Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:09 AM GMT

PDB ID	:	3H9Q
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

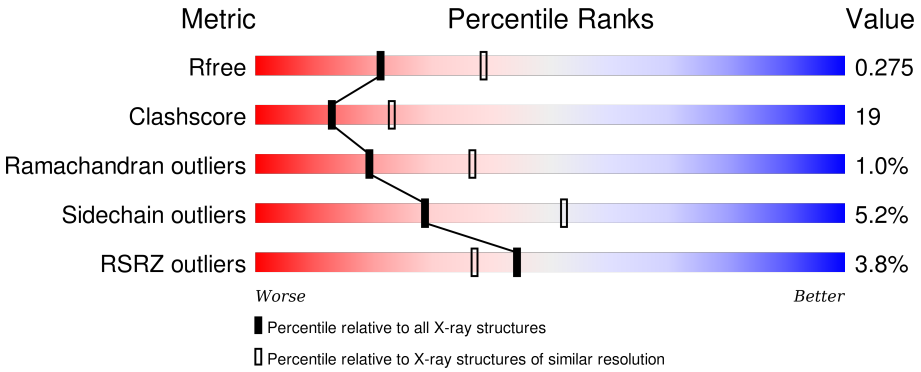
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 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}	91344	3377 (2.68-2.60)
Clashscore	102246	3781 (2.68-2.60)
Ramachandran outliers	100387	3722 (2.68-2.60)
Sidechain outliers	100360	3722 (2.68-2.60)
RSRZ outliers	91569	3388 (2.68-2.60)

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	353	% 65% 28% • 5%
1	B	353	4% 62% 30% • 6%
1	C	353	3% 69% 27% • •
1	D	353	4% 60% 30% • 6%
2	E	7	57% 14% 43% 14% 29%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	7	14% 14% 14% 71%
2	G	7	71% 43% 57%
2	H	7	14% 14% 71%

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	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			

Continued on next page...

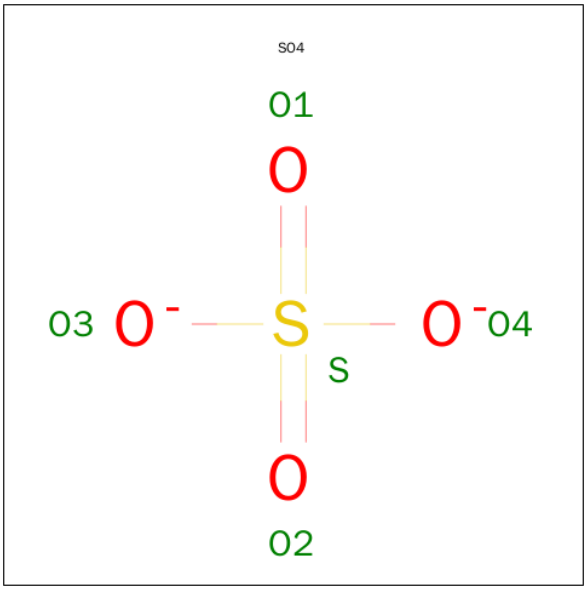
Continued from previous page...

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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is water.

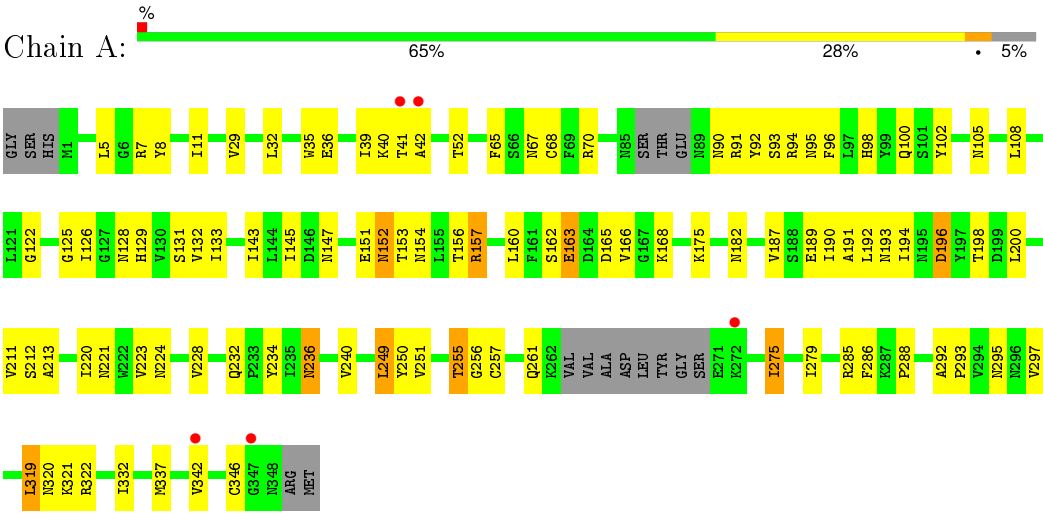
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	40	Total O 40 40	0	0
5	B	39	Total O 39 39	0	0
5	C	36	Total O 36 36	0	0
5	D	23	Total O 23 23	0	0
5	F	1	Total O 1 1	0	0
5	G	2	Total O 2 2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

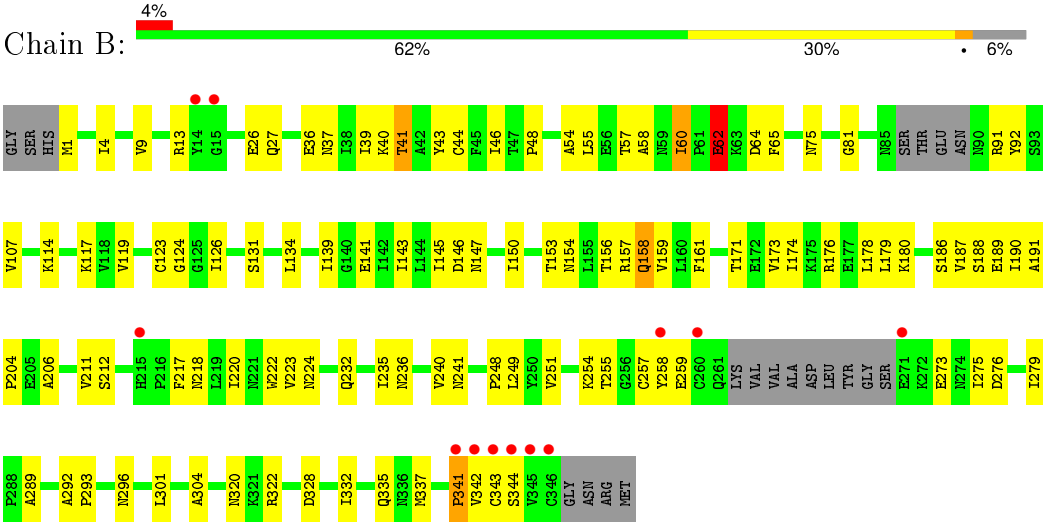
- Molecule 1: MccB protein

Chain A:



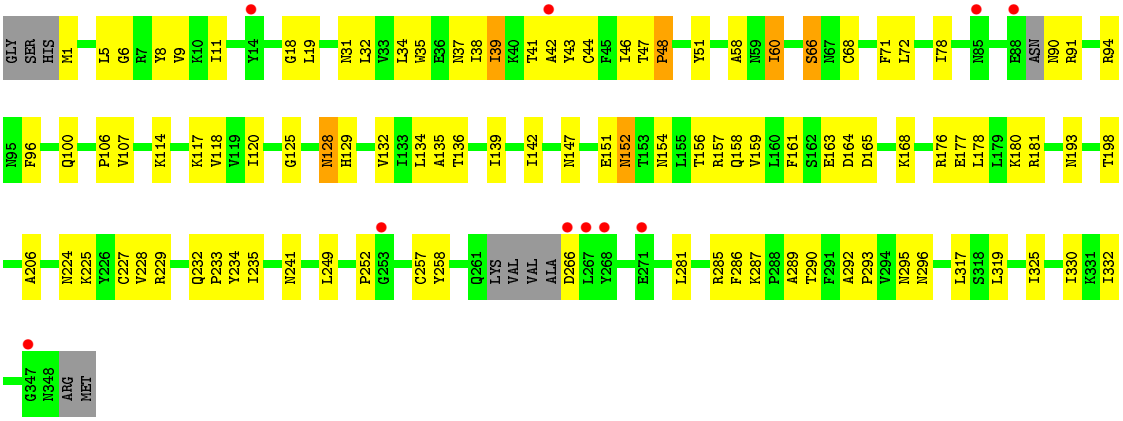
- Molecule 1: MccB protein

Chain B:



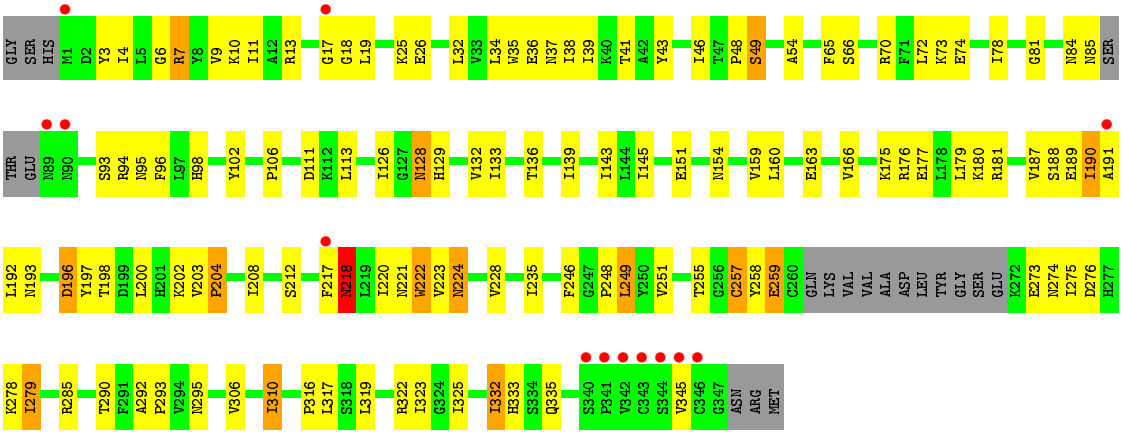
- Molecule 1: MccB protein

Chain C:



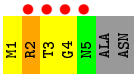
• Molecule 1: MccB protein

Chain D:



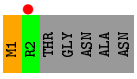
• Molecule 2: Microcin C7 ANALOG

Chain E:



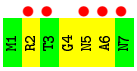
• Molecule 2: Microcin C7 ANALOG

Chain F:



• Molecule 2: Microcin C7 ANALOG

Chain G:



• Molecule 2: Microcin C7 ANALOG

Chain H:

4 Data and refinement statistics (i)

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 19.88 – 2.62	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.63) 99.6 (19.88-2.62)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.87 (at 2.63Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.207 , 0.273 0.208 , 0.275	Depositor DCC
R_{free} test set	1864 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	48.2	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 35.4	EDS
Estimated twinning fraction	0.040 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 37032 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.40	0/2632	0.64	0/3579
1	B	0.42	0/2606	0.64	0/3543
1	C	0.43	0/2696	0.65	0/3665
1	D	0.39	0/2583	0.61	0/3519
2	E	0.52	0/35	0.83	0/44
2	F	0.88	0/18	1.45	0/21
2	G	0.67	0/51	1.26	0/65
2	H	1.85	0/8	3.83	2/9 (22.2%)
All	All	0.42	0/10629	0.65	2/14445 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	1	MSE	CB-CG-SE	-9.26	84.91	112.70
2	H	1	MSE	CG-SE-CE	6.44	113.07	98.90

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	94	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2553	0	2480	116	0
1	C	2636	0	2555	98	0
1	D	2526	0	2415	129	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
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	391	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 19.

All (391) 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:D:11:ILE:HD13	1:D:39:ILE:HD13	1.56	0.87
1:B:156:THR:HG23	1:B:157:ARG:HG3	1.57	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:B:251:VAL:HG11	1:B:254:LYS:HE3	1.59	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:THR:HG22	1:A:65:PHE:CD1	2.13	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
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:HD22	1:A:152:ASN:H	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: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:C:163:GLU:HG3	1:D:180:LYS:O	1.92	0.69
1:B:206:ALA:H	1:B:232:GLN:HE22	1.38	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:A:189:GLU:C	1:A:190:ILE:HD12	2.13	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:H	1:B:60:ILE:HD13	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:ILE:HB	1:D:249:LEU:HD22	1.78	0.66
1:D:9:VAL:O	1:D:9:VAL:HG23	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: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:C:18:GLY:HA3	1:C:35:TRP:CE2	2.31	0.64
1:B:107:VAL:HG23	5:B:396:HOH:O	1.97	0.64
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:275:ILE:O	1:A:279:ILE:HG12	1.97	0.64
1:A:192:LEU:HD12	1:A:193:ASN:H	1.63	0.64
1:C:46:ILE:CG2	1:D:285:ARG:HH11	2.11	0.63
1:B:157:ARG:HH11	1:B:157:ARG:HG3	1.62	0.63
1:C:58:ALA:HB1	1:C:60:ILE:CD1	2.27	0.63
1:D:113:LEU:HD23	1:D:310:ILE:CD1	2.27	0.63
1:C:128:ASN:O	1:C:132:VAL:HG23	1.98	0.63
1:A:32:LEU:HG	1:A:36:GLU:OE2	1.99	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: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:B:322:ARG:HD3	5:B:398:HOH:O	2.00	0.61
1:B:117:LYS:O	1:B:206:ALA:HB1	1.99	0.61
1:C:285:ARG:O	1:D:7:ARG:HG3	2.00	0.61
1:D:335:GLN:HG3	2:H:1:MSE:CE	2.31	0.61
1:C:43:TYR:CG	1:D:278:LYS:HD3	2.36	0.61
1:B:224:ASN:ND2	1:B:257:CYS:HB2	2.15	0.61
1:D:4:ILE:CD1	1:D:48:PRO:HG3	2.31	0.61
1:C:224:ASN:O	1:C:228:VAL:HG23	2.00	0.61
1:C:176:ARG:NH1	1:C:177:GLU:OE2	2.33	0.61
1:C:72:LEU:HB3	1:C:78:ILE:HG23	1.83	0.61
1:A:147:ASN:OD1	1:A:191:ALA:HB1	1.99	0.61
1:D:128:ASN:O	1:D:132:VAL:HG23	2.01	0.61
1:C:107:VAL:HG23	5:C:361:HOH:O	2.00	0.61
1:D:133:ILE:O	1:D:136:THR:HG22	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:PHE:CE1	1:D:10:LYS:HG3	2.36	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:N	1:A:152:ASN:HD22	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
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
2:G:4:GLY:O	2:G:5:ASN:C	2.41	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:D:323:ILE:CG2	1:D:332:ILE:HD11	2.34	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:A:11:ILE:C	1:A:11:ILE:HD12	2.25	0.57
1:B:173:VAL:HG13	1:B:176:ARG:NH2	2.18	0.57
1:A:224:ASN:HD21	1:A:257:CYS:HB2	1.69	0.57
1:D:145:ILE:CD1	1:D:203:VAL:HG13	2.35	0.57
1:B:95:ASN:HD22	1:B:95:ASN:N	2.03	0.57
1:C:286:PHE:CZ	2:G:6:ALA:HB1	2.39	0.57
1:A:105:ASN:HB3	1:A:108:LEU:HB2	1.87	0.57
1:B:224:ASN:HD21	1:B:257:CYS:CB	2.18	0.57
1:B:224:ASN:HD21	1:B:257:CYS:HB2	1.70	0.56
1:B:1:MET:HA	5:B:391:HOH:O	2.04	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:4:ILE:HG12	1:D:48:PRO:HG3	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:A:206:ALA:H	1:A:232:GLN:HE22	1.54	0.54
1:B:154:ASN:HB3	1:B:158:GLN:NE2	2.22	0.54
1:A:122:GLY:HA3	1:A:213:ALA:HB2	1.90	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:D:197:TYR:N	1:D:222:TRP:CZ2	2.77	0.53
1:C:281:LEU:HD23	1:D:43:TYR:HE1	1.73	0.53
1:D:275:ILE:O	1:D:279:ILE:HG23	2.09	0.53
1:B:44:CYS:SG	1:B:58:ALA:HB2	2.49	0.53
1:A:129:HIS:O	1:A:133:ILE:HG12	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:D:93:SER:O	1:D:96:PHE:HB2	2.08	0.53
1:C:164:ASP:O	1:C:168:LYS:HE3	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:275:ILE:HG23	1:B:39:ILE:CD1	2.37	0.52
1:D:166:VAL:HG13	1:D:166:VAL:O	2.10	0.52
