Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:38 AM GMT

PDB ID	:	2RGK
Title	:	Functional annotation of Escherichia coli yihS-encoded protein
Authors	:	Itoh, T.; Mikami, B.; Hashimoto, W.; Murata, K.
Deposited on	:	2007-10-03
Resolution	:	2.50 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:

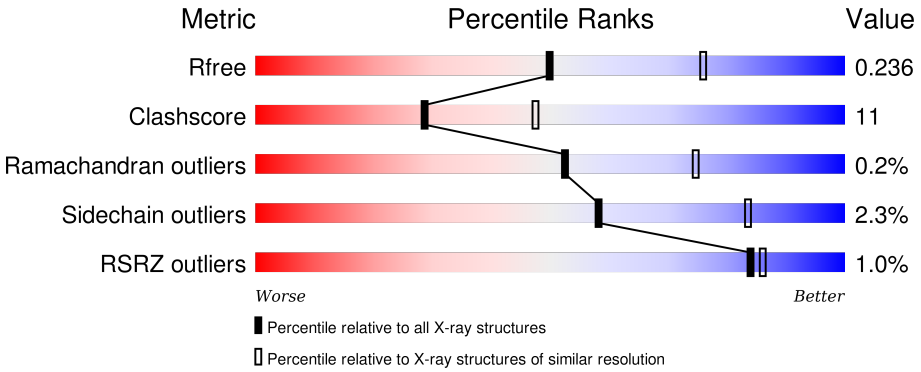
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	421	76% 20%
1	B	421	2% 79% 18%
1	C	421	% 75% 20%
1	D	421	% 75% 21%
1	E	421	% 76% 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	421	

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
2	EPE	A	3001	-	-	-	X
2	EPE	B	3002	-	-	-	X
2	EPE	D	3004	-	-	-	X
2	EPE	E	3005	-	-	-	X
2	EPE	F	3006	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21377 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 Uncharacterized sugar isomerase yihS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	0	0
			3317	2128	575	598	16			
1	B	409	Total	C	N	O	S	0	0	0
			3317	2128	575	598	16			
1	C	409	Total	C	N	O	S	0	0	0
			3317	2128	575	598	16			
1	D	409	Total	C	N	O	S	0	0	0
			3317	2128	575	598	16			
1	E	409	Total	C	N	O	S	0	0	0
			3317	2128	575	598	16			
1	F	409	Total	C	N	O	S	0	0	0
			3317	2128	575	598	16			

There are 48 discrepancies between the modelled and reference sequences:

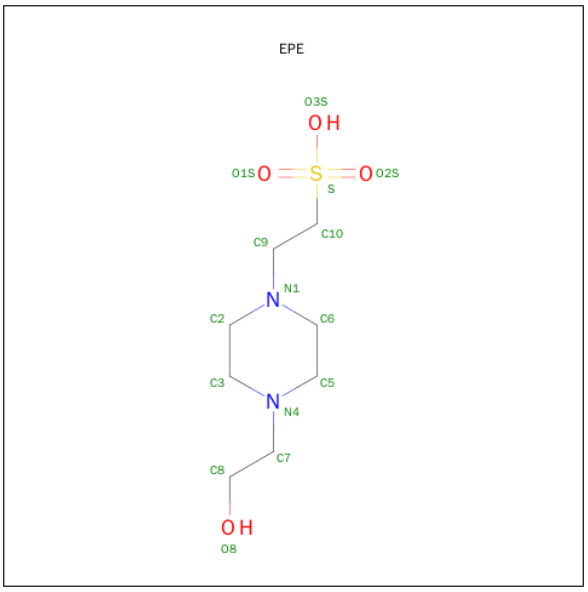
Chain	Residue	Modelled	Actual	Comment	Reference
A	414	LEU	-	EXPRESSION TAG	UNP P32140
A	415	GLU	-	EXPRESSION TAG	UNP P32140
A	416	HIS	-	EXPRESSION TAG	UNP P32140
A	417	HIS	-	EXPRESSION TAG	UNP P32140
A	418	HIS	-	EXPRESSION TAG	UNP P32140
A	419	HIS	-	EXPRESSION TAG	UNP P32140
A	420	HIS	-	EXPRESSION TAG	UNP P32140
A	421	HIS	-	EXPRESSION TAG	UNP P32140
B	414	LEU	-	EXPRESSION TAG	UNP P32140
B	415	GLU	-	EXPRESSION TAG	UNP P32140
B	416	HIS	-	EXPRESSION TAG	UNP P32140
B	417	HIS	-	EXPRESSION TAG	UNP P32140
B	418	HIS	-	EXPRESSION TAG	UNP P32140
B	419	HIS	-	EXPRESSION TAG	UNP P32140
B	420	HIS	-	EXPRESSION TAG	UNP P32140
B	421	HIS	-	EXPRESSION TAG	UNP P32140
C	414	LEU	-	EXPRESSION TAG	UNP P32140

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	415	GLU	-	EXPRESSION TAG	UNP P32140
C	416	HIS	-	EXPRESSION TAG	UNP P32140
C	417	HIS	-	EXPRESSION TAG	UNP P32140
C	418	HIS	-	EXPRESSION TAG	UNP P32140
C	419	HIS	-	EXPRESSION TAG	UNP P32140
C	420	HIS	-	EXPRESSION TAG	UNP P32140
C	421	HIS	-	EXPRESSION TAG	UNP P32140
D	414	LEU	-	EXPRESSION TAG	UNP P32140
D	415	GLU	-	EXPRESSION TAG	UNP P32140
D	416	HIS	-	EXPRESSION TAG	UNP P32140
D	417	HIS	-	EXPRESSION TAG	UNP P32140
D	418	HIS	-	EXPRESSION TAG	UNP P32140
D	419	HIS	-	EXPRESSION TAG	UNP P32140
D	420	HIS	-	EXPRESSION TAG	UNP P32140
D	421	HIS	-	EXPRESSION TAG	UNP P32140
E	414	LEU	-	EXPRESSION TAG	UNP P32140
E	415	GLU	-	EXPRESSION TAG	UNP P32140
E	416	HIS	-	EXPRESSION TAG	UNP P32140
E	417	HIS	-	EXPRESSION TAG	UNP P32140
E	418	HIS	-	EXPRESSION TAG	UNP P32140
E	419	HIS	-	EXPRESSION TAG	UNP P32140
E	420	HIS	-	EXPRESSION TAG	UNP P32140
E	421	HIS	-	EXPRESSION TAG	UNP P32140
F	414	LEU	-	EXPRESSION TAG	UNP P32140
F	415	GLU	-	EXPRESSION TAG	UNP P32140
F	416	HIS	-	EXPRESSION TAG	UNP P32140
F	417	HIS	-	EXPRESSION TAG	UNP P32140
F	418	HIS	-	EXPRESSION TAG	UNP P32140
F	419	HIS	-	EXPRESSION TAG	UNP P32140
F	420	HIS	-	EXPRESSION TAG	UNP P32140
F	421	HIS	-	EXPRESSