



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:30 pm BST

PDB ID : 6IGX  
Title : Crystal structure of human CAP-G in complex with CAP-H  
Authors : Hara, K.; Migita, T.; Shimizu, K.; Hashimoto, H.  
Deposited on : 2018-09-26  
Resolution : 3.00 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](mailto: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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

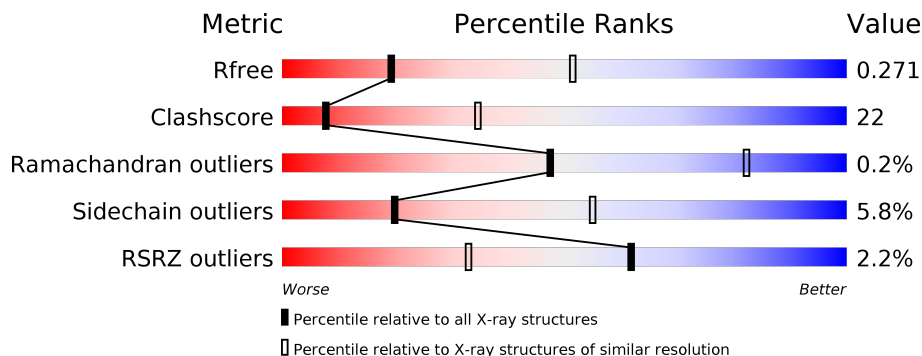
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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  $\geq 3$ , 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	B	839	<div style="display: flex; align-items: center;"> <div style="width: 10%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 41%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">% 51% 33% • 13%</p>
1	D	839	<div style="display: flex; align-items: center;"> <div style="width: 10%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 39%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 36%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">% 49% 36% • 13%</p>
2	A	57	<div style="display: flex; align-items: center;"> <div style="width: 11%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 54%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">11% 65% 18% 5% 12%</p>
2	C	57	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 52%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">9% 61% 19% 5% 14%</p>

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 12379 atoms, of which 17 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 Condensin complex subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	730	Total	C	N	O	S	0	0	0
			5748	3699	964	1055	30			
1	D	731	Total	C	N	O	S	0	0	0
			5767	3714	967	1056	30			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	MET	-	expression tag	UNP Q9BPX3
B	-12	GLY	-	expression tag	UNP Q9BPX3
B	-11	SER	-	expression tag	UNP Q9BPX3
B	-10	SER	-	expression tag	UNP Q9BPX3
B	-9	HIS	-	expression tag	UNP Q9BPX3
B	-8	HIS	-	expression tag	UNP Q9BPX3
B	-7	HIS	-	expression tag	UNP Q9BPX3
B	-6	HIS	-	expression tag	UNP Q9BPX3
B	-5	HIS	-	expression tag	UNP Q9BPX3
B	-4	HIS	-	expression tag	UNP Q9BPX3
B	-3	SER	-	expression tag	UNP Q9BPX3
B	-2	GLN	-	expression tag	UNP Q9BPX3
B	-1	ASP	-	expression tag	UNP Q9BPX3
B	0	PRO	-	expression tag	UNP Q9BPX3
D	-13	MET	-	expression tag	UNP Q9BPX3
D	-12	GLY	-	expression tag	UNP Q9BPX3
D	-11	SER	-	expression tag	UNP Q9BPX3
D	-10	SER	-	expression tag	UNP Q9BPX3
D	-9	HIS	-	expression tag	UNP Q9BPX3
D	-8	HIS	-	expression tag	UNP Q9BPX3
D	-7	HIS	-	expression tag	UNP Q9BPX3
D	-6	HIS	-	expression tag	UNP Q9BPX3
D	-5	HIS	-	expression tag	UNP Q9BPX3
D	-4	HIS	-	expression tag	UNP Q9BPX3
D	-3	SER	-	expression tag	UNP Q9BPX3

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	GLN	-	expression tag	UNP Q9BPX3
D	-1	ASP	-	expression tag	UNP Q9BPX3
D	0	PRO	-	expression tag	UNP Q9BPX3

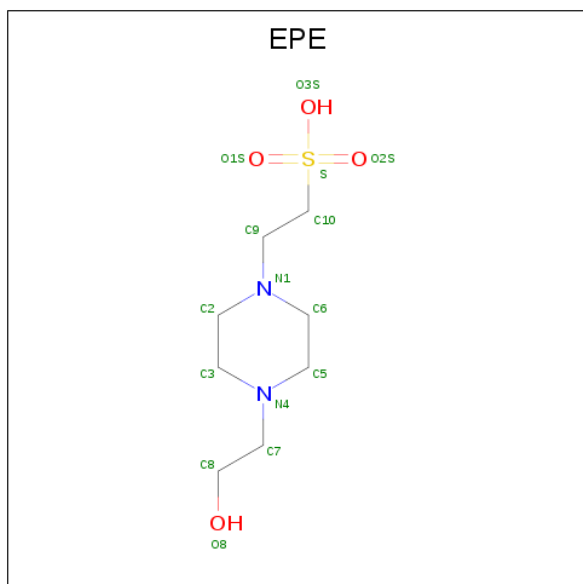
- Molecule 2 is a protein called Condensin complex subunit 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	A	50	Total	C	N	O	0	0	0
			420	271	68	81			
2	C	49	Total	C	N	O	0	0	0
			406	259	67	80			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	459	MET	-	initiating methionine	UNP Q15003
C	459	MET	-	initiating methionine	UNP Q15003

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			S
3	D	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		

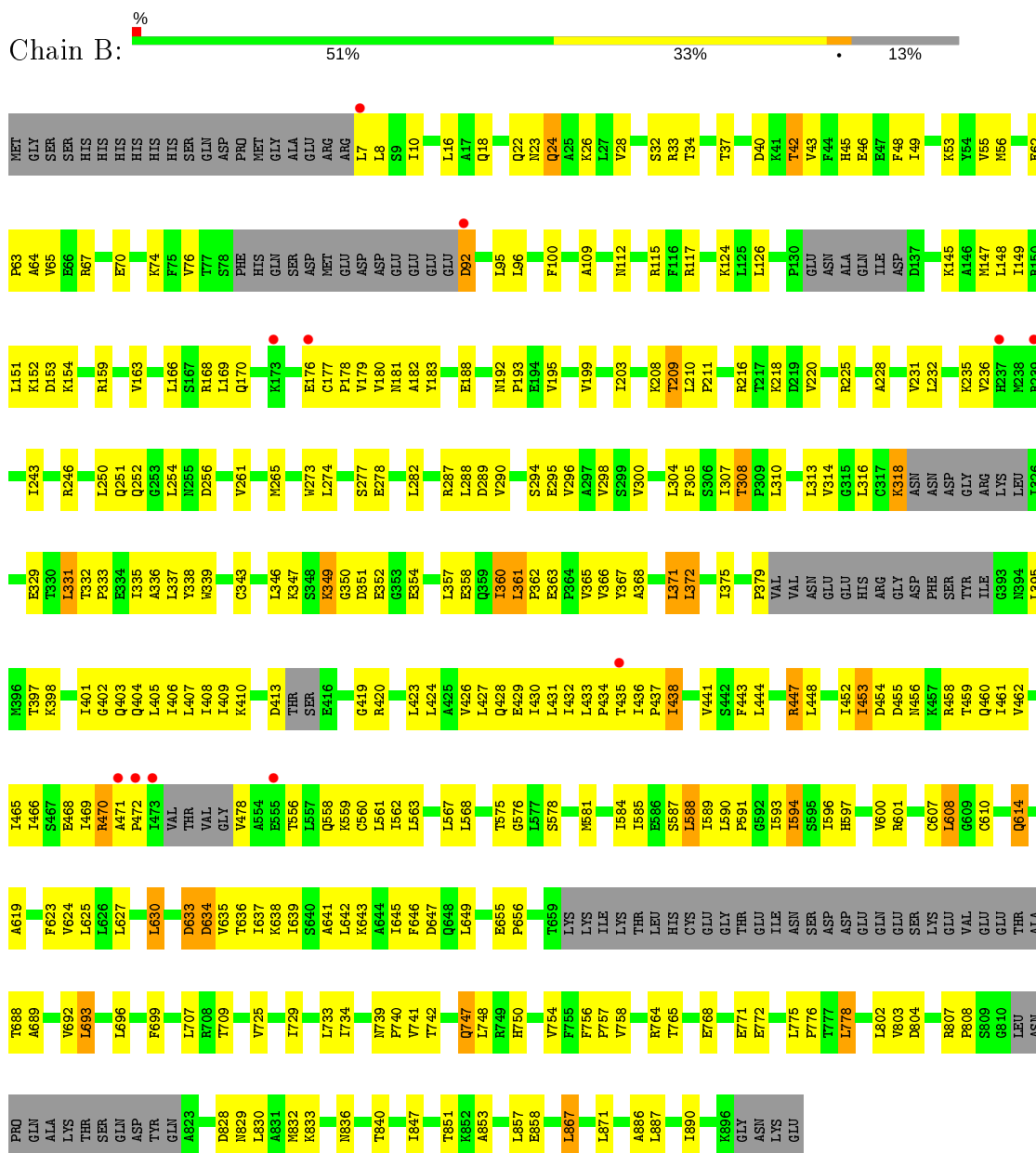
- Molecule 4 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
4	B	4	Total O 4 4	0	0
4	D	2	Total O 2 2	0	0

### 3 Residue-property plots i

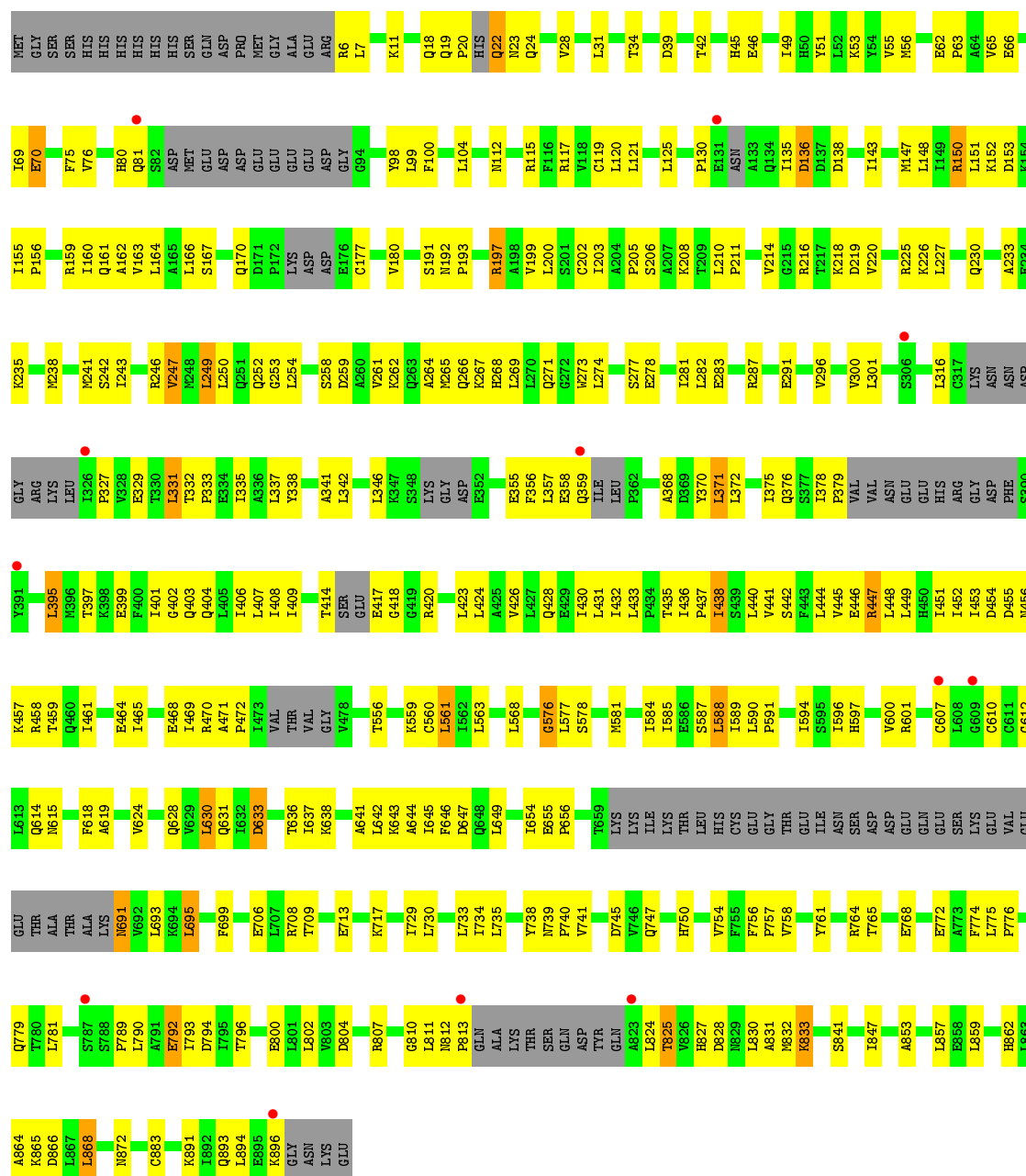
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Condensin complex subunit 3



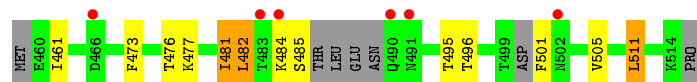
- Molecule 1: Condensin complex subunit 3

Chain D:  %



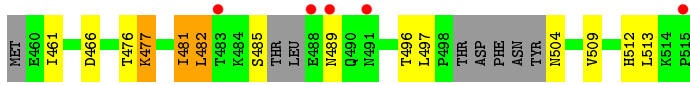
• Molecule 2: Condensin complex subunit 2

Chain A:  %



• Molecule 2: Condensin complex subunit 2

Chain C:  %





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.43Å 62.00Å 130.88Å 90.00° 93.47° 90.00°	Depositor
Resolution (Å)	19.81 – 3.00 19.81 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (19.81-3.00) 99.0 (19.81-3.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.44 (at 2.98Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.212 , 0.272 0.215 , 0.271	Depositor DCC
$R_{free}$ test set	1982 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.0	Xtrriage
Anisotropy	0.222	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 45.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12379	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: EPE

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	B	0.21	0/5829	0.41	0/7886
1	D	0.21	0/5847	0.41	0/7908
2	A	0.24	0/427	0.50	0/577
2	C	0.25	0/412	0.50	0/557
All	All	0.22	0/12515	0.42	0/16928

There are no bond length outliers.

There are no bond angle outliers.

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	B	5748	0	6025	260	0
1	D	5767	0	6033	271	0
2	A	420	0	407	27	0
2	C	406	0	395	15	0
3	D	15	17	17	0	0
4	B	4	0	0	0	0
4	D	2	0	0	1	0
All	All	12362	17	12877	550	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 22.

