Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:48 PM GMT

PDB ID	:	1H8T
Title	:	Echovirus 11
Authors	:	Stuart, A.; Mckee, T.; Williams, P.A.; Harley, C.; Stuart, D.I.; Brown, T.D.K.; Lea, S.M.
Deposited on	:	2001-02-15
Resolution	:	2.90 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:

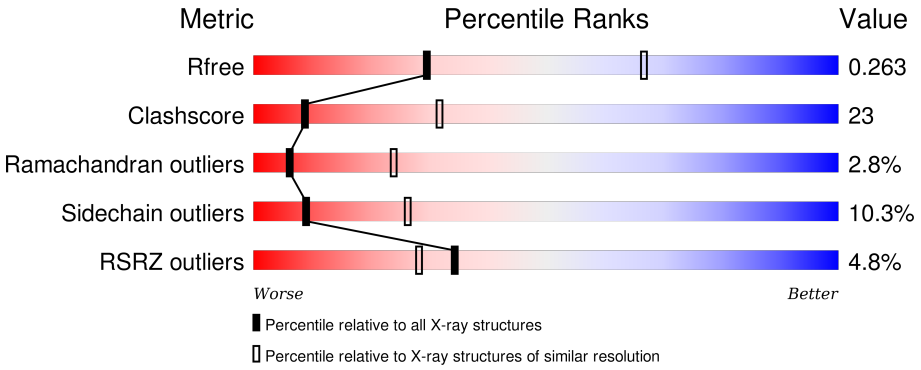
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	292	7% 60% 32% 8%
2	B	262	2% 65% 25% 5%
3	C	238	66% 27% 5%
4	D	68	19% 40% 37% 13% 10%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	DOA	A	1000	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6575 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 ECHOVIRUS 11 COAT PROTEIN VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	1
			2284	1439	399	435	11			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	VAL	MET	CONFLICT	UNP P29813
A	78	GLU	GLY	CONFLICT	UNP P29813
A	84	SER	THR	CONFLICT	UNP P29813
A	131	THR	SER	CONFLICT	UNP P29813
A	132	GLN	ARG	CONFLICT	UNP P29813
A	161	THR	ALA	CONFLICT	UNP P29813
A	267	SER	THR	CONFLICT	UNP P29813
A	270	ASP	ASN	CONFLICT	UNP P29813
A	271	ILE	VAL	CONFLICT	UNP P29813
A	276	ASN	THR	CONFLICT	UNP P29813
A	279	THR	ASN	CONFLICT	UNP P29813
A	283	ASP	GLU	CONFLICT	UNP P29813
A	289	VAL	LEU	CONFLICT	UNP P29813
A	292	HIS	TYR	CONFLICT	UNP P29813

- Molecule 2 is a protein called ECHOVIRUS 11 COAT PROTEIN VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	253	Total	C	N	O	S	0	0	1
			1964	1240	332	376	16			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1043	ARG	LYS	CONFLICT	UNP P29813
B	1045	ASP	ASN	CONFLICT	UNP P29813

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1073	LYS	ARG	CONFLICT	UNP P29813
B	1108	ILE	LEU	CONFLICT	UNP P29813
B	1136	THR	GLN	CONFLICT	UNP P29813
B	1157	ALA	SER	CONFLICT	UNP P29813
B	1159	GLY	SER	CONFLICT	UNP P29813
B	1168	SER	THR	CONFLICT	UNP P29813
B	1185	PHE	TYR	CONFLICT	UNP P29813
B	1230	ASN	ASP	CONFLICT	UNP P29813
B	1235	PHE	SER	CONFLICT	UNP P29813
B	1260	ALA	SER	CONFLICT	UNP P29813

- Molecule 3 is a protein called ECHOVIRUS 11 COAT PROTEIN VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	238	Total	C	N	O	S	0	0	0
			1819	1161	299	346	13			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2005	ILE	MET	CONFLICT	UNP P29813
C	2059	ALA	GLU	CONFLICT	UNP P29813
C	2061	ASN	LYS	CONFLICT	UNP P29813
C	2063	GLU	ASP	CONFLICT	UNP P29813
C	2066	ASP	GLU	CONFLICT	UNP P29813
C	2067	ILE	VAL	CONFLICT	UNP P29813
C	2080	SER	ASP	CONFLICT	UNP P29813
C	2093	GLY	SER	CONFLICT	UNP P29813
C	2107	TYR	PHE	CONFLICT	UNP P29813
C	2144	SER	ASN	CONFLICT	UNP P29813
C	2168	ILE	VAL	CONFLICT	UNP P29813
C	2232	GLN	GLU	CONFLICT	UNP P29813
C	2234	ALA	THR	CONFLICT	UNP P29813

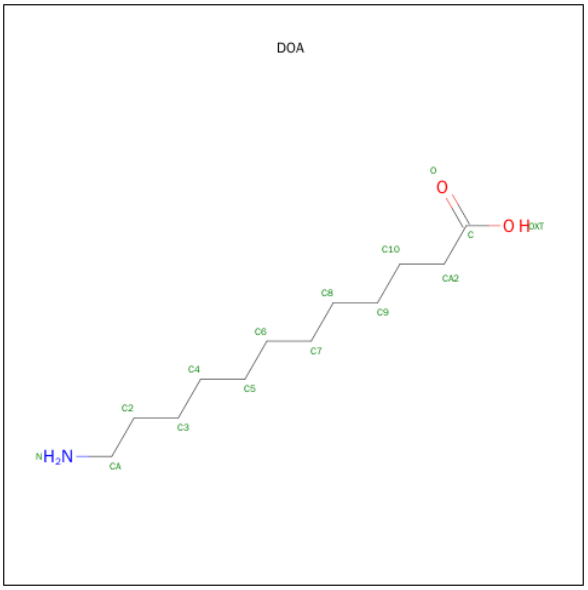
- Molecule 4 is a protein called ECHOVIRUS 11 COAT PROTEIN VP4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	61	Total	C	N	O	S	0	0	1
			467	289	82	95	1			

There are 4 discrepancies between the modelled and reference sequences:

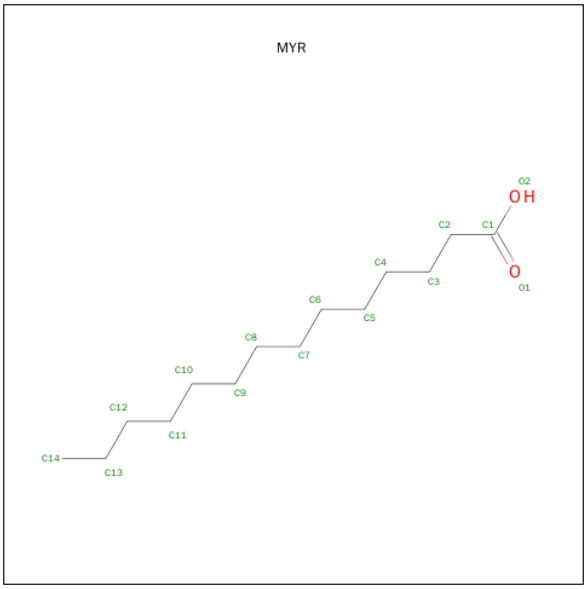
Chain	Residue	Modelled	Actual	Comment	Reference
D	3018	ARG	ASN	CONFLICT	UNP P29813
D	3022	ASN	SER	CONFLICT	UNP P29813
D	3045	ASP	GLU	CONFLICT	UNP P29813
D	3047	THR	SER	CONFLICT	UNP P29813

- Molecule 5 is 12-AMINO-DODECANOIC ACID (three-letter code: DOA) (formula: $C_{12}H_{25}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			15	12	1	2		

- Molecule 6 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total C O 15 14 1	0	0

- Molecule 7 is water.

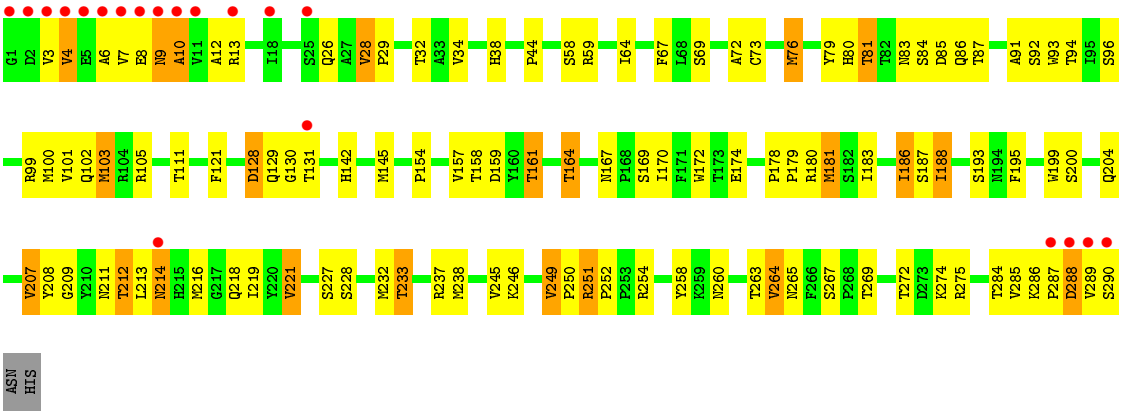
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total O 2 2	0	0
7	B	4	Total O 4 4	0	0
7	C	5	Total O 5 5	0	0

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.

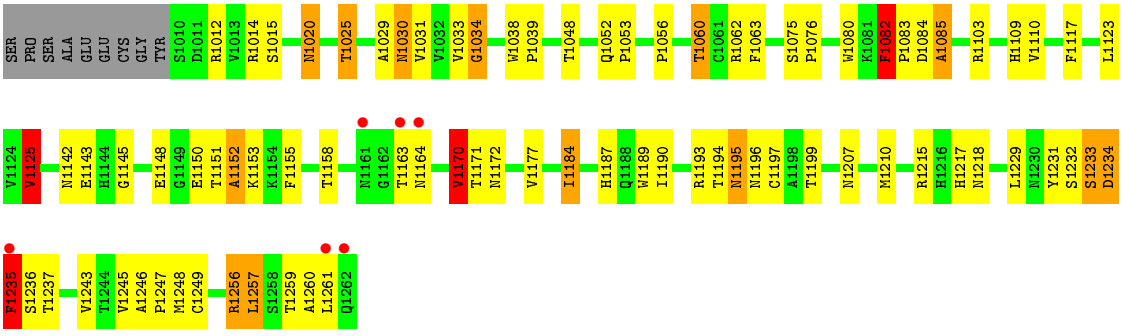
- Molecule 1: ECHOVIRUS 11 COAT PROTEIN VP1

Chain A:



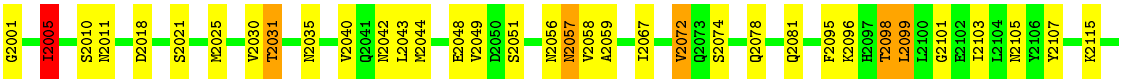
- Molecule 2: ECHOVIRUS 11 COAT PROTEIN VP2

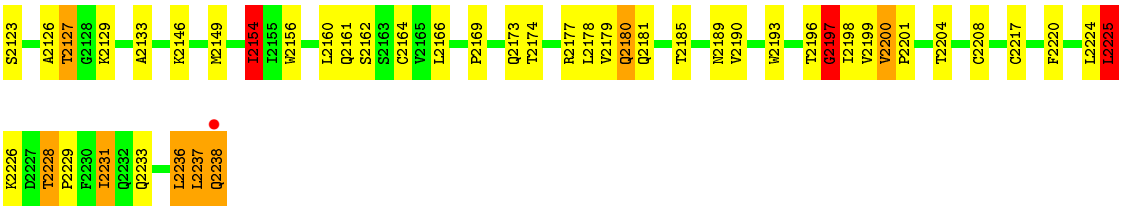
Chain B:



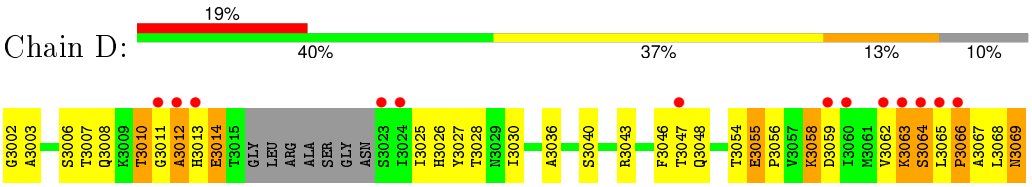
- Molecule 3: ECHOVIRUS 11 COAT PROTEIN VP3

Chain C:





- Molecule 4: ECHOVIRUS 11 COAT PROTEIN VP4



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	300.85Å 300.85Å 1476.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	100.00 – 2.90 39.78 – 2.86	Depositor EDS
% Data completeness (in resolution range)	71.3 (100.00-2.90) 69.7 (39.78-2.86)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 2.86Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.246 , 0.255 0.265 , 0.263	Depositor DCC
R_{free} test set	2014 reflections (0.50%)	DCC
Wilson B-factor (Å^2)	22.7	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.95 , 36.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Outliers	0 of 411034 reflections	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	6575	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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: DOA, MYR

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	0.77	1/2349 (0.0%)	0.95	3/3208 (0.1%)
2	B	0.77	0/2016	1.05	8/2755 (0.3%)
3	C	0.76	1/1866 (0.1%)	0.99	6/2549 (0.2%)
4	D	0.89	0/475	1.04	3/641 (0.5%)
All	All	0.78	2/6706 (0.0%)	1.00	20/9153 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	76	MET	SD-CE	6.53	2.14	1.77
3	C	2001	GLY	N-CA	6.04	1.55	1.46

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1195	ASN	N-CA-CB	-8.60	95.12	110.60
2	B	1082	PHE	N-CA-C	8.59	134.20	111.00
3	C	2237	LEU	CB-CG-CD1	-7.95	97.48	111.00
3	C	2197	GLY	N-CA-C	7.88	132.79	113.10
1	A	237	ARG	NE-CZ-NH2	-7.44	116.58	120.30
3	C	2237	LEU	CB-CG-CD2	6.78	122.52	111.00
2	B	1014	ARG	NE-CZ-NH2	-6.68	116.96	120.30
3	C	2005	ILE	CB-CA-C	-5.94	99.72	111.60
3	C	2225	LEU	CA-CB-CG	5.94	128.97	115.30
2	B	1029	ALA	N-CA-C	-5.86	95.17	111.00
2	B	1125	VAL	CB-CA-C	-5.78	100.42	111.40
4	D	3012	ALA	N-CA-C	5.62	126.18	111.00
2	B	1215	ARG	CG-CD-NE	5.62	123.61	111.80
2	B	1082	PHE	C-N-CA	-5.57	98.59	122.00
1	A	284	THR	N-CA-C	-5.55	96.01	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	2154	ILE	CB-CA-C	-5.43	100.74	111.60
1	A	128	ASP	CB-CG-OD2	-5.24	113.58	118.30
4	D	3058	LYS	N-CA-C	-5.23	96.88	111.00
2	B	1170	VAL	CB-CA-C	-5.10	101.71	111.40
4	D	3064	SER	N-CA-C	-5.06	97.33	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2284	0	2212	150	0
2	B	1964	0	1874	65	0
3	C	1819	0	1772	111	0
4	D	467	0	447	47	0
5	A	15	0	24	2	0
6	D	15	0	27	1	0
7	A	2	0	0	1	0
7	B	4	0	0	0	0
7	C	5	0	0	0	0
All	All	6575	0	6356	303	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 23.