1:A:94:ARG:HG2	1:B:153:THR:OG1	2.08	0.52
1:C:31:ASN:HD22	1:C:34:LEU:HB2	1.73	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:A:251:VAL:H	1:A:255:THR:CG2	2.23	0.52
1:C:43:TYR:CD1	1:D:278:LYS:HD3	2.45	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:LYS:HG3	1:D:187:VAL:HB	1.92	0.52
1:D:159:VAL:O	1:D:159:VAL:HG22	2.09	0.52
1:C:11:ILE:HD13	1:C:39:ILE:HB	1.92	0.52
1:C:38:ILE:HD12	1:C:71:PHE:CD2	2.44	0.52
1:D:10:LYS:HZ3	2:G:6:ALA:HB2	1.75	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
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:C:94:ARG:HD2	1:D:290:THR:CG2	2.39	0.51
1:B:60:ILE:HD11	1:B:65:PHE:HD1	1.71	0.51
1:A:35:TRP:CZ2	1:A:39:ILE:HD11	2.45	0.51
1:B:217:PHE:CG	1:B:218:ASN:N	2.79	0.51
1:D:96:PHE:CD2	1:D:106:PRO:HB2	2.46	0.51
1:C:290:THR:HG21	1:D:94:ARG:HD3	1.92	0.51
1:A:322:ARG:NH2	2:E:3:THR:O	2.44	0.51
1:C:18:GLY:HA3	1:C:35:TRP:NE1	2.26	0.51
1:B:240:VAL:HG21	2:F:1:MSE:HA	1.93	0.50
1:B:58:ALA:CB	1:B:60:ILE:HD12	2.42	0.50
1:C:287:LYS:HB2	1:D:7:ARG:HG2	1.92	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:B:4:ILE:HD12	1:B:48:PRO:HD3	1.93	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:HH11	1:D:176:ARG:HG3	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: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:B:58:ALA:HB1	1:B:60:ILE:HD12	1.95	0.49
1:A:293:PRO:O	1:A:297:VAL:HG23	2.13	0.49
1:C:94:ARG:HB3	1:D:290:THR:OG1	2.13	0.49
1:B:106:PRO:HG2	5:B:396:HOH:O	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:GLN:HE21	1:B:158:GLN:H	1.60	0.48
1:A:120:ILE:CD1	1:A:131:SER:HB3	2.43	0.48
1:C:120:ILE:HD12	1:C:120:ILE:N	2.28	0.48
1:C:227:CYS:SG	1:C:232[B]:GLN:CG	3.01	0.48
1:D:246:PHE:CE1	1:D:323:ILE:HB	2.49	0.48
1:D:32:LEU:O	1:D:36:GLU:HG3	2.14	0.48
1:B:322:ARG:HH12	2:F:1:MSE:C	2.16	0.48
1:C:118:VAL:HG21	1:C:139:ILE:HD13	1.94	0.48
1:B:94:ARG:HG2	1:B:94:ARG:HH11	1.78	0.48
1:D:10:LYS:NZ	2:G:6:ALA:HB2	2.29	0.48
1:C:330:ILE:HG12	1:D:317:LEU:HD22	1.95	0.48
1:D:192:LEU:HD22	1:D:193:ASN:O	2.14	0.48
1:D:41:THR:HG22	1:D:65:PHE:CE1	2.49	0.48
1:C:224:ASN:HD21	1:C:257:CYS:HB2	1.78	0.48
1:A:5:LEU:HD13	1:A:42:ALA:HB1	1.95	0.48
1:C:114:LYS:HB2	1:C:114:LYS:HE3	1.58	0.48
1:B:156:THR:CG2	1:B:157:ARG:HH11	2.27	0.48
1:A:255:THR:HG23	1:A:256:GLY:N	2.28	0.48
1:B:220:ILE:HD11	1:B:236:ASN:HB2	1.95	0.48
1:D:26:GLU:CD	2:G:2:ARG:HB3	2.35	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:B:26:GLU:OE1	2:E:2:ARG:HD3	2.15	0.47
1:A:240:VAL:HG22	2:E:4:GLY:O	2.14	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:241:ASN:ND2	1:B:289:ALA:H	2.12	0.47
1:B:43:TYR:O	1:B:46:ILE:HG12	2.15	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:134:LEU:HB3	1:C:139:ILE:HD12	1.97	0.46
1:C:91:ARG:NH2	1:C:181:ARG:O	2.48	0.46
1:D:224:ASN:ND2	1:D:224:ASN:C	2.69	0.46
1:B:54:ALA:O	1:B:57:THR:HB	2.15	0.46
1:D:139:ILE:HG22	1:D:139:ILE:O	2.14	0.46
1:C:37:ASN:HB3	1:C:68:CYS:SG	2.56	0.46
1:A:151:GLU:H	1:A:154:ASN:HD22	1.63	0.46
1:B:146:ASP:O	1:B:191:ALA:HA	2.15	0.46
1:D:4:ILE:HG13	1:D:81:GLY:HA2	1.97	0.46
1:B:196:ASP:HA	1:B:222:TRP:CH2	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:ILE:HD13	1:B:236:ASN:ND2	2.31	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
1:B:4:ILE:HG22	1:B:81:GLY:HA2	1.98	0.45
1:D:113:LEU:HD23	1:D:310:ILE:CG1	2.47	0.45
1:D:224:ASN:HD22	1:D:224:ASN:C	2.20	0.45
1:A:220:ILE:HD13	1:A:236:ASN:OD1	2.16	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:C:47:THR:HG23	1:C:48:PRO:HD2	1.99	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:208:ILE:HD13	1:D:306:VAL:HG22	1.98	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:B:157:ARG:HG3	1:B:157:ARG:NH1	2.31	0.45
1:B:60:ILE:N	1:B:60:ILE:HD13	2.29	0.45
1:D:66:SER:O	1:D:70:ARG:HG3	2.17	0.45
1:A:105:ASN:HB3	1:A:108:LEU:HD12	1.98	0.45
1:D:218:ASN:HA	1:D:221:ASN:HD22	1.81	0.45
1:D:235:ILE:HA	1:D:248:PRO:O	2.17	0.45
1:D:143:ILE:HG13	1:D:188:SER:OG	2.17	0.45
1:A:102:TYR:OH	1:B:328:ASP:HB3	2.17	0.45
1:B:224:ASN:OD1	1:B:259:GLU:HG2	2.17	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:D:3:TYR:HE2	1:D:73:LYS:HE2	1.82	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:O	1:C:9:VAL:HG13	2.17	0.44
1:D:4:ILE:CG1	1:D:48:PRO:HG3	2.47	0.44
1:C:330:ILE:O	1:C:330:ILE:HG22	2.18	0.44
1:D:332:ILE:O	1:D:332:ILE:HG23	2.17	0.44
1:C:176:ARG:O	1:C:180:LYS:HG3	2.17	0.44
1:D:41:THR:HG22	1:D:65:PHE:CD1	2.53	0.44
1:B:322:ARG:HH12	2:F:1:MSE:CA	2.31	0.44
1:A:125:GLY:C	1:A:295:ASN:HD21	2.21	0.44
1:D:273:GLU:O	1:D:276:ASP:HB2	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:200:LEU:C	1:D:202:LYS:H	2.21	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:196:ASP:HB2	1:A:198:THR:HG22	1.99	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: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:A:67:ASN:OD1	1:A:70:ARG:NH1	2.51	0.43
1:A:320:ASN:C	1:A:321:LYS:HG3	2.39	0.43
1:D:133:ILE:HA	1:D:136:THR:HG22	2.00	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:4:ILE:HD11	1:D:48:PRO:HG3	2.00	0.43
1:B:292:ALA:O	1:B:293:PRO:C	2.55	0.43
1:A:126:ILE:HB	1:A:212:SER:CB	2.48	0.43
1:B:145:ILE:O	1:B:146:ASP:HB2	2.19	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: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:152:ASN:ND2	1:A:152:ASN:H	2.10	0.42
1:A:304:ALA:HB2	1:B:293:PRO:CB	2.49	0.42
1:A:95:ASN:O	1:A:98:HIS:HB3	2.19	0.42
1:B:156:THR:HG23	1:B:157:ARG:HH11	1.84	0.42
1:D:9:VAL:O	1:D:9:VAL:CG2	2.66	0.42
1:B:343:CYS:SG	1:B:344:SER:N	2.92	0.42
1:B:275:ILE:HG13	1:B:276:ASP:N	2.35	0.42
1:D:151:GLU:H	1:D:154:ASN:ND2	2.13	0.42
1:B:55:LEU:HD21	1:B:62:GLU:HG2	2.02	0.42
1:A:261:GLN:HG3	1:A:337:MET:HA	2.02	0.42
1:C:44:CYS:SG	1:C:58:ALA:HB2	2.60	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:D:322:ARG:O	2:H:1:MSE:HE1	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:123:CYS:HB3	1:B:174:ILE:CD1	2.50	0.42
1:D:332:ILE:CG2	1:D:332:ILE:O	2.68	0.41
1:C:39:ILE:HD13	1:D:279:ILE:HG22	2.01	0.41
1:B:91:ARG:HD2	1:B:92:TYR:CE1	2.55	0.41
1:B:154:ASN:C	1:B:156:THR:H	2.24	0.41
1:A:90:ASN:HD21	1:A:92:TYR:HD2	1.67	0.41
1:D:126:ILE:HB	1:D:212:SER:CB	2.50	0.41
1:A:91:ARG:CZ	1:A:182:ASN:ND2	2.82	0.41
1:C:158:GLN:OE1	1:C:161:PHE:HE2	2.04	0.41
1:A:285:ARG:HG3	1:A:285:ARG:O	2.20	0.41
1:C:135:ALA:HB2	1:C:178:LEU:HD22	2.01	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:A:7:ARG:HB3	1:B:287:LYS:HG2	2.03	0.41
1:C:193:ASN:HD22	1:C:193:ASN:HA	1.69	0.41
1:A:234:TYR:CD1	1:A:234:TYR:C	2.92	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:C:234:TYR:CD1	1:C:234:TYR:C	2.93	0.41
1:C:233:PRO:HG3	1:C:252:PRO:HD2	2.03	0.41
1:B:281:LEU:HD13	1:B:281:LEU:O	2.20	0.41
1:B:301:LEU:HA	1:B:301:LEU:HD23	1.84	0.41
1:B:27:GLN:HE22	1:B:75:ASN:CG	2.23	0.41
1:B:126:ILE:CD1	1:B:126:ILE:N	2.84	0.41
1:D:200:LEU:C	1:D:202:LYS:N	2.74	0.41
1:C:8:TYR:HE2	1:C:100:GLN:HE21	1.69	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:B:180:LYS:HG2	5:B:390:HOH:O	2.20	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:C:5:LEU:HD13	1:C:42:ALA:HB1	2.03	0.40
1:B:248:PRO:HG3	1:B:337:MET:HE2	2.04	0.40
1:D:203:VAL:HA	1:D:204:PRO:HD2	1.92	0.40
1:A:319:LEU:HD12	1:A:319:LEU:HA	1.95	0.40
1:D:292:ALA:O	1:D:295:ASN:HB3	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LYS:HE2	1:A:312:LYS:HE3	2.04	0.40
1:A:93:SER:O	1:A:96:PHE:HB2	2.21	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:D:26:GLU:OE1	2:G:2:ARG:HB2	2.22	0.40
1:C:285:ARG:NH2	1:D:7:ARG:CD	2.84	0.40
1:C:51:TYR:OH	1:C:66:SER:HA	2.21	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%)	46 70
1	B	327/353 (93%)	287 (88%)	34 (10%)	6 (2%)	11 19
1	C	338/353 (96%)	310 (92%)	26 (8%)	2 (1%)	30 53
1	D	328/353 (93%)	297 (90%)	27 (8%)	4 (1%)	16 31
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%)	19 37

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	271/304 (89%)	260 (96%)	11 (4%)	37 64
1	B	269/304 (88%)	259 (96%)	10 (4%)	41 67
1	C	279/304 (92%)	267 (96%)	12 (4%)	35 62
1	D	263/304 (86%)	242 (92%)	21 (8%)	15 28
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
2	H	1/4 (25%)	1 (100%)	0	100 100
All	All	1093/1232 (89%)	1036 (95%)	57 (5%)	29 52

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	VAL
1	A	52	THR
1	A	152	ASN
1	A	157	ARG
1	A	163	GLU
1	A	196	ASP
1	A	236	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	249	LEU
1	A	255	THR
1	A	275	ILE
1	A	319	LEU
1	B	9	VAL
1	B	13	ARG
1	B	41	THR
1	B	60	ILE
1	B	62	GLU
1	B	94	ARG
1	B	95	ASN
1	B	114	LYS
1	B	158	GLN
1	B	179	LEU
1	C	32	LEU
1	C	39	ILE
1	C	60	ILE
1	C	66	SER
1	C	90	ASN
1	C	128	ASN
1	C	129	HIS
1	C	152	ASN
1	C	198	THR
1	C	266	ASP
1	C	317	LEU
1	C	319	LEU
1	D	7	ARG
1	D	49	SER
1	D	85	ASN
1	D	111	ASP
1	D	128	ASN
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	224	ASN
1	D	249	LEU
1	D	257	CYS
1	D	259	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) 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	129	HIS
1	A	152	ASN
1	A	154	ASN
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
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	224	ASN
1	B	232	GLN
1	B	236	ASN
1	B	241	ASN
1	B	296	ASN
1	C	31	ASN
1	C	59	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	90	ASN
1	C	95	ASN
1	C	98	HIS
1	C	100	GLN
1	C	110	GLN
1	C	149	GLN
1	C	152	ASN
1	C	154	ASN
1	C	193	ASN
1	C	215	HIS
1	C	224	ASN
1	C	236	ASN
1	C	241	ASN
1	C	277	HIS
1	C	295	ASN
1	C	296	ASN
1	D	95	ASN
1	D	98	HIS
1	D	100	GLN
1	D	129	HIS
1	D	154	ASN
1	D	158	GLN
1	D	218	ASN
1	D	221	ASN
1	D	224	ASN
1	D	236	ASN
1	D	241	ASN
1	D	296	ASN

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

There are no carbohydrates 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	0.13	0	6,6,6	0.14	0
4	SO4	B	360	-	4,4,4	0.22	0	6,6,6	0.25	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
4	SO4	B	359	-	-	0/0/0/0	0/0/0/0
4	SO4	B	360	-	-	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 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

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	337/353 (95%)	-0.14	5 (1%) 76 71	23, 47, 72, 86	0
1	B	333/353 (94%)	-0.02	14 (4%) 40 33	24, 46, 84, 103	0
1	C	343/353 (97%)	-0.12	10 (2%) 55 49	25, 47, 72, 100	0
1	D	333/353 (94%)	0.13	13 (3%) 43 36	32, 55, 85, 97	0
2	E	4/7 (57%)	4.47	4 (100%) 0 0	99, 109, 111, 113	0
2	F	1/7 (14%)	2.48	1 (100%) 0 0	97, 97, 97, 97	0
2	G	6/7 (85%)	3.12	5 (83%) 0 0	96, 101, 104, 105	0
2	H	0/7	-	-	-	-
All	All	1357/1440 (94%)	-0.01	52 (3%) 44 37	23, 49, 82, 113	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	4	GLY	6.2
1	D	341	PRO	6.1
1	B	341	PRO	6.0
2	E	3	THR	5.1
1	B	344	SER	5.0
1	B	342	VAL	4.8
1	B	215	HIS	4.7
1	D	342	VAL	4.4
2	E	5	ASN	4.3
2	G	3	THR	4.1
2	G	6	ALA	4.0
2	G	7	ASN	3.9
1	D	340	SER	3.7
1	C	266	ASP	3.6
1	B	343	CYS	3.5
1	B	258	TYR	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	272	LYS	3.0
1	C	85	ASN	3.0
1	D	90	ASN	3.0
1	A	42	ALA	2.9
1	D	1	MET	2.9
2	G	2	ARG	2.9
1	B	260	CYS	2.9
1	D	343	CYS	2.9
1	A	41	THR	2.8
1	D	89	ASN	2.8
1	D	191	ALA	2.7
1	A	342	VAL	2.7
1	C	14	TYR	2.6
2	G	5	ASN	2.6
1	C	267	LEU	2.6
1	B	271	GLU	2.5
1	D	345	VAL	2.5
1	C	253	GLY	2.5
2	F	2	ARG	2.5
1	B	346	CYS	2.5
1	D	217	PHE	2.5
1	C	347	GLY	2.5
1	A	347	GLY	2.4
1	B	196	ASP	2.4
1	D	344	SER	2.3
2	E	2	ARG	2.3
1	C	42	ALA	2.3
1	B	94	ARG	2.2
1	C	268	TYR	2.2
1	B	15	GLY	2.2
1	D	346	CYS	2.2
1	B	14	TYR	2.1
1	C	271	GLU	2.1
1	B	345	VAL	2.1
1	C	88	GLU	2.1
1	D	17	GLY	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	SO4	B	359	5/5	0.92	0.29	2.93	118,118,118,118	0
3	ZN	C	500	1/1	0.99	0.05	-1.73	45,45,45,45	0
3	ZN	D	500	1/1	0.87	0.06	-2.61	104,104,104,104	0
3	ZN	A	500	1/1	0.98	0.04	-2.82	74,74,74,74	0
3	ZN	B	500	1/1	0.97	0.05	-4.54	98,98,98,98	0
4	SO4	B	360	5/5	0.94	0.11	-	74,74,75,75	0

6.5 Other polymers (i)

There are no such residues in this entry.