All (550) 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:B:395:LEU:HD13	1:B:398:LYS:HE3	1.33	1.09
2:C:485:SER:HA	2:C:489:ASN:HB2	1.34	1.07
1:D:430:ILE:HG22	1:D:436:ILE:HD11	1.08	1.05
1:D:576:GLY:HA2	1:D:614:GLN:HG3	1.47	0.95
1:D:893:GLN:HA	1:D:896:LYS:HE3	1.48	0.94
1:D:577:LEU:HG	1:D:614:GLN:HB3	1.51	0.93
1:B:576:GLY:HA2	1:B:614:GLN:HG3	1.54	0.89
1:B:469:ILE:HD13	1:B:559:LYS:HD2	1.57	0.85
1:D:148:LEU:HD23	1:D:151:LEU:HD12	1.59	0.84
1:B:593:ILE:HD11	1:B:608:LEU:HD12	1.60	0.82
1:D:430:ILE:HG22	1:D:436:ILE:CD1	2.03	0.82
1:D:830:LEU:HD23	1:D:857:LEU:HD21	1.62	0.81
1:D:409:ILE:HB	1:D:447:ARG:HG2	1.64	0.79
1:D:56:MET:HA	1:D:117:ARG:HG3	1.64	0.78
1:B:395:LEU:HD13	1:B:398:LYS:CE	2.13	0.77
1:D:636:THR:HG23	1:D:637:ILE:HD12	1.68	0.76
1:B:756:PHE:HB2	1:B:757:PRO:HD3	1.67	0.76
1:D:238:MET:HE3	1:D:246:ARG:HD2	1.67	0.75
1:D:250:LEU:HA	1:D:265:MET:HE3	1.68	0.75
1:D:150:ARG:NH1	1:D:153:ASP:OD2	2.20	0.74
2:A:482:LEU:HD22	2:A:485:SER:H	1.51	0.74
1:D:250:LEU:HA	1:D:265:MET:CE	2.18	0.74
1:B:177:CYS:HB3	1:B:180:VAL:HG22	1.68	0.74
1:D:81:GLN:HG3	1:D:130:PRO:HG3	1.70	0.73
2:A:482:LEU:HD23	2:A:484:LYS:HB2	1.70	0.73
1:D:424:LEU:HD22	1:D:448:LEU:HD12	1.70	0.73
1:B:601:ARG:NH1	1:B:633:ASP:OD1	2.22	0.73
1:B:447:ARG:HA	1:B:447:ARG:HH11	1.54	0.73
1:D:332:THR:HB	1:D:333:PRO:HD2	1.68	0.73
1:D:633:ASP:O	1:D:638:LYS:NZ	2.21	0.73
1:B:218:LYS:HG2	1:B:252:GLN:OE1	1.88	0.73
1:B:447:ARG:HA	1:B:447:ARG:NH1	2.04	0.73
1:D:115:ARG:HD2	1:D:150:ARG:NH1	2.02	0.73
1:D:112:ASN:OD1	1:D:115:ARG:NH2	2.23	0.72
1:D:115:ARG:HD2	1:D:150:ARG:HH12	1.54	0.72
1:D:20:PRO:C	1:D:22:GLN:HB2	2.10	0.71
1:D:81:GLN:HA	1:D:130:PRO:HG2	1.72	0.71
1:B:591:PRO:HA	1:B:594:ILE:HD11	1.72	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:ARG:NH1	1:D:261:VAL:HG21	2.06	0.70
2:C:482:LEU:HD22	2:C:482:LEU:H	1.54	0.70
1:B:148:LEU:HD23	1:B:151:LEU:HD12	1.74	0.70
1:B:646:PHE:CE1	1:B:696:LEU:HD13	2.25	0.70
1:B:290:VAL:HG13	1:B:337:LEU:HD22	1.73	0.70
1:B:154:LYS:HA	2:A:481:ILE:HG23	1.74	0.69
1:D:7:LEU:HD12	1:D:34:THR:HA	1.74	0.69
2:A:482:LEU:H	2:A:482:LEU:HD13	1.58	0.69
1:D:708:ARG:NH1	1:D:745:ASP:OD2	2.26	0.69
1:B:243:ILE:HG21	1:B:289:ASP:HB2	1.74	0.69
1:D:197:ARG:NE	1:D:227:LEU:HD22	2.08	0.68
1:D:577:LEU:HD12	1:D:615:ASN:HB2	1.75	0.68
1:B:362:PRO:HB2	1:B:366:VAL:CG2	2.23	0.68
1:D:230:GLN:HG2	1:D:268:HIS:CD2	2.28	0.68
1:B:438:ILE:HG22	1:B:562:ILE:HD12	1.75	0.68
1:B:343:CYS:SG	1:B:361:LEU:HD11	2.33	0.68
1:B:560:CYS:HB3	1:B:588:LEU:HD11	1.74	0.68
1:B:7:LEU:CD1	1:B:37:THR:HG21	2.23	0.68
1:D:756:PHE:HB2	1:D:757:PRO:HD3	1.75	0.68
1:B:404:GLN:O	1:B:408:ILE:HG13	1.94	0.68
2:A:482:LEU:HD23	2:A:484:LYS:HD2	1.76	0.67
1:D:812:ASN:HB2	1:D:813:PRO:HD3	1.76	0.67
1:B:56:MET:HA	1:B:117:ARG:HG3	1.75	0.67
2:A:482:LEU:CD2	2:A:484:LYS:HB2	2.23	0.67
1:B:332:THR:HB	1:B:333:PRO:HD2	1.76	0.67
1:D:197:ARG:HE	1:D:227:LEU:HD22	1.58	0.67
1:D:160:ILE:O	1:D:163:VAL:HG22	1.94	0.67
1:D:654:ILE:HD13	1:D:693:LEU:HD11	1.76	0.67
1:B:426:VAL:O	1:B:430:ILE:HG13	1.95	0.67
1:D:225:ARG:HH12	1:D:261:VAL:HG21	1.60	0.67
1:D:433:LEU:HD13	1:D:435:THR:HB	1.75	0.66
1:B:590:LEU:HB2	1:B:591:PRO:HD3	1.77	0.66
1:B:316:LEU:HD12	1:B:338:TYR:CZ	2.30	0.66
1:B:742:THR:HG21	1:B:748:LEU:HD22	1.78	0.66
1:D:430:ILE:O	1:D:433:LEU:HG	1.95	0.66
1:D:643:LYS:HD3	2:C:512:HIS:HB3	1.78	0.66
1:B:633:ASP:O	1:B:638:LYS:NZ	2.29	0.65
1:D:368:ALA:HB1	1:D:426:VAL:HG21	1.79	0.65
1:D:283:GLU:OE2	1:D:287:ARG:NH2	2.30	0.65
1:B:576:GLY:HA2	1:B:614:GLN:CG	2.25	0.64
1:B:764:ARG:NH1	1:B:768:GLU:OE2	2.30	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:576:GLY:CA	1:B:614:GLN:HG3	2.27	0.64
1:D:893:GLN:HA	1:D:896:LYS:CE	2.27	0.64
1:D:790:LEU:O	1:D:793:ILE:HD12	1.97	0.64
1:B:589:ILE:HD13	1:B:607:CYS:HB3	1.78	0.64
1:B:225:ARG:NH1	1:B:261:VAL:HG21	2.12	0.64
1:D:428:GLN:HG2	1:D:465:ILE:HD11	1.78	0.64
1:B:152:LYS:O	2:A:481:ILE:HG12	1.98	0.64
1:B:277:SER:O	1:B:278:GLU:HB2	1.97	0.64
1:B:406:ILE:HD13	1:B:444:LEU:HG	1.80	0.64
1:D:18:GLN:HE22	2:C:461:ILE:HB	1.63	0.64
1:D:409:ILE:HB	1:D:447:ARG:CG	2.27	0.64
1:B:115:ARG:NH1	1:B:153:ASP:OD2	2.32	0.63
1:D:274:LEU:HD21	1:D:281:ILE:HG12	1.80	0.63
1:B:431:LEU:HD21	1:B:444:LEU:HB3	1.81	0.63
1:D:226:LYS:HG3	1:D:264:ALA:HB2	1.80	0.63
1:B:410:LYS:HD3	1:B:447:ARG:NH2	2.14	0.63
1:D:465:ILE:O	1:D:469:ILE:HG13	1.98	0.63
1:B:624:VAL:HG21	1:B:688:THR:HB	1.79	0.63
1:D:438:ILE:HA	1:D:441:VAL:HG23	1.81	0.63
1:B:804:ASP:O	1:B:807:ARG:HG3	1.99	0.62
1:D:447:ARG:NH1	1:D:447:ARG:HA	2.14	0.62
1:B:428:GLN:HG2	1:B:465:ILE:HD11	1.80	0.62
1:D:66:GLU:O	1:D:70:GLU:HB2	1.99	0.62
2:A:482:LEU:H	2:A:482:LEU:CD1	2.12	0.62
1:D:81:GLN:CG	1:D:130:PRO:HG3	2.30	0.62
1:D:740:PRO:HG2	1:D:789:PRO:HB2	1.81	0.62
1:D:404:GLN:O	1:D:408:ILE:HG13	2.00	0.61
1:B:55:VAL:HG12	2:A:461:ILE:CD1	2.29	0.61
2:A:482:LEU:CD2	2:A:485:SER:H	2.13	0.61
1:B:232:LEU:HA	1:B:236:VAL:HG13	1.81	0.61
1:B:346:LEU:HD12	1:B:360:ILE:HD11	1.83	0.61
1:B:63:PRO:O	1:B:67:ARG:HG3	2.00	0.61
1:D:449:LEU:HD12	1:D:458:ARG:HD3	1.82	0.61
1:B:438:ILE:HA	1:B:441:VAL:HG23	1.83	0.61
1:D:864:ALA:HA	1:D:894:LEU:HD22	1.81	0.61
1:D:282:LEU:HG	1:D:316:LEU:HD22	1.82	0.61
1:B:294:SER:O	1:B:298:VAL:HG23	2.01	0.61
1:B:62:GLU:HG3	1:B:63:PRO:HD2	1.83	0.61
1:B:55:VAL:HG12	2:A:461:ILE:HD13	1.82	0.60
1:B:624:VAL:CG2	1:B:688:THR:HB	2.31	0.60
1:B:409:ILE:HB	1:B:447:ARG:HD2	1.82	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:CYS:SG	1:D:180:VAL:HG13	2.42	0.60
1:B:452:ILE:CD1	1:B:461:ILE:HD12	2.32	0.60
1:B:351:ASP:OD2	1:D:418:GLY:N	2.34	0.60
1:B:371:LEU:CD1	1:B:409:ILE:HD11	2.32	0.60
1:B:429:GLU:O	1:B:433:LEU:HG	2.02	0.60
1:B:362:PRO:HB2	1:B:366:VAL:HG23	1.83	0.59
1:D:642:LEU:HD22	1:D:646:PHE:HE2	1.67	0.59
1:B:40:ASP:O	1:B:43:VAL:HG22	2.03	0.59
1:B:593:ILE:CD1	1:B:608:LEU:HD12	2.31	0.59
1:B:210:LEU:N	1:B:211:PRO:HD2	2.18	0.59
1:B:639:ILE:O	1:B:643:LYS:HG3	2.03	0.59
1:B:406:ILE:HG23	1:B:444:LEU:HD23	1.85	0.59
1:D:282:LEU:HG	1:D:316:LEU:CD2	2.33	0.59
1:D:642:LEU:HD22	1:D:646:PHE:CE2	2.38	0.59
2:A:482:LEU:HD23	2:A:484:LYS:CB	2.33	0.58
1:D:246:ARG:HG3	1:D:273:TRP:CH2	2.38	0.58
1:B:166:LEU:HD23	1:B:169:LEU:HD12	1.85	0.58
1:D:115:ARG:NH1	1:D:153:ASP:OD2	2.36	0.58
1:D:148:LEU:HD23	1:D:151:LEU:CD1	2.32	0.58
1:D:42:THR:O	1:D:46:GLU:HG3	2.03	0.58
1:B:734:ILE:HD13	1:B:802:LEU:HD21	1.86	0.58
1:D:119:CYS:SG	1:D:150:ARG:HG2	2.43	0.58
1:B:254:LEU:HD13	1:B:265:MET:CE	2.34	0.58
1:B:452:ILE:HD13	1:B:461:ILE:HD12	1.86	0.58
1:D:200:LEU:O	1:D:203:ILE:HD11	2.04	0.58
1:D:218:LYS:HG2	1:D:252:GLN:OE1	2.03	0.58
1:D:167:SER:O	1:D:170:GLN:HG2	2.03	0.58
1:D:205:PRO:HG2	1:D:235:LYS:HB3	1.85	0.58
1:B:365:VAL:CG2	1:B:419:GLY:HA2	2.33	0.57
1:D:371:LEU:HD22	1:D:375:ILE:CD1	2.33	0.57
1:B:290:VAL:HG13	1:B:337:LEU:CD2	2.33	0.57
1:B:591:PRO:HA	1:B:594:ILE:CD1	2.34	0.57
1:D:631:GLN:OE1	1:D:695:LEU:HD21	2.04	0.57
1:D:768:GLU:O	1:D:772:GLU:HG3	2.04	0.57
1:B:568:LEU:HB3	1:B:610:CYS:HB3	1.85	0.57
1:D:18:GLN:NE2	2:C:461:ILE:HB	2.18	0.57
1:D:445:VAL:HG21	1:D:563:LEU:HG	1.86	0.57
2:C:482:LEU:HD23	2:C:485:SER:OG	2.03	0.57
1:B:254:LEU:HD13	1:B:265:MET:HE1	1.87	0.57
1:D:199:VAL:O	1:D:203:ILE:HG13	2.03	0.57
1:B:148:LEU:HD23	1:B:151:LEU:CD1	2.34	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:GLN:O	1:D:28:VAL:HG23	2.05	0.57
1:D:406:ILE:HG23	1:D:444:LEU:HD23	1.86	0.57
1:B:689:ALA:O	1:B:692:VAL:HG23	2.05	0.57
1:D:641:ALA:O	1:D:645:ILE:HG13	2.05	0.57
1:B:225:ARG:NH1	1:B:256:ASP:OD1	2.37	0.56
1:D:576:GLY:CA	1:D:614:GLN:HG3	2.28	0.56
1:D:709:THR:HG21	1:D:747:GLN:CG	2.35	0.56
1:D:630:LEU:HD22	1:D:699:PHE:CZ	2.40	0.56
1:B:10:ILE:HD13	1:B:48:PHE:HA	1.88	0.56
1:D:612:GLY:HA2	1:D:618:PHE:HD2	1.70	0.56
1:B:420:ARG:O	1:B:424:LEU:HG	2.06	0.56
1:D:45:HIS:HB3	1:D:98:TYR:CE2	2.40	0.56
1:B:454:ASP:O	1:B:458:ARG:HG3	2.05	0.56
1:D:152:LYS:O	2:C:481:ILE:HB	2.06	0.55
1:D:775:LEU:N	1:D:776:PRO:HD2	2.22	0.55
1:B:371:LEU:HD22	1:B:375:ILE:CD1	2.36	0.55
1:B:630:LEU:O	1:B:638:LYS:HE3	2.05	0.55
1:B:70:GLU:HB3	1:B:74:LYS:HE3	1.88	0.55
1:D:449:LEU:HD12	1:D:458:ARG:CG	2.37	0.55
1:D:655:GLU:N	1:D:656:PRO:HD2	2.21	0.55
1:D:327:PRO:HB3	1:D:370:TYR:CE2	2.42	0.55
1:D:601:ARG:NH1	1:D:633:ASP:OD2	2.40	0.55
1:D:734:ILE:HD13	1:D:802:LEU:HD21	1.87	0.55
1:B:375:ILE:CG2	1:B:436:ILE:HG12	2.37	0.55
1:B:466:ILE:HG23	1:B:560:CYS:SG	2.47	0.55
1:B:630:LEU:HD13	1:B:699:PHE:CE1	2.42	0.55
1:B:395:LEU:CD1	1:B:398:LYS:HE3	2.23	0.54
1:B:405:LEU:HD23	1:B:408:ILE:HD12	1.89	0.54
1:B:585:ILE:HA	1:B:589:ILE:HB	1.89	0.54
1:B:729:ILE:O	1:B:733:LEU:HG	2.06	0.54
1:D:259:ASP:HA	1:D:262:LYS:HB2	1.89	0.54
1:D:274:LEU:HD13	1:D:274:LEU:O	2.07	0.54
1:B:339:TRP:HE1	1:B:360:ILE:HB	1.72	0.54
1:D:812:ASN:HB2	1:D:813:PRO:CD	2.37	0.54
1:B:176:GLU:HA	1:B:208:LYS:NZ	2.22	0.54
1:B:349:LYS:NZ	1:B:352:GLU:OE1	2.40	0.54
1:B:871:LEU:HD11	1:B:887:LEU:HD22	1.88	0.54
1:D:39:ASP:OD1	1:D:39:ASP:N	2.34	0.54
1:D:469:ILE:HD13	1:D:559:LYS:HD2	1.87	0.54
1:B:18:GLN:HG3	1:B:64:ALA:HB1	1.90	0.54
2:A:476:THR:O	2:A:477:LYS:HG3	2.07	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:THR:O	1:B:46:GLU:HG3	2.08	0.54
1:D:433:LEU:HD12	1:D:435:THR:H	1.73	0.54
1:D:828:ASP:O	1:D:832:MET:HG2	2.08	0.54
1:B:578:SER:O	1:B:581:MET:N	2.40	0.54
1:B:470:ARG:NH2	1:B:588:LEU:HG	2.21	0.54
1:D:230:GLN:HG2	1:D:268:HIS:CG	2.43	0.54
1:D:424:LEU:HD21	1:D:451:ILE:HB	1.88	0.54
1:B:232:LEU:HA	1:B:236:VAL:CG1	2.38	0.54
1:D:327:PRO:HB3	1:D:370:TYR:CZ	2.43	0.54
1:B:754:VAL:O	1:B:758:VAL:HG13	2.08	0.54
1:D:597:HIS:HB2	1:D:600:VAL:HG23	1.90	0.54
1:D:589:ILE:HD13	1:D:607:CYS:HB3	1.90	0.53
1:D:233:ALA:HB2	1:D:269:LEU:HA	1.90	0.53
1:D:455:ASP:O	1:D:459:THR:HG23	2.09	0.53
1:B:709:THR:HG21	1:B:747:GLN:HB3	1.91	0.53
1:B:332:THR:OG1	1:B:335:ILE:HG13	2.08	0.53
1:B:456:ASN:O	1:B:460:GLN:HG3	2.08	0.53
2:C:485:SER:HA	2:C:489:ASN:CB	2.22	0.53
1:D:449:LEU:HD12	1:D:458:ARG:HB3	1.91	0.53
1:D:775:LEU:O	1:D:779:GLN:HG3	2.09	0.53
1:B:147:MET:CB	1:B:166:LEU:HG	2.39	0.53
1:B:147:MET:HB3	1:B:166:LEU:HG	1.91	0.53
1:B:277:SER:OG	1:B:287:ARG:NH1	2.41	0.53
1:D:397:THR:O	1:D:401:ILE:HG13	2.09	0.53
1:B:28:VAL:O	1:B:32:SER:HB2	2.09	0.53
1:B:427:LEU:O	1:B:431:LEU:HG	2.09	0.53
1:B:461:ILE:O	1:B:465:ILE:HG13	2.08	0.53
1:B:830:LEU:HD23	1:B:857:LEU:HD21	1.91	0.53
1:B:828:ASP:O	1:B:832:MET:HG2	2.09	0.53
1:D:210:LEU:N	1:D:211:PRO:HD2	2.24	0.53
1:D:159:ARG:O	1:D:163:VAL:HG13	2.08	0.53
1:D:22:GLN:HG3	1:D:23:ASN:N	2.24	0.53
1:D:355:GLU:O	1:D:358:GLU:HG2	2.08	0.52
1:D:561:LEU:CD1	1:D:588:LEU:HD22	2.38	0.52
1:D:590:LEU:N	1:D:591:PRO:HD2	2.24	0.52
1:B:750:HIS:CE1	2:A:501:PHE:HB3	2.45	0.52
1:B:365:VAL:HG22	1:B:419:GLY:HA2	1.91	0.52
1:D:402:GLY:O	1:D:406:ILE:HG13	2.10	0.52
1:B:163:VAL:HG13	1:B:183:TYR:CE1	2.45	0.52
1:B:471:ALA:N	1:B:472:PRO:HD2	2.25	0.52
1:D:277:SER:O	1:D:278:GLU:HB2	2.10	0.52

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:796:THR:O	1:D:800:GLU:HG3	2.09	0.52
1:D:833:LYS:HB2	1:D:833:LYS:NZ	2.25	0.52
1:B:371:LEU:HD11	1:B:409:ILE:HD11	1.91	0.52
1:B:424:LEU:O	1:B:428:GLN:HG3	2.10	0.52
1:B:459:THR:HG22	1:B:567:LEU:HD21	1.92	0.52
1:D:372:LEU:O	1:D:376:GLN:HG3	2.10	0.52
1:B:754:VAL:HG11	2:A:505:VAL:HG22	1.92	0.52
1:B:250:LEU:O	1:B:254:LEU:HB2	2.09	0.52
1:B:333:PRO:HA	1:B:401:ILE:HG12	1.92	0.52
1:B:597:HIS:HB2	1:B:600:VAL:HG23	1.92	0.52
1:B:8:LEU:O	1:B:34:THR:HG21	2.09	0.52
1:D:561:LEU:HD13	1:D:588:LEU:HD22	1.92	0.52
1:D:104:LEU:HD21	1:D:143:ILE:HA	1.92	0.51
1:B:112:ASN:OD1	1:B:115:ARG:NH2	2.44	0.51
1:B:177:CYS:HB3	1:B:180:VAL:CG2	2.40	0.51
1:D:644:ALA:HA	2:C:513:LEU:HD11	1.91	0.51
1:D:291:GLU:OE1	1:D:397:THR:HG22	2.09	0.51
1:B:561:LEU:HD21	1:B:588:LEU:HD22	1.92	0.51
1:D:424:LEU:CD2	1:D:448:LEU:HD12	2.38	0.51
1:B:148:LEU:N	1:B:166:LEU:HD11	2.25	0.51
1:B:430:ILE:O	1:B:436:ILE:HD12	2.11	0.51
1:D:81:GLN:HA	1:D:130:PRO:CG	2.40	0.51
1:B:228:ALA:O	1:B:232:LEU:HG	2.11	0.51
1:D:464:GLU:O	1:D:468:GLU:HB2	2.11	0.51
1:D:559:LYS:O	1:D:563:LEU:HD13	2.11	0.51
1:B:250:LEU:HD12	1:B:288:LEU:HD22	1.93	0.51
1:B:332:THR:H	1:B:335:ILE:HD12	1.76	0.51
1:B:76:VAL:HG12	1:B:96:LEU:HD13	1.93	0.51
1:D:379:PRO:HB2	1:D:395:LEU:HD21	1.92	0.51
1:B:655:GLU:N	1:B:656:PRO:HD2	2.26	0.51
1:D:62:GLU:O	1:D:66:GLU:HG2	2.11	0.51
1:D:804:ASP:OD1	1:D:807:ARG:NH2	2.44	0.51
1:D:568:LEU:HB3	1:D:610:CYS:HB3	1.92	0.51
1:B:438:ILE:HG22	1:B:562:ILE:CD1	2.41	0.51
1:B:771:GLU:OE2	1:B:833:LYS:HE3	2.11	0.50
1:D:80:HIS:O	1:D:130:PRO:HG2	2.11	0.50
1:B:584:ILE:HA	1:B:587:SER:OG	2.11	0.50
1:B:803:VAL:HG13	1:B:857:LEU:HD23	1.93	0.50
1:D:62:GLU:CD	1:D:63:PRO:HD2	2.32	0.50
1:D:792:GLU:OE1	1:D:792:GLU:N	2.45	0.50
1:B:176:GLU:HG2	1:B:181:ASN:OD1	2.10	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:PRO:HB2	1:B:366:VAL:HG21	1.92	0.50
1:B:627:LEU:HD11	1:B:692:VAL:HG22	1.94	0.50
1:B:642:LEU:HD22	1:B:646:PHE:CE2	2.46	0.50
1:B:645:ILE:O	1:B:649:LEU:HG	2.12	0.50
1:D:211:PRO:HA	1:D:214:VAL:HG22	1.93	0.50
1:D:436:ILE:HG23	1:D:437:PRO:HD2	1.93	0.50
1:D:49:ILE:O	1:D:53:LYS:HG3	2.11	0.50
1:D:22:GLN:HE21	1:D:23:ASN:HA	1.77	0.50
1:D:238:MET:CE	1:D:246:ARG:HD2	2.41	0.50
1:D:267:LYS:O	1:D:271:GLN:HB2	2.12	0.49
1:D:148:LEU:HA	1:D:151:LEU:HD12	1.93	0.49
1:D:585:ILE:HA	1:D:589:ILE:HB	1.94	0.49
1:D:216:ARG:NH1	1:D:219:ASP:OD1	2.44	0.49
1:D:449:LEU:CD1	1:D:458:ARG:HB3	2.42	0.49
1:D:691:ASN:N	1:D:691:ASN:HD22	2.10	0.49
1:B:310:LEU:O	1:B:314:VAL:HG12	2.12	0.49
1:B:318:LYS:O	1:B:318:LYS:HD3	2.12	0.49
1:B:65:VAL:HG22	2:A:461:ILE:HD11	1.95	0.49
1:D:20:PRO:O	1:D:22:GLN:HB2	2.13	0.49
1:B:282:LEU:HG	1:B:316:LEU:HD13	1.93	0.49
1:B:375:ILE:HG23	1:B:436:ILE:HG12	1.94	0.49
1:B:853:ALA:O	1:B:857:LEU:HG	2.13	0.49
1:B:329:GLU:O	1:B:331:LEU:HG	2.12	0.49
1:D:471:ALA:HB3	1:D:472:PRO:CD	2.43	0.49
1:B:836:ASN:O	1:B:840:THR:OG1	2.29	0.49
1:D:150:ARG:HB3	1:D:162:ALA:HB2	1.95	0.49
1:D:22:GLN:NE2	1:D:23:ASN:HA	2.27	0.49
1:D:804:ASP:O	1:D:807:ARG:HG2	2.12	0.49
1:D:342:LEU:HD21	1:D:346:LEU:CD1	2.43	0.48
1:D:645:ILE:O	1:D:649:LEU:HG	2.13	0.48
1:B:375:ILE:HG21	1:B:436:ILE:CD1	2.42	0.48
1:D:372:LEU:HD23	1:D:430:ILE:HG12	1.95	0.48
1:B:23:ASN:HB3	1:B:26:LYS:HD2	1.95	0.48
2:C:482:LEU:N	2:C:482:LEU:HD13	2.28	0.48
1:B:45:HIS:CE1	1:B:95:LEU:HB2	2.49	0.48
1:B:647:ASP:OD2	2:A:511:LEU:HB3	2.13	0.48
1:B:336:ALA:HB2	1:B:401:ILE:HG23	1.96	0.48
1:B:829:ASN:O	1:B:833:LYS:HG3	2.13	0.48
1:B:216:ARG:HH22	2:A:496:THR:CG2	2.26	0.48
1:B:203:ILE:CD1	1:B:209:THR:HG23	2.44	0.48
1:B:367:TYR:OH	1:B:408:ILE:HB	2.14	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:634:ASP:HB3	1:B:637:ILE:HD13	1.94	0.48
1:D:471:ALA:N	1:D:472:PRO:HD2	2.29	0.48
1:D:471:ALA:HB3	1:D:472:PRO:HD3	1.96	0.48
1:D:296:VAL:O	1:D:300:VAL:HG23	2.14	0.48
1:D:11:LYS:HD3	1:D:51:TYR:CE1	2.49	0.48
1:B:871:LEU:CD1	1:B:887:LEU:HD22	2.44	0.47
1:B:92:ASP:OD1	1:B:92:ASP:N	2.45	0.47
2:C:509:VAL:HG12	2:C:509:VAL:O	2.14	0.47
1:D:449:LEU:HD12	1:D:458:ARG:CD	2.44	0.47
1:B:778:LEU:HD13	1:B:778:LEU:N	2.30	0.47
1:B:220:VAL:N	2:A:495:THR:O	2.43	0.47
1:B:754:VAL:CG1	2:A:505:VAL:HG22	2.43	0.47
1:B:593:ILE:HD11	1:B:608:LEU:CD1	2.40	0.47
1:B:635:VAL:HA	1:B:638:LYS:HD2	1.96	0.47
1:B:742:THR:HG22	1:B:742:THR:O	2.14	0.47
1:D:596:ILE:HG23	1:D:597:HIS:CD2	2.49	0.47
1:B:331:LEU:H	1:B:331:LEU:HD12	1.79	0.47
1:D:414:THR:O	1:D:417:GLU:HA	2.15	0.47
1:D:831:ALA:HB2	1:D:859:LEU:HD21	1.97	0.47
2:A:482:LEU:N	2:A:482:LEU:HD13	2.26	0.47
1:B:220:VAL:HG23	2:A:495:THR:O	2.13	0.47
1:D:210:LEU:O	1:D:214:VAL:HG22	2.15	0.47
2:A:482:LEU:HD23	2:A:484:LYS:CD	2.44	0.47
1:B:177:CYS:SG	1:B:178:PRO:HD2	2.55	0.47
1:B:354:GLU:O	1:B:358:GLU:HG3	2.15	0.47
1:D:403:GLN:HG3	1:D:440:LEU:CD2	2.44	0.47
1:D:431:LEU:HD21	1:D:444:LEU:CB	2.45	0.47
1:B:594:ILE:HD13	1:B:594:ILE:H	1.80	0.47
1:D:220:VAL:HA	2:C:497:LEU:HG	1.96	0.47
1:D:250:LEU:HD23	1:D:265:MET:CE	2.45	0.47
1:D:45:HIS:HB3	1:D:98:TYR:CD2	2.50	0.47
1:B:768:GLU:O	1:B:772:GLU:HG3	2.15	0.47
1:B:151:LEU:O	1:B:159:ARG:HD2	2.16	0.46
1:B:33:ARG:O	1:B:37:THR:HG22	2.15	0.46
1:D:180:VAL:HG21	1:D:208:LYS:NZ	2.30	0.46
1:D:761:TYR:HB3	1:D:810:GLY:O	2.16	0.46
1:B:402:GLY:O	1:B:406:ILE:HG13	2.15	0.46
1:D:120:LEU:HA	1:D:161:GLN:OE1	2.14	0.46
1:D:206:SER:OG	1:D:208:LYS:HG2	2.16	0.46
1:D:454:ASP:HB3	1:D:457:LYS:HG3	1.95	0.46
1:B:478:VAL:O	1:B:556:THR:OG1	2.28	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:469:ILE:HD13	1:D:559:LYS:CD	2.46	0.46
1:D:713:GLU:O	1:D:717:LYS:HG3	2.16	0.46
1:B:368:ALA:HB1	1:B:426:VAL:HG21	1.97	0.46
1:D:709:THR:CG2	1:D:747:GLN:HG3	2.45	0.46
1:D:864:ALA:O	1:D:868:LEU:HB2	2.16	0.46
1:B:465:ILE:O	1:B:469:ILE:HG13	2.15	0.46
1:D:266:GLN:O	1:D:271:GLN:HG2	2.16	0.46
1:D:740:PRO:CG	1:D:789:PRO:HB2	2.46	0.46
1:B:363:GLU:O	1:B:366:VAL:HG22	2.15	0.46
1:D:561:LEU:HA	1:D:561:LEU:HD12	1.75	0.46
1:D:739:ASN:OD1	1:D:741:VAL:HG13	2.16	0.46
1:B:619:ALA:O	1:B:623:PHE:HB2	2.15	0.46
1:B:33:ARG:HD2	1:B:33:ARG:HA	1.79	0.46
1:B:630:LEU:HD23	1:B:630:LEU:HA	1.80	0.46
1:D:774:PHE:HA	1:D:802:LEU:HD13	1.98	0.46
1:B:372:LEU:HD12	1:B:426:VAL:HG13	1.97	0.45
1:D:156:PRO:HA	1:D:159:ARG:CZ	2.46	0.45
1:D:368:ALA:HB2	1:D:423:LEU:HD23	1.99	0.45
1:D:136:ASP:OD1	1:D:136:ASP:N	2.49	0.45
1:D:226:LYS:HG3	1:D:264:ALA:CB	2.44	0.45
1:D:375:ILE:HA	1:D:378:ILE:HD12	1.98	0.45
1:D:865:LYS:HG3	1:D:866:ASP:N	2.30	0.45
1:D:156:PRO:HG2	4:D:1101:HOH:O	2.16	0.45
1:D:647:ASP:OD2	2:C:512:HIS:N	2.46	0.45
1:B:145:LYS:O	1:B:149:ILE:HG13	2.17	0.45
1:B:375:ILE:HD13	1:B:430:ILE:HD13	1.98	0.45
1:B:431:LEU:HD21	1:B:444:LEU:CB	2.46	0.45
1:D:243:ILE:H	1:D:243:ILE:HD12	1.81	0.45
1:B:147:MET:HE2	1:B:147:MET:HA	1.98	0.45
1:B:596:ILE:HG23	1:B:597:HIS:CD2	2.52	0.45
1:D:433:LEU:HD12	1:D:433:LEU:O	2.16	0.45
1:B:455:ASP:O	1:B:459:THR:HG23	2.17	0.45
1:D:177:CYS:O	1:D:180:VAL:HG22	2.16	0.45
1:D:164:LEU:HD23	1:D:202:CYS:SG	2.57	0.45
1:D:31:LEU:HD23	1:D:75:PHE:CE1	2.52	0.45
1:B:18:GLN:OE1	2:A:461:ILE:N	2.41	0.45
1:B:192:ASN:HA	1:B:193:PRO:HD3	1.84	0.45
1:D:333:PRO:HA	1:D:401:ILE:HG12	1.99	0.45
1:D:452:ILE:CD1	1:D:461:ILE:HD12	2.47	0.45
1:B:423:LEU:O	1:B:427:LEU:HG	2.17	0.44
1:B:867:LEU:HD23	1:B:867:LEU:HA	1.80	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ARG:HA	1:B:273:TRP:CH2	2.52	0.44
1:B:590:LEU:CB	1:B:591:PRO:HD3	2.47	0.44
1:D:258:SER:OG	1:D:261:VAL:HG23	2.17	0.44
1:D:445:VAL:CG2	1:D:563:LEU:HG	2.47	0.44
1:B:251:GLN:HG3	1:B:296:VAL:HG22	2.00	0.44
1:B:225:ARG:HH12	1:B:261:VAL:HG21	1.83	0.44
1:B:430:ILE:HG22	1:B:436:ILE:HD13	1.99	0.44
1:D:709:THR:HG21	1:D:747:GLN:HG3	1.99	0.44
1:D:738:TYR:HB3	1:D:793:ILE:HG12	1.97	0.44
1:D:395:LEU:O	1:D:399:GLU:HG3	2.17	0.44
1:D:414:THR:O	1:D:420:ARG:HG3	2.18	0.44
1:B:250:LEU:HD13	1:B:300:VAL:HG21	1.99	0.44
1:D:243:ILE:O	1:D:247:VAL:HG13	2.17	0.44
1:D:612:GLY:O	1:D:619:ALA:HB2	2.18	0.44
1:D:764:ARG:NH2	1:D:824:LEU:O	2.51	0.44
1:D:847:ILE:HG13	1:D:883:CYS:SG	2.58	0.44
1:B:403:GLN:HG2	1:B:443:PHE:CD2	2.52	0.44
1:D:254:LEU:HD12	1:D:254:LEU:HA	1.83	0.44
1:D:253:GLY:O	1:D:262:LYS:HG2	2.17	0.44
1:D:301:LEU:HD11	1:D:337:LEU:HD13	2.00	0.44
1:D:342:LEU:HD21	1:D:346:LEU:HD12	2.00	0.44
1:B:246:ARG:HA	1:B:273:TRP:HH2	1.82	0.43
1:D:76:VAL:HG21	1:D:99:LEU:HD22	2.00	0.43
1:B:195:VAL:O	1:B:199:VAL:HG23	2.18	0.43
1:B:24:GLN:O	1:B:28:VAL:HG23	2.19	0.43
1:B:347:LYS:NZ	1:B:410:LYS:O	2.39	0.43
1:B:436:ILE:HG23	1:B:437:PRO:HD2	2.01	0.43
1:B:274:LEU:HD22	1:B:304:LEU:HD11	2.00	0.43
2:C:476:THR:O	2:C:477:LYS:HG3	2.19	0.43
1:D:19:GLN:HA	1:D:20:PRO:HD3	1.84	0.43
1:D:406:ILE:HD13	1:D:444:LEU:HG	2.00	0.43
1:D:65:VAL:O	1:D:69:ILE:HG12	2.18	0.43
1:B:371:LEU:HD12	1:B:409:ILE:HD11	2.01	0.43
1:B:593:ILE:O	1:B:601:ARG:HG2	2.18	0.43
1:D:121:LEU:O	1:D:125:LEU:HG	2.18	0.43
1:D:454:ASP:OD1	1:D:456:ASN:HB2	2.19	0.43
1:D:55:VAL:HB	1:D:65:VAL:HG13	2.00	0.43
1:D:807:ARG:HB3	1:D:827:HIS:CE1	2.53	0.43
1:B:76:VAL:CG1	1:B:96:LEU:HD13	2.49	0.43
1:B:452:ILE:O	1:B:453:ILE:HB	2.18	0.43
1:D:872:ASN:OD1	1:D:891:LYS:HE3	2.19	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:THR:O	1:B:401:ILE:HG13	2.19	0.43
1:B:558:GLN:O	1:B:562:ILE:HG13	2.18	0.43
1:B:304:LEU:HD12	1:B:307:ILE:HD11	2.00	0.43
1:B:627:LEU:HD23	1:B:645:ILE:HD13	2.01	0.43
1:B:847:ILE:O	1:B:851:THR:HG23	2.19	0.43
1:D:735:LEU:CD2	1:D:781:LEU:HD21	2.49	0.43
1:D:729:ILE:O	1:D:733:LEU:HG	2.19	0.42
1:D:560:CYS:HB3	1:D:588:LEU:HD11	2.01	0.42
1:B:16:LEU:HB3	1:B:22:GLN:HE21	1.84	0.42
1:D:403:GLN:HG3	1:D:440:LEU:HD23	2.02	0.42
1:D:754:VAL:O	1:D:758:VAL:HG13	2.19	0.42
1:B:188:GLU:HG2	1:B:216:ARG:HH21	1.84	0.42
1:B:368:ALA:HB1	1:B:426:VAL:CG2	2.48	0.42
1:D:647:ASP:CG	2:C:512:HIS:H	2.21	0.42
1:D:407:LEU:HD23	1:D:407:LEU:HA	1.92	0.42
1:D:655:GLU:N	1:D:656:PRO:CD	2.83	0.42
1:B:368:ALA:O	1:B:426:VAL:HG11	2.20	0.42
1:B:693:LEU:HD22	1:B:693:LEU:HA	1.68	0.42
1:D:192:ASN:HA	1:D:193:PRO:HD3	1.81	0.42
1:B:232:LEU:O	1:B:236:VAL:HG13	2.19	0.42
1:B:70:GLU:OE2	1:B:124:LYS:HE3	2.20	0.42
1:B:407:LEU:HD23	1:B:407:LEU:HA	1.93	0.42
1:B:438:ILE:HA	1:B:441:VAL:CG2	2.48	0.42
1:D:597:HIS:HB2	1:D:600:VAL:CG2	2.50	0.42
1:B:151:LEU:HD13	1:B:182:ALA:HB1	2.02	0.42
1:B:775:LEU:HB2	1:B:776:PRO:HD3	2.02	0.42
1:B:357:LEU:HD11	1:B:361:LEU:CD1	2.49	0.42
1:B:371:LEU:O	1:B:375:ILE:HD12	2.20	0.42
1:D:357:LEU:C	1:D:357:LEU:HD23	2.40	0.42
1:B:430:ILE:HG21	1:B:444:LEU:HD11	2.02	0.41
1:D:332:THR:OG1	1:D:335:ILE:HG13	2.20	0.41
1:D:739:ASN:HA	1:D:740:PRO:HD2	1.94	0.41
1:B:371:LEU:HD22	1:B:375:ILE:HD11	2.01	0.41
1:B:434:PRO:C	1:B:436:ILE:H	2.24	0.41
1:B:304:LEU:O	1:B:308:THR:HG22	2.21	0.41
1:B:34:THR:HA	1:B:37:THR:HG22	2.02	0.41
1:B:432:ILE:HG21	1:B:468:GLU:HG2	2.02	0.41
1:B:608:LEU:HA	1:B:608:LEU:HD23	1.87	0.41
1:D:337:LEU:HD22	1:D:337:LEU:O	2.20	0.41
1:D:452:ILE:HG22	1:D:453:ILE:N	2.35	0.41
1:D:750:HIS:O	1:D:754:VAL:HG23	2.20	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:ARG:HB3	1:D:7:LEU:H	1.50	0.41
1:D:853:ALA:O	1:D:857:LEU:HG	2.20	0.41
1:B:379:PRO:O	1:B:435:THR:HG23	2.20	0.41
1:B:561:LEU:CD2	1:B:588:LEU:HD22	2.50	0.41
1:B:699:PHE:CE2	1:B:707:LEU:HD13	2.55	0.41
1:D:438:ILE:HA	1:D:441:VAL:CG2	2.48	0.41
1:D:793:ILE:HG22	1:D:794:ASP:N	2.35	0.41
1:D:331:LEU:CD1	1:D:401:ILE:HG21	2.51	0.41
1:D:735:LEU:HD22	1:D:781:LEU:HD21	2.02	0.41
2:A:482:LEU:O	2:A:482:LEU:HD22	2.19	0.41
1:B:458:ARG:O	1:B:462:VAL:HG23	2.20	0.41
1:B:886:ALA:O	1:B:890:ILE:HG13	2.21	0.41
1:D:155:ILE:HA	1:D:156:PRO:HD2	1.88	0.41
1:D:316:LEU:HD13	1:D:338:TYR:OH	2.21	0.41
1:D:431:LEU:HA	1:D:436:ILE:HD12	2.01	0.41
1:D:449:LEU:HD12	1:D:458:ARG:CB	2.51	0.41
1:D:301:LEU:HD13	1:D:341:ALA:HB3	2.01	0.41
1:D:356:PHE:O	1:D:359:GLN:HB2	2.21	0.41
1:B:254:LEU:HD12	1:B:254:LEU:HA	1.80	0.41
1:B:559:LYS:O	1:B:563:LEU:HD13	2.21	0.41
1:D:578:SER:O	1:D:581:MET:N	2.47	0.41
1:D:584:ILE:HA	1:D:587:SER:OG	2.20	0.41
1:B:109:ALA:HB1	2:A:473:PHE:HA	2.03	0.41
1:B:231:VAL:O	1:B:235:LYS:HB2	2.21	0.41
1:B:409:ILE:HB	1:B:447:ARG:CD	2.50	0.41
1:B:427:LEU:HB2	1:B:448:LEU:HD13	2.03	0.41
1:B:49:ILE:O	1:B:53:LYS:HG3	2.21	0.41
1:B:575:THR:OG1	1:B:575:THR:O	2.36	0.41
1:D:426:VAL:O	1:D:430:ILE:HG13	2.21	0.41
1:D:147:MET:CB	1:D:166:LEU:HG	2.51	0.41
1:D:203:ILE:O	1:D:203:ILE:HD12	2.21	0.41
1:D:211:PRO:HA	1:D:214:VAL:CG2	2.51	0.41
1:D:241:MET:CE	1:D:249:LEU:HD21	2.51	0.41
1:D:250:LEU:HD23	1:D:265:MET:HE2	2.02	0.41
1:D:409:ILE:CB	1:D:447:ARG:HG2	2.42	0.41
1:D:730:LEU:O	1:D:734:ILE:HG13	2.20	0.41
1:B:739:ASN:HA	1:B:740:PRO:HD3	1.99	0.40
1:B:163:VAL:O	1:B:183:TYR:OH	2.38	0.40
1:B:808:PRO:HD2	1:B:858:GLU:OE1	2.21	0.40
1:D:406:ILE:HD12	1:D:440:LEU:HD22	2.03	0.40
1:D:642:LEU:HD23	1:D:642:LEU:HA	1.92	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:706:GLU:OE1	1:D:706:GLU:N	2.54	0.40
1:D:824:LEU:HD12	1:D:862:HIS:NE2	2.37	0.40
1:B:296:VAL:O	1:B:300:VAL:HG23	2.21	0.40
1:D:420:ARG:O	1:D:424:LEU:HG	2.21	0.40
1:D:428:GLN:O	1:D:432:ILE:HG13	2.21	0.40
1:D:431:LEU:HD21	1:D:444:LEU:HB3	2.02	0.40
1:D:831:ALA:HB2	1:D:859:LEU:CD2	2.51	0.40
1:B:34:THR:HA	1:B:37:THR:CG2	2.52	0.40
1:B:641:ALA:O	1:B:645:ILE:HG13	2.21	0.40
1:D:375:ILE:HD13	1:D:430:ILE:HD13	2.02	0.40
1:D:447:ARG:CZ	1:D:447:ARG:HA	2.52	0.40
2:A:511:LEU:HD22	2:A:511:LEU:N	2.36	0.40
1:B:170:GLN:HG2	1:B:179:VAL:CG1	2.51	0.40
1:B:305:PHE:CD1	1:B:313:LEU:HD13	2.56	0.40
1:B:432:ILE:HD13	1:B:468:GLU:HG2	2.03	0.40
1:B:455:ASP:OD2	1:B:575:THR:HG21	2.22	0.40
1:B:642:LEU:HA	1:B:642:LEU:HD23	1.96	0.40
1:D:442:SER:O	1:D:446:GLU:HB2	2.21	0.40
1:D:630:LEU:O	1:D:638:LYS:HE3	2.21	0.40
1:D:825:THR:OG1	1:D:828:ASP:OD2	2.34	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	B	712/839 (85%)	683 (96%)	27 (4%)	2 (0%)	41	76
1	D	705/839 (84%)	685 (97%)	19 (3%)	1 (0%)	51	85
2	A	44/57 (77%)	41 (93%)	3 (7%)	0	100	100
2	C	43/57 (75%)	39 (91%)	4 (9%)	0	100	100
All	All	1504/1792 (84%)	1448 (96%)	53 (4%)	3 (0%)	47	82



All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	453	ILE
1	D	576	GLY
1	B	350	GLY

### 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	B	651/749 (87%)	615 (94%)	36 (6%)	21	57
1	D	654/749 (87%)	618 (94%)	36 (6%)	21	57
2	A	47/54 (87%)	44 (94%)	3 (6%)	17	51
2	C	46/54 (85%)	40 (87%)	6 (13%)	4	19
All	All	1398/1606 (87%)	1317 (94%)	81 (6%)	20	55

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	24	GLN
1	B	42	THR
1	B	92	ASP
1	B	100	PHE
1	B	126	LEU
1	B	168	ARG
1	B	209	THR
1	B	295	GLU
1	B	308	THR
1	B	318	LYS
1	B	331	LEU
1	B	349	LYS
1	B	360	ILE
1	B	361	LEU
1	B	371	LEU
1	B	372	LEU
1	B	413	ASP

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	438	ILE
1	B	447	ARG
1	B	470	ARG
1	B	588	LEU
1	B	594	ILE
1	B	608	LEU
1	B	614	GLN
1	B	625	LEU
1	B	630	LEU
1	B	633	ASP
1	B	634	ASP
1	B	636	THR
1	B	693	LEU
1	B	725	VAL
1	B	741	VAL
1	B	747	GLN
1	B	765	THR
1	B	778	LEU
1	B	867	LEU
2	A	481	ILE
2	A	482	LEU
2	A	511	LEU
1	D	22	GLN
1	D	70	GLU
1	D	100	PHE
1	D	135	ILE
1	D	136	ASP
1	D	138	ASP
1	D	150	ARG
1	D	191	SER
1	D	197	ARG
1	D	242	SER
1	D	247	VAL
1	D	249	LEU
1	D	329	GLU
1	D	331	LEU
1	D	371	LEU
1	D	395	LEU
1	D	438	ILE
1	D	447	ARG
1	D	470	ARG
1	D	556	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	561	LEU
1	D	588	LEU
1	D	594	ILE
1	D	624	VAL
1	D	628	GLN
1	D	630	LEU
1	D	633	ASP
1	D	691	ASN
1	D	695	LEU
1	D	765	THR
1	D	792	GLU
1	D	811	LEU
1	D	825	THR
1	D	833	LYS
1	D	841	SER
1	D	868	LEU
2	C	466	ASP
2	C	477	LYS
2	C	481	ILE
2	C	482	LEU
2	C	496	THR
2	C	504	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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
3	EPE	D	1001	-	15,15,15	0.85	1 (6%)	18,20,20	1.51	4 (22%)

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
3	EPE	D	1001	-	-	4/9/19/19	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1001	EPE	C10-S	2.90	1.81	1.77

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1001	EPE	C7-N4-C3	3.27	119.60	111.23
3	D	1001	EPE	O2S-S-C10	2.72	110.19	106.92
3	D	1001	EPE	C5-N4-C3	2.27	113.94	108.83
3	D	1001	EPE	O3S-S-C10	2.26	109.42	105.77

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1001	EPE	C9-C10-S-O1S
3	D	1001	EPE	C9-C10-S-O3S
3	D	1001	EPE	C8-C7-N4-C3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	D	1001	EPE	C9-C10-S-O2S

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	B	730/839 (87%)	-0.01	11 (1%) 73 46	36, 70, 106, 122	0
1	D	731/839 (87%)	0.01	12 (1%) 72 44	45, 75, 109, 129	0
2	A	50/57 (87%)	0.38	6 (12%) 4 1	46, 78, 99, 104	0
2	C	49/57 (85%)	0.30	5 (10%) 6 2	49, 81, 106, 114	0
All	All	1560/1792 (87%)	0.02	34 (2%) 62 33	36, 73, 107, 129	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	490	GLN	4.0
2	C	515	PRO	3.8
1	D	359	GLN	3.4
1	D	391	TYR	3.1
1	D	81	GLN	3.1
1	B	92	ASP	3.1
1	B	176	GLU	3.0
1	D	131	GLU	3.0
1	D	896	LYS	3.0
1	B	472	PRO	2.9
1	B	435	THR	2.8
1	D	787	SER	2.8
1	B	239	ARG	2.7
2	A	484	LYS	2.6
2	A	466	ASP	2.6
2	C	483	THR	2.6
1	B	173	LYS	2.6
2	C	489	ASN	2.5
1	D	609	GLY	2.5
2	A	491	ASN	2.4
1	B	471	ALA	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	607	CYS	2.4
2	A	502	ASN	2.4
2	C	488	GLU	2.4
1	B	555	GLU	2.4
1	B	473	ILE	2.4
1	D	326	ILE	2.3
1	D	813	PRO	2.3
1	D	306	SER	2.3
1	B	237	HIS	2.3
2	C	491	ASN	2.2
1	B	7	LEU	2.2
1	D	823	ALA	2.0
2	A	483	THR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EPE	D	1001	15/15	0.78	0.24	64,103,127,132	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.