All (303) 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:76:MET:SD	1:A:76:MET:CE	2.14	1.34
1:A:260:ASN:OD1	1:A:263:THR:HG22	1.49	1.09
3:C:2098:THR:HG22	3:C:2101:GLY:H	1.20	1.04
4:D:3054:THR:O	4:D:3055:GLU:HB2	1.51	1.04
3:C:2233:GLN:NE2	3:C:2238:GLN:HG2	1.73	1.04
1:A:101:VAL:HB	3:C:2238:GLN:OE1	1.60	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1234:ASP:O	2:B:1236:SER:N	1.92	1.01
3:C:2196:THR:O	3:C:2196:THR:HG23	1.58	0.99
2:B:1025:THR:HG21	2:B:1197:CYS:SG	2.03	0.98
1:A:275:ARG:HE	3:C:2057:ASN:HD21	1.08	0.93
3:C:2233:GLN:HE22	3:C:2238:GLN:HG2	1.34	0.92
3:C:2233:GLN:CD	3:C:2238:GLN:HE21	1.74	0.90
1:A:101:VAL:HB	3:C:2238:GLN:CD	1.92	0.89
2:B:1082:PHE:O	2:B:1083:PRO:C	2.01	0.86
1:A:38:HIS:HD2	4:D:3055:GLU:HG3	1.39	0.85
3:C:2129:LYS:HB2	3:C:2196:THR:HG22	1.59	0.84
2:B:1030:ASN:HD21	4:D:3059:ASP:HB2	1.42	0.84
1:A:252:PRO:HD3	2:B:1184:ILE:HD11	1.57	0.84
3:C:2154:ILE:HD11	3:C:2166:LEU:HA	1.59	0.84
3:C:2233:GLN:HB3	3:C:2238:GLN:NE2	1.93	0.83
1:A:159:ASP:OD1	1:A:161:THR:HB	1.78	0.83
1:A:128:ASP:OD2	1:A:233:THR:HG22	1.77	0.83
4:D:3002:GLY:N	6:D:3500:MYR:O1	2.13	0.82
1:A:101:VAL:HB	3:C:2238:GLN:NE2	1.95	0.81
4:D:3047:THR:HG22	4:D:3048:GLN:H	1.44	0.80
1:A:6:ALA:O	1:A:7:VAL:HG23	1.82	0.80
1:A:59:ARG:NH1	4:D:3048:GLN:HE22	1.79	0.80
3:C:2057:ASN:H	3:C:2057:ASN:HD22	1.27	0.79
1:A:83:ASN:ND2	1:A:84:SER:H	1.80	0.79
3:C:2196:THR:O	3:C:2196:THR:CG2	2.29	0.79
3:C:2042:ASN:HD22	3:C:2044:MET:H	1.28	0.79
4:D:3054:THR:O	4:D:3055:GLU:CB	2.31	0.79
2:B:1233:SER:O	2:B:1235:PHE:CD2	2.36	0.79
2:B:1193:ARG:HG3	2:B:1194:THR:HG23	1.63	0.78
3:C:2095:PHE:O	3:C:2098:THR:HB	1.82	0.78
3:C:2228:THR:HG22	3:C:2229:PRO:HD2	1.65	0.78
1:A:81:THR:HG21	1:A:232:MET:HB2	1.64	0.78
1:A:4:VAL:CG1	4:D:3036:ALA:HB1	2.14	0.78
1:A:38:HIS:CD2	4:D:3055:GLU:HG3	2.19	0.76
3:C:2057:ASN:HA	3:C:2067:ILE:HG13	1.67	0.76
1:A:128:ASP:OD2	1:A:233:THR:CG2	2.36	0.74
1:A:164:THR:HG21	1:A:169:SER:OG	1.87	0.74
4:D:3058:LYS:O	4:D:3059:ASP:HB2	1.86	0.74
2:B:1117:PHE:CD2	3:C:2204:THR:HG22	2.22	0.74
1:A:32:THR:HB	4:D:3063:LYS:HE3	1.70	0.74
1:A:99:ARG:C	3:C:2238:GLN:HB2	2.10	0.72
3:C:2057:ASN:HD22	3:C:2057:ASN:N	1.87	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1190:ILE:HA	2:B:1195:ASN:ND2	2.05	0.72
1:A:32:THR:HA	4:D:3063:LYS:HE2	1.71	0.72
1:A:3:VAL:HG23	1:A:3:VAL:O	1.90	0.70
1:A:269:THR:H	2:B:1172:ASN:HD21	1.39	0.70
1:A:81:THR:HG22	1:A:232:MET:O	1.92	0.70
1:A:101:VAL:CG1	3:C:2238:GLN:NE2	2.55	0.69
2:B:1142:ASN:HB3	2:B:1145:GLY:H	1.55	0.69
3:C:2173:GLN:HG2	3:C:2174:THR:HG23	1.74	0.69
1:A:209:GLY:O	1:A:212:THR:HG23	1.91	0.69
3:C:2005:ILE:H	3:C:2005:ILE:HD12	1.58	0.69
3:C:2107:TYR:O	3:C:2226:LYS:HE3	1.92	0.69
3:C:2072:VAL:HG13	3:C:2198:ILE:CD1	2.23	0.68
4:D:3007:THR:HA	4:D:3026:HIS:HB3	1.73	0.68
3:C:2233:GLN:HB3	3:C:2238:GLN:HE21	1.57	0.68
1:A:99:ARG:O	3:C:2238:GLN:HB2	1.93	0.68
2:B:1151:THR:O	2:B:1152:ALA:HB2	1.93	0.68
1:A:4:VAL:HG12	4:D:3036:ALA:HB1	1.75	0.67
1:A:85:ASP:O	1:A:87:THR:N	2.25	0.67
4:D:3003:ALA:HB2	4:D:3030:ILE:HG12	1.77	0.67
3:C:2236:LEU:C	3:C:2238:GLN:N	2.48	0.67
1:A:6:ALA:HB1	4:D:3040:SER:OG	1.94	0.66
1:A:105:ARG:HD3	3:C:2231:ILE:HG12	1.76	0.66
2:B:1194:THR:HG21	3:C:2162:SER:HB3	1.78	0.66
1:A:100:MET:CA	3:C:2238:GLN:HG3	2.26	0.66
1:A:101:VAL:CB	3:C:2238:GLN:OE1	2.43	0.66
3:C:2180:GLN:O	3:C:2180:GLN:HG3	1.94	0.66
1:A:263:THR:HG23	1:A:265:ASN:H	1.61	0.65
3:C:2098:THR:HG22	3:C:2101:GLY:N	2.04	0.65
1:A:101:VAL:CB	3:C:2238:GLN:NE2	2.60	0.64
2:B:1084:ASP:O	2:B:1085:ALA:CB	2.46	0.64
1:A:12:ALA:HB2	4:D:3046:PHE:HB3	1.80	0.64
3:C:2129:LYS:HB2	3:C:2196:THR:CG2	2.28	0.64
4:D:3055:GLU:H	4:D:3056:PRO:CD	2.11	0.64
3:C:2200:VAL:HG22	3:C:2201:PRO:HD2	1.79	0.64
1:A:286:LYS:HD2	1:A:289:VAL:HB	1.80	0.63
4:D:3066:PRO:O	4:D:3067:ALA:HB3	1.98	0.63
2:B:1184:ILE:N	2:B:1184:ILE:HD12	2.14	0.63
1:A:80:HIS:CD2	1:A:233:THR:HB	2.32	0.63
1:A:101:VAL:CG1	3:C:2238:GLN:HE22	2.10	0.63
1:A:145:MET:SD	1:A:164:THR:HG23	2.39	0.63
1:A:72:ALA:CB	1:A:103:MET:HG2	2.29	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:THR:CG2	1:A:232:MET:H	2.12	0.62
2:B:1117:PHE:HD2	3:C:2204:THR:HG22	1.63	0.62
3:C:2072:VAL:HG13	3:C:2198:ILE:HD12	1.80	0.62
1:A:101:VAL:HG12	3:C:2238:GLN:NE2	2.15	0.62
1:A:101:VAL:HB	3:C:2238:GLN:HE22	1.65	0.62
4:D:3006:SER:O	4:D:3026:HIS:HB2	2.00	0.62
3:C:2228:THR:HG22	3:C:2229:PRO:CD	2.29	0.62
1:A:164:THR:HG22	1:A:167:ASN:HB2	1.82	0.62
1:A:207:VAL:HG22	1:A:212:THR:HG22	1.82	0.61
3:C:2018:ASP:OD2	4:D:3043:ARG:HD2	2.01	0.61
2:B:1056:PRO:HB2	2:B:1060:THR:HB	1.82	0.61
4:D:3047:THR:HG22	4:D:3048:GLN:N	2.15	0.61
1:A:200:SER:HB3	1:A:207:VAL:HG13	1.83	0.61
1:A:105:ARG:HD3	3:C:2231:ILE:CG1	2.31	0.60
2:B:1151:THR:O	2:B:1152:ALA:CB	2.48	0.60
1:A:13:ARG:HH11	1:A:13:ARG:HG3	1.66	0.60
2:B:1184:ILE:HD12	2:B:1184:ILE:H	1.66	0.60
3:C:2233:GLN:CB	3:C:2238:GLN:HE21	2.15	0.59
1:A:72:ALA:HB3	1:A:103:MET:HG2	1.83	0.59
1:A:286:LYS:C	1:A:288:ASP:H	2.04	0.59
2:B:1020:ASN:HD21	2:B:1062:ARG:HH21	1.51	0.59
1:A:100:MET:HA	3:C:2238:GLN:HG3	1.82	0.59
1:A:81:THR:HG21	1:A:232:MET:CB	2.32	0.59
1:A:81:THR:CG2	1:A:232:MET:HB2	2.31	0.58
2:B:1151:THR:OG1	2:B:1152:ALA:N	2.34	0.58
4:D:3055:GLU:H	4:D:3056:PRO:HD3	1.67	0.58
3:C:2042:ASN:ND2	3:C:2044:MET:H	1.99	0.58
3:C:2057:ASN:ND2	3:C:2057:ASN:H	2.00	0.58
1:A:195:PHE:CE1	1:A:251:ARG:HD2	2.39	0.58
1:A:3:VAL:HG21	1:A:246:LYS:HG3	1.86	0.57
1:A:59:ARG:NH1	4:D:3048:GLN:NE2	2.50	0.57
1:A:85:ASP:O	1:A:85:ASP:OD1	2.22	0.57
3:C:2233:GLN:CD	3:C:2238:GLN:NE2	2.54	0.57
1:A:252:PRO:HG2	2:B:1177:VAL:HG11	1.86	0.57
1:A:12:ALA:HB2	4:D:3046:PHE:CB	2.35	0.56
3:C:2233:GLN:CG	3:C:2238:GLN:HE21	2.18	0.56
1:A:9:ASN:O	1:A:10:ALA:HB3	2.04	0.56
3:C:2107:TYR:CE2	3:C:2225:LEU:HD13	2.40	0.56
1:A:44:PRO:HB3	3:C:2169:PRO:HB3	1.87	0.56
3:C:2049:VAL:HA	4:D:3054:THR:HG22	1.87	0.56
1:A:99:ARG:HA	3:C:2238:GLN:HB2	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:VAL:HG22	1:A:249:VAL:O	2.05	0.55
2:B:1012:ARG:HH11	2:B:1012:ARG:HG3	1.71	0.55
1:A:59:ARG:HH11	4:D:3048:GLN:NE2	2.05	0.55
1:A:272:THR:HG22	3:C:2067:ILE:HD11	1.88	0.55
4:D:3066:PRO:O	4:D:3067:ALA:CB	2.54	0.55
1:A:101:VAL:CB	3:C:2238:GLN:CD	2.71	0.55
2:B:1193:ARG:NH1	3:C:2123:SER:O	2.40	0.54
1:A:32:THR:CB	4:D:3063:LYS:HE3	2.37	0.54
2:B:1063:PHE:CD1	2:B:1246:ALA:HB2	2.41	0.54
3:C:2154:ILE:HD11	3:C:2166:LEU:CA	2.35	0.54
1:A:180:ARG:C	1:A:181:MET:HG3	2.28	0.54
1:A:245:VAL:HG12	1:A:246:LYS:N	2.23	0.54
1:A:289:VAL:CG1	1:A:290:SER:N	2.70	0.54
1:A:99:ARG:O	3:C:2238:GLN:CG	2.56	0.54
1:A:83:ASN:ND2	1:A:84:SER:N	2.54	0.53
1:A:7:VAL:HG22	4:D:3027:TYR:OH	2.08	0.53
4:D:3062:VAL:HB	4:D:3065:LEU:HD13	1.91	0.53
3:C:2107:TYR:O	3:C:2179:VAL:HG11	2.09	0.53
1:A:13:ARG:NH1	1:A:13:ARG:HG3	2.24	0.53
3:C:2236:LEU:C	3:C:2238:GLN:H	2.11	0.53
1:A:275:ARG:HE	3:C:2057:ASN:ND2	1.92	0.52
1:A:59:ARG:HH11	4:D:3048:GLN:HE22	1.55	0.52
2:B:1233:SER:O	2:B:1235:PHE:HD2	1.90	0.52
3:C:2180:GLN:O	3:C:2180:GLN:CG	2.57	0.52
2:B:1084:ASP:O	2:B:1085:ALA:HB2	2.09	0.52
1:A:93:TRP:O	1:A:218:GLN:HB2	2.08	0.52
3:C:2005:ILE:N	3:C:2005:ILE:HD12	2.25	0.52
2:B:1012:ARG:NH1	2:B:1012:ARG:HG3	2.24	0.52
1:A:28:VAL:O	1:A:28:VAL:HG13	2.10	0.52
1:A:73:CYS:SG	1:A:100:MET:CE	2.98	0.52
1:A:79:TYR:OH	1:A:142:HIS:HD2	1.93	0.52
1:A:28:VAL:N	1:A:29:PRO:HD3	2.24	0.51
1:A:79:TYR:OH	1:A:142:HIS:CD2	2.63	0.51
1:A:99:ARG:O	3:C:2238:GLN:CB	2.57	0.51
1:A:183:ILE:HG12	5:A:1000:DOA:H31	1.92	0.51
3:C:2051:SER:HB3	3:C:2099:LEU:HD22	1.93	0.51
1:A:101:VAL:CB	3:C:2238:GLN:HE22	2.23	0.51
1:A:170:ILE:HD11	1:A:181:MET:HG2	1.92	0.51
4:D:3011:GLY:O	4:D:3013:HIS:N	2.41	0.51
1:A:99:ARG:CA	3:C:2238:GLN:HB2	2.41	0.50
1:A:129:GLN:NE2	1:A:130:GLY:H	2.10	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1125:VAL:HG13	2:B:1187:HIS:HB3	1.93	0.50
1:A:99:ARG:HD3	3:C:2237:LEU:HA	1.92	0.50
1:A:172:TRP:CD1	1:A:179:PRO:HG3	2.47	0.50
1:A:64:ILE:HD12	3:C:2040:VAL:O	2.12	0.50
1:A:101:VAL:CG2	3:C:2231:ILE:HG13	2.42	0.50
1:A:286:LYS:O	1:A:288:ASP:N	2.44	0.50
1:A:250:PRO:HD3	3:C:2040:VAL:CG2	2.42	0.50
1:A:111:THR:OG1	1:A:249:VAL:HG22	2.11	0.49
2:B:1148:GLU:OE2	2:B:1153:LYS:HE3	2.12	0.49
1:A:157:VAL:HG23	1:A:158:THR:HG23	1.94	0.49
3:C:2133:ALA:O	3:C:2190:VAL:HA	2.13	0.49
3:C:2233:GLN:CD	3:C:2238:GLN:HG2	2.32	0.49
1:A:275:ARG:NE	3:C:2057:ASN:HD21	1.92	0.49
1:A:154:PRO:HG3	1:A:161:THR:CG2	2.43	0.49
1:A:249:VAL:O	1:A:249:VAL:CG2	2.60	0.49
2:B:1052:GLN:HE21	2:B:1053:PRO:HD2	1.78	0.49
3:C:2173:GLN:HG2	3:C:2174:THR:N	2.28	0.49
2:B:1080:TRP:CE2	2:B:1152:ALA:HB2	2.47	0.49
1:A:99:ARG:O	3:C:2238:GLN:HG3	2.12	0.48
2:B:1033:VAL:O	2:B:1034:GLY:C	2.51	0.48
2:B:1031:VAL:HB	4:D:3058:LYS:HG2	1.94	0.48
1:A:3:VAL:O	1:A:3:VAL:CG2	2.59	0.48
1:A:263:THR:HG21	1:A:265:ASN:HB2	1.96	0.48
3:C:2072:VAL:HG13	3:C:2198:ILE:HD11	1.94	0.48
1:A:85:ASP:OD1	1:A:87:THR:HB	2.13	0.48
1:A:81:THR:HG23	1:A:232:MET:H	1.78	0.47
1:A:101:VAL:HG21	3:C:2231:ILE:HD12	1.94	0.47
1:A:264:VAL:HG23	7:A:2001:HOH:O	2.14	0.47
1:A:285:VAL:HG12	1:A:285:VAL:O	2.14	0.47
2:B:1234:ASP:C	2:B:1236:SER:H	2.08	0.47
2:B:1062:ARG:HG3	2:B:1062:ARG:HH11	1.80	0.47
1:A:128:ASP:CG	1:A:233:THR:HG22	2.34	0.47
2:B:1020:ASN:HD21	2:B:1062:ARG:HE	1.62	0.47
4:D:3010:THR:O	4:D:3010:THR:CG2	2.61	0.47
2:B:1109:HIS:HD2	2:B:1199:THR:OG1	1.97	0.47
1:A:9:ASN:O	1:A:10:ALA:CB	2.63	0.47
3:C:2057:ASN:ND2	3:C:2057:ASN:N	2.59	0.47
2:B:1189:TRP:O	2:B:1195:ASN:ND2	2.47	0.47
1:A:121:PHE:CZ	1:A:238:MET:HE2	2.50	0.47
1:A:172:TRP:CG	1:A:179:PRO:HG3	2.50	0.47
3:C:2115:LYS:HG3	3:C:2217:CYS:SG	2.55	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1103:ARG:HB2	2:B:1210:MET:HG2	1.96	0.46
1:A:274:LYS:HD2	3:C:2059:ALA:HB2	1.97	0.46
1:A:263:THR:HG23	1:A:265:ASN:N	2.30	0.46
3:C:2156:TRP:CD1	3:C:2164:CYS:HB2	2.50	0.46
3:C:2044:MET:HE2	3:C:2220:PHE:HD1	1.79	0.46
3:C:2231:ILE:HA	3:C:2231:ILE:HD13	1.76	0.46
2:B:1234:ASP:C	2:B:1236:SER:N	2.66	0.46
1:A:286:LYS:HD2	1:A:289:VAL:CB	2.45	0.46
1:A:263:THR:CG2	1:A:265:ASN:HB2	2.46	0.46
1:A:154:PRO:CA	1:A:161:THR:HG21	2.46	0.46
1:A:81:THR:CG2	1:A:232:MET:O	2.62	0.46
3:C:2177:ARG:HG2	3:C:2185:THR:HB	1.98	0.46
2:B:1020:ASN:HD21	2:B:1062:ARG:NH2	2.14	0.46
1:A:81:THR:HG22	1:A:232:MET:C	2.37	0.45
3:C:2201:PRO:HG2	3:C:2204:THR:HG21	1.99	0.45
2:B:1142:ASN:HB2	2:B:1164:ASN:HB3	1.98	0.45
1:A:154:PRO:HG3	1:A:161:THR:HG21	1.99	0.45
2:B:1232:SER:C	2:B:1234:ASP:H	2.19	0.45
1:A:267:SER:O	1:A:269:THR:HG23	2.17	0.45
1:A:188:ILE:HD13	1:A:188:ILE:HG21	1.62	0.45
3:C:2010:SER:O	3:C:2011:ASN:HB2	2.17	0.45
3:C:2196:THR:O	3:C:2197:GLY:O	2.34	0.45
1:A:211:ASN:HA	1:A:211:ASN:HD22	1.53	0.45
1:A:105:ARG:HG3	1:A:254:ARG:HB3	1.99	0.44
1:A:81:THR:CG2	1:A:232:MET:N	2.81	0.44
1:A:121:PHE:CZ	1:A:238:MET:CE	3.01	0.44
1:A:260:ASN:CG	1:A:263:THR:HG22	2.29	0.44
1:A:252:PRO:HD3	2:B:1184:ILE:CD1	2.37	0.44
4:D:3063:LYS:CD	4:D:3067:ALA:HB2	2.48	0.44
4:D:3068:LEU:O	4:D:3069:ASN:HB2	2.17	0.44
3:C:2129:LYS:CB	3:C:2196:THR:HG22	2.40	0.44
3:C:2044:MET:O	3:C:2048:GLU:HG3	2.18	0.43
1:A:193:SER:HB2	2:B:1207:ASN:ND2	2.33	0.43
2:B:1083:PRO:HD2	2:B:1217:HIS:HA	2.01	0.43
2:B:1193:ARG:HG3	2:B:1194:THR:CG2	2.42	0.43
3:C:2072:VAL:CG1	3:C:2198:ILE:HD11	2.49	0.43
1:A:92:SER:HA	1:A:219:ILE:O	2.17	0.43
1:A:187:SER:O	3:C:2031:THR:HG21	2.19	0.43
2:B:1248:MET:O	2:B:1249:CYS:HB2	2.18	0.43
3:C:2160:LEU:HD21	4:D:3069:ASN:H	1.82	0.43
4:D:3067:ALA:O	4:D:3068:LEU:HD23	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:TRP:O	1:A:218:GLN:CB	2.67	0.43
3:C:2146:LYS:HB2	3:C:2146:LYS:HE2	1.68	0.43
3:C:2074:SER:HA	3:C:2198:ILE:O	2.19	0.43
1:A:101:VAL:N	3:C:2238:GLN:CD	2.72	0.43
1:A:199:TRP:CZ3	1:A:208:TYR:HB2	2.54	0.42
2:B:1190:ILE:HA	2:B:1195:ASN:HD21	1.81	0.42
4:D:3010:THR:O	4:D:3010:THR:HG22	2.18	0.42
2:B:1184:ILE:H	2:B:1184:ILE:CD1	2.28	0.42
1:A:245:VAL:CG1	1:A:246:LYS:N	2.82	0.42
3:C:2201:PRO:HG2	3:C:2204:THR:CG2	2.50	0.42
1:A:12:ALA:O	1:A:58:SER:HA	2.19	0.42
1:A:91:ALA:HB3	1:A:221:VAL:HG13	2.01	0.42
1:A:204:GLN:NE2	2:B:1143:GLU:HG2	2.34	0.42
1:A:142:HIS:HE1	1:A:174:GLU:OE1	2.02	0.42
2:B:1259:THR:HG22	2:B:1260:ALA:N	2.35	0.42
3:C:2193:TRP:N	3:C:2193:TRP:CD1	2.87	0.42
2:B:1256:ARG:HD2	2:B:1257:LEU:O	2.18	0.42
1:A:67:PHE:CG	3:C:2043:LEU:HD11	2.55	0.41
4:D:3047:THR:CG2	4:D:3048:GLN:H	2.24	0.41
2:B:1196:ASN:C	2:B:1196:ASN:OD1	2.59	0.41
3:C:2127:THR:HG22	3:C:2199:VAL:HB	2.02	0.41
1:A:186:ILE:HD11	3:C:2025:MET:CE	2.50	0.41
1:A:213:LEU:HA	1:A:213:LEU:HD23	1.61	0.41
1:A:216:MET:HE1	5:A:1000:DOA:H101	2.01	0.41
2:B:1231:TYR:CE1	2:B:1237:THR:HG22	2.55	0.41
2:B:1075:SER:HA	2:B:1076:PRO:HD3	1.89	0.41
1:A:129:GLN:NE2	1:A:130:GLY:N	2.68	0.41
4:D:3014:GLU:HA	4:D:3014:GLU:OE2	2.20	0.41
1:A:101:VAL:O	1:A:102:GLN:C	2.59	0.41
2:B:1083:PRO:HD3	2:B:1218:ASN:H	1.86	0.41
2:B:1233:SER:O	2:B:1235:PHE:N	2.53	0.41
3:C:2161:GLN:NE2	4:D:3066:PRO:HB3	2.35	0.41
2:B:1256:ARG:HD3	2:B:1257:LEU:HD23	2.03	0.41
2:B:1038:TRP:CD1	2:B:1039:PRO:HD2	2.55	0.41
4:D:3003:ALA:HB2	4:D:3030:ILE:CG1	2.47	0.41
2:B:1155:PHE:HB3	2:B:1170:VAL:HG13	2.02	0.41
1:A:101:VAL:HG21	3:C:2231:ILE:CD1	2.50	0.41
2:B:1123:LEU:HB2	2:B:1189:TRP:CZ3	2.56	0.41
3:C:2018:ASP:OD1	4:D:3040:SER:HB2	2.20	0.41
4:D:3008:GLN:HG3	4:D:3026:HIS:HA	2.04	0.40
2:B:1246:ALA:HA	2:B:1247:PRO:HD3	1.95	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ILE:CD1	1:A:238:MET:HE1	2.51	0.40
3:C:2105:ASN:HB3	3:C:2228:THR:HG23	2.02	0.40
1:A:178:PRO:HA	1:A:179:PRO:HD3	1.83	0.40
3:C:2115:LYS:HE3	3:C:2115:LYS:HB2	1.75	0.40
3:C:2081:GLN:HB2	3:C:2193:TRP:CZ3	2.56	0.40
2:B:1110:VAL:HG22	2:B:1243:VAL:HG22	2.03	0.40
1:A:101:VAL:HG23	1:A:258:TYR:CE2	2.56	0.40
4:D:3003:ALA:CB	4:D:3030:ILE:HG12	2.49	0.40
3:C:2126:ALA:HA	3:C:2200:VAL:HG23	2.03	0.40
1:A:129:GLN:HE21	1:A:130:GLY:N	2.20	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	288/292 (99%)	259 (90%)	20 (7%)	9 (3%)	5 21
2	B	251/262 (96%)	220 (88%)	23 (9%)	8 (3%)	5 20
3	C	236/238 (99%)	224 (95%)	10 (4%)	2 (1%)	24 60
4	D	57/68 (84%)	44 (77%)	9 (16%)	4 (7%)	1 4
All	All	832/860 (97%)	747 (90%)	62 (8%)	23 (3%)	6 24

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	9	ASN
1	A	214	ASN
1	A	228	SER
2	B	1152	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	1234	ASP
2	B	1235	PHE
2	B	1261	LEU
3	C	2197	GLY
4	D	3012	ALA
4	D	3055	GLU
4	D	3064	SER
1	A	227	SER
2	B	1034	GLY
2	B	1085	ALA
3	C	2236	LEU
4	D	3063	LYS
1	A	10	ALA
2	B	1150	GLU
1	A	86	GLN
2	B	1082	PHE
1	A	4	VAL
1	A	287	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	259/262 (99%)	236 (91%)	23 (9%)	12 35
2	B	217/225 (96%)	199 (92%)	18 (8%)	14 38
3	C	204/204 (100%)	176 (86%)	28 (14%)	4 13
4	D	51/56 (91%)	45 (88%)	6 (12%)	6 19
All	All	731/747 (98%)	656 (90%)	75 (10%)	9 26

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	28	VAL
1	A	34	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	69	SER
1	A	81	THR
1	A	94	THR
1	A	96	SER
1	A	103	MET
1	A	131	THR
1	A	161	THR
1	A	164	THR
1	A	181	MET
1	A	186	ILE
1	A	188	ILE
1	A	207	VAL
1	A	212	THR
1	A	214	ASN
1	A	221	VAL
1	A	233	THR
1	A	249	VAL
1	A	251	ARG
1	A	264	VAL
1	A	288	ASP
2	B	1015	SER
2	B	1020	ASN
2	B	1025	THR
2	B	1030	ASN
2	B	1048	THR
2	B	1060	THR
2	B	1125	VAL
2	B	1158	THR
2	B	1163	THR
2	B	1170	VAL
2	B	1171	THR
2	B	1184	ILE
2	B	1229	LEU
2	B	1233	SER
2	B	1235	PHE
2	B	1245	VAL
2	B	1256	ARG
2	B	1257	LEU
3	C	2005	ILE
3	C	2021	SER
3	C	2030	VAL
3	C	2031	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	2035	ASN
3	C	2056	ASN
3	C	2057	ASN
3	C	2058	VAL
3	C	2072	VAL
3	C	2078	GLN
3	C	2096	LYS
3	C	2098	THR
3	C	2099	LEU
3	C	2103	ILE
3	C	2127	THR
3	C	2149	MET
3	C	2154	ILE
3	C	2178	LEU
3	C	2180	GLN
3	C	2181	GLN
3	C	2189	ASN
3	C	2200	VAL
3	C	2208	CYS
3	C	2224	LEU
3	C	2225	LEU
3	C	2228	THR
3	C	2231	ILE
3	C	2238	GLN
4	D	3010	THR
4	D	3014	GLU
4	D	3025	ILE
4	D	3028	THR
4	D	3066	PRO
4	D	3069	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	HIS
1	A	83	ASN
1	A	129	GLN
1	A	142	HIS
1	A	201	HIS
1	A	204	GLN
1	A	211	ASN
1	A	214	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	1020	ASN
2	B	1030	ASN
2	B	1052	GLN
2	B	1109	HIS
2	B	1119	GLN
2	B	1172	ASN
2	B	1195	ASN
3	C	2012	GLN
3	C	2035	ASN
3	C	2042	ASN
3	C	2056	ASN
3	C	2057	ASN
3	C	2088	GLN
3	C	2140	ASN
3	C	2189	ASN
3	C	2238	GLN
4	D	3044	GLN
4	D	3048	GLN

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

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	DOA	A	1000	-	11,14,14	0.50	0	11,14,14	1.58	4 (36%)
6	MYR	D	3500	-	14,14,15	0.63	0	12,13,15	1.13	1 (8%)

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
5	DOA	A	1000	-	-	0/10/12/12	0/0/0/0
6	MYR	D	3500	-	-	0/11/12/13	0/0/0/0

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1000	DOA	C5-C4-C3	-2.85	99.83	114.53
5	A	1000	DOA	C7-C6-C5	-2.55	101.36	114.53
6	D	3500	MYR	C7-C6-C5	-2.45	101.89	114.53
5	A	1000	DOA	C3-C2-CA	-2.35	102.94	114.01
5	A	1000	DOA	C10-C9-C8	-2.27	102.80	114.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1000	DOA	2	0
6	D	3500	MYR	1	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	290/292 (99%)	0.33	20 (6%) 20 14	1, 12, 71, 119	0
2	B	253/262 (96%)	0.00	6 (2%) 62 57	2, 9, 37, 85	0
3	C	238/238 (100%)	-0.18	1 (0%) 93 92	1, 8, 29, 75	0
4	D	61/68 (89%)	0.88	13 (21%) 1 0	6, 40, 83, 106	0
All	All	842/860 (97%)	0.13	40 (4%) 34 28	1, 10, 60, 119	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	GLY	13.3
1	A	289	VAL	12.4
1	A	4	VAL	10.3
2	B	1262	GLN	10.1
1	A	2	ASP	9.7
1	A	7	VAL	8.0
1	A	3	VAL	6.5
1	A	5	GLU	6.4
1	A	8	GLU	6.0
1	A	290	SER	5.8
1	A	6	ALA	5.5
4	D	3060	ILE	5.5
4	D	3065	LEU	5.5
1	A	288	ASP	5.0
4	D	3013	HIS	4.8
2	B	1235	PHE	4.4
3	C	2238	GLN	4.1
1	A	287	PRO	3.6
4	D	3023	SER	3.3
1	A	10	ALA	3.2
2	B	1163	THR	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	13	ARG	3.1
1	A	25	SER	3.1
1	A	9	ASN	3.0
2	B	1261	LEU	2.7
4	D	3064	SER	2.6
4	D	3062	VAL	2.6
4	D	3066	PRO	2.4
4	D	3012	ALA	2.4
4	D	3059	ASP	2.4
4	D	3011	GLY	2.3
1	A	18	ILE	2.3
2	B	1164	ASN	2.3
1	A	131	THR	2.3
1	A	11	VAL	2.2
4	D	3047	THR	2.1
2	B	1161	ASN	2.1
1	A	214	ASN	2.0
4	D	3024	ILE	2.0
4	D	3063	LYS	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
5	DOA	A	1000	15/15	0.92	0.24	3.08	7,19,41,52	0
6	MYR	D	3500	15/16	0.71	0.43	-	24,51,73,75	0

6.5 Other polymers (i)

There are no such residues in this entry.