1:B:156:THR:CG2	1:B:157:ARG:NH1	2.82	0.43
1:B:157:ARG:NH2	4:B:359:SO4:O3	2.52	0.43
1:B:226:TYR:CD2	1:B:226:TYR:C	2.96	0.43
1:C:325:ILE:HG12	1:C:332:ILE:CD1	2.40	0.43
1:D:132:VAL:O	1:D:136:THR:HB	2.18	0.43
1:B:189:GLU:O	1:B:190:ILE:HD13	2.18	0.43
1:C:135:ALA:CB	1:C:178:LEU:HD22	2.48	0.43
1:D:133:ILE:HA	1:D:136:THR:HG22	2.00	0.43
1:B:10:LYS:C	1:B:11:ILE:HG13	2.44	0.43
1:D:4:ILE:HD11	1:D:48:PRO:HG3	2.00	0.43
1:A:126:ILE:HB	1:A:212:SER:CB	2.48	0.43
1:C:117:LYS:NZ	1:C:205:GLU:O	2.49	0.43
1:B:217:PHE:CD1	1:B:218:ASN:N	2.87	0.43
5:C:365:HOH:O	1:D:129:HIS:HD2	2.01	0.43
1:B:145:ILE:O	1:B:146:ASP:HB2	2.19	0.42
1:C:125:GLY:C	1:C:295:ASN:HD21	2.27	0.42
1:D:251:VAL:HB	1:D:255:THR:HG23	2.01	0.42
1:C:157:ARG:NH1	5:C:389:HOH:O	2.53	0.42
1:A:95:ASN:O	1:A:98:HIS:HB3	2.19	0.42
1:A:152:ASN:H	1:A:152:ASN:ND2	2.10	0.42
1:A:304:ALA:HB2	1:B:293:PRO:CB	2.49	0.42
1:D:82:GLU:C	1:D:84:ASN:H	2.27	0.42
1:B:156:THR:HG23	1:B:157:ARG:HH11	1.84	0.42
1:B:343:CYS:SG	1:B:344:SER:N	2.92	0.42
1:C:138:GLY:O	1:C:139:ILE:C	2.62	0.42
1:D:9:VAL:O	1:D:9:VAL:CG2	2.66	0.42
1:B:275:ILE:HG13	1:B:276:ASP:N	2.35	0.42
1:D:28:TYR:CD1	1:D:28:TYR:C	2.98	0.42
1:A:261:GLN:HG3	1:A:337:MET:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:LEU:HD21	1:B:62:GLU:HG2	2.02	0.42
1:B:154:ASN:C	1:B:156:THR:N	2.76	0.42
1:D:151:GLU:H	1:D:154:ASN:ND2	2.13	0.42
1:A:224:ASN:O	1:A:225:LYS:C	2.62	0.42
1:A:292:ALA:O	1:A:293:PRO:C	2.62	0.42
1:C:44:CYS:SG	1:C:58:ALA:HB2	2.60	0.42
1:A:105:ASN:O	1:A:106:PRO:C	2.62	0.42
1:D:6:GLY:O	1:D:9:VAL:HG22	2.20	0.42
1:D:98:HIS:NE2	1:D:102:TYR:HE2	2.17	0.42
1:A:194:ILE:HD12	1:A:194:ILE:N	2.35	0.42
1:B:211:VAL:HG21	1:B:223:VAL:HG11	2.02	0.42
1:D:322:ARG:O	2:H:1:MSE:HE1	2.20	0.42
1:B:123:CYS:HB3	1:B:174:ILE:CD1	2.50	0.42
1:C:325:ILE:HG12	1:C:332:ILE:HG23	2.02	0.42
1:D:19:LEU:HD11	2:G:2:ARG:HG2	2.01	0.42
1:D:26:GLU:OE1	2:G:2:ARG:CB	2.68	0.42
1:B:91:ARG:HD2	1:B:92:TYR:CE1	2.55	0.41
1:C:39:ILE:HD13	1:D:279:ILE:HG22	2.01	0.41
1:C:291:PHE:O	1:C:292:ALA:C	2.63	0.41
1:D:332:ILE:O	1:D:332:ILE:CG2	2.68	0.41
1:A:90:ASN:HD21	1:A:92:TYR:HD2	1.67	0.41
1:A:91:ARG:CZ	1:A:182:ASN:ND2	2.82	0.41
1:A:285:ARG:O	1:A:285:ARG:HG3	2.20	0.41
1:C:158:GLN:OE1	1:C:161:PHE:HE2	2.04	0.41
1:D:126:ILE:HB	1:D:212:SER:CB	2.50	0.41
1:C:135:ALA:HB2	1:C:178:LEU:HD22	2.01	0.41
1:A:7:ARG:HB3	1:B:287:LYS:HG2	2.03	0.41
1:B:281:LEU:C	1:B:281:LEU:HD13	2.46	0.41
1:C:193:ASN:HD22	1:C:193:ASN:HA	1.69	0.41
1:D:113:LEU:HD22	1:D:139:ILE:HD12	2.01	0.41
1:D:176:ARG:O	1:D:180:LYS:HG3	2.19	0.41
1:D:192:LEU:HD13	1:D:192:LEU:C	2.46	0.41
1:D:37:ASN:O	1:D:41:THR:HG23	2.21	0.41
1:B:171:THR:HB	1:B:189:GLU:CB	2.51	0.41
1:B:281:LEU:HD13	1:B:281:LEU:O	2.20	0.41
1:B:328:ASP:OD1	1:B:328:ASP:C	2.64	0.41
1:C:233:PRO:HG3	1:C:252:PRO:HD2	2.03	0.41
1:D:133:ILE:C	1:D:136:THR:HG22	2.45	0.41
1:B:301:LEU:HD23	1:B:301:LEU:HA	1.84	0.41
1:D:274:ASN:C	1:D:276:ASP:H	2.28	0.41
1:B:126:ILE:N	1:B:126:ILE:CD1	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:ALA:O	1:B:231:ASN:C	2.64	0.41
1:C:8:TYR:HE2	1:C:100:GLN:HE21	1.69	0.41
1:C:88:GLU:H	1:C:88:GLU:CD	2.28	0.41
1:D:332:ILE:HD13	1:D:332:ILE:C	2.46	0.41
1:A:220:ILE:HG23	1:A:221:ASN:N	2.36	0.41
1:A:156:THR:CG2	1:B:95:ASN:HD21	2.27	0.40
1:A:251:VAL:H	1:A:255:THR:HG21	1.86	0.40
1:A:293:PRO:CB	1:B:304:ALA:HB2	2.50	0.40
1:B:180:LYS:HG2	5:B:390:HOH:O	2.20	0.40
1:C:5:LEU:HD13	1:C:42:ALA:HB1	2.03	0.40
1:A:319:LEU:HD12	1:A:319:LEU:HA	1.95	0.40
1:D:203:VAL:HA	1:D:204:PRO:HD2	1.92	0.40
1:A:93:SER:O	1:A:96:PHE:HB2	2.21	0.40
1:A:112:LYS:HE2	1:A:312:LYS:HE3	2.04	0.40
1:D:292:ALA:O	1:D:295:ASN:HB3	2.22	0.40
1:B:187:VAL:CG1	1:B:188:SER:N	2.82	0.40
1:D:257:CYS:SG	1:D:258:TYR:N	2.94	0.40
1:C:51:TYR:OH	1:C:66:SER:HA	2.21	0.40
1:C:285:ARG:NH2	1:D:7:ARG:CD	2.84	0.40
1:D:26:GLU:OE1	2:G:2:ARG:HB2	2.22	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	331/353 (94%)	291 (88%)	39 (12%)	1 (0%)	36	50
1	B	327/353 (93%)	287 (88%)	34 (10%)	6 (2%)	6	9
1	C	338/353 (96%)	310 (92%)	26 (8%)	2 (1%)	21	31
1	D	328/353 (93%)	297 (90%)	27 (8%)	4 (1%)	10	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	G	5/7 (71%)	4 (80%)	1 (20%)	0	100	100
All	All	1332/1426 (93%)	1191 (89%)	128 (10%)	13 (1%)	12	18

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	273	GLU
1	B	197	TYR
1	D	191	ALA
1	B	62	GLU
1	D	190	ILE
1	D	218	ASN
1	B	258	TYR
1	A	342	VAL
1	C	48	PRO
1	C	159	VAL
1	D	204	PRO
1	B	204	PRO
1	B	341	PRO

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	271/304 (89%)	260 (96%)	11 (4%)	27	44
1	B	269/304 (88%)	255 (95%)	14 (5%)	21	34
1	C	279/304 (92%)	268 (96%)	11 (4%)	28	47
1	D	263/304 (86%)	244 (93%)	19 (7%)	13	21
2	E	3/4 (75%)	1 (33%)	2 (67%)	0	0
2	F	2/4 (50%)	1 (50%)	1 (50%)	0	0
2	G	5/4 (125%)	5 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	1/4 (25%)	1 (100%)	0	100	100
All	All	1093/1232 (89%)	1035 (95%)	58 (5%)	20	34

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	VAL
1	A	52	THR
1	A	120	ILE
1	A	152	ASN
1	A	163	GLU
1	A	196	ASP
1	A	231	ASN
1	A	249	LEU
1	A	255	THR
1	A	275	ILE
1	A	319	LEU
1	B	9	VAL
1	B	39	ILE
1	B	41	THR
1	B	60	ILE
1	B	62	GLU
1	B	74	GLU
1	B	78	ILE
1	B	95	ASN
1	B	114	LYS
1	B	119	VAL
1	B	158	GLN
1	B	172	GLU
1	B	179	LEU
1	B	219	LEU
1	C	32	LEU
1	C	39	ILE
1	C	60	ILE
1	C	128	ASN
1	C	129	HIS
1	C	152	ASN
1	C	153	THR
1	C	198	THR
1	C	266	ASP
1	C	317	LEU
1	C	319	LEU

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Mol	Chain	Res	Type
1	D	7	ARG
1	D	49	SER
1	D	85	ASN
1	D	139	ILE
1	D	179	LEU
1	D	196	ASP
1	D	198	THR
1	D	218	ASN
1	D	220	ILE
1	D	222	TRP
1	D	223	VAL
1	D	249	LEU
1	D	257	CYS
1	D	259	GLU
1	D	274	ASN
1	D	279	ILE
1	D	310	ILE
1	D	325	ILE
1	D	332	ILE
2	E	1	MSE
2	E	2	ARG
2	F	1	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	90	ASN
1	A	100	GLN
1	A	110	GLN
1	A	152	ASN
1	A	193	ASN
1	A	201	HIS
1	A	224	ASN
1	A	232	GLN
1	A	236	ASN
1	A	241	ASN
1	A	274	ASN
1	A	295	ASN
1	A	296	ASN
1	B	27	GLN
1	B	37	ASN

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Mol	Chain	Res	Type
1	B	75	ASN
1	B	95	ASN
1	B	98	HIS
1	B	100	GLN
1	B	115	ASN
1	B	129	HIS
1	B	158	GLN
1	B	182	ASN
1	B	224	ASN
1	B	232	GLN
1	B	236	ASN
1	B	241	ASN
1	B	296	ASN
1	B	336	ASN
1	C	31	ASN
1	C	59	ASN
1	C	84	ASN
1	C	90	ASN
1	C	95	ASN
1	C	100	GLN
1	C	110	GLN
1	C	147	ASN
1	C	152	ASN
1	C	154	ASN
1	C	193	ASN
1	C	201	HIS
1	C	224	ASN
1	C	241	ASN
1	C	295	ASN
1	C	296	ASN
1	D	95	ASN
1	D	100	GLN
1	D	129	HIS
1	D	154	ASN
1	D	158	GLN
1	D	169	ASN
1	D	201	HIS
1	D	218	ASN
1	D	221	ASN
1	D	224	ASN
1	D	236	ASN
1	D	241	ASN

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Mol	Chain	Res	Type
1	D	296	ASN
2	G	5	ASN
2	G	7	ASN

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 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\# Z > 2$
4	SO4	B	359	-	4,4,4	0.30	0	6,6,6	0.12	0
4	SO4	B	360	-	4,4,4	0.36	0	6,6,6	0.22	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 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	359	SO4	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	337/353 (95%)	-0.36	1 (0%) 90 89	23, 47, 72, 86	0
1	B	333/353 (94%)	-0.27	1 (0%) 90 89	24, 46, 84, 103	0
1	C	343/353 (97%)	-0.35	1 (0%) 90 89	25, 47, 72, 100	1 (0%)
1	D	333/353 (94%)	-0.14	2 (0%) 85 83	32, 55, 85, 97	1 (0%)
2	E	4/7 (57%)	1.81	2 (50%) 0 0	99, 109, 111, 113	0
2	F	1/7 (14%)	0.69	0 100 100	97, 97, 97, 97	0
2	G	6/7 (85%)	0.90	0 100 100	96, 101, 104, 105	0
2	H	0/7	-	-	-	-
All	All	1357/1440 (94%)	-0.27	7 (0%) 87 85	23, 49, 82, 113	2 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	5	ASN	3.2
1	A	348	ASN	2.9
1	D	341	PRO	2.5
1	D	232[A]	GLN	2.3
2	E	4	GLY	2.2
1	B	256	GLY	2.1
1	C	348	ASN	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(Å ²)	Q<0.9
4	SO4	B	359	5/5	0.73	0.16	118,118,118,118	0
4	SO4	B	360	5/5	0.88	0.08	74,74,75,75	0
3	ZN	D	500	1/1	0.92	0.06	104,104,104,104	0
3	ZN	B	500	1/1	0.97	0.06	98,98,98,98	0
3	ZN	A	500	1/1	0.98	0.03	74,74,74,74	0
3	ZN	C	500	1/1	0.99	0.01	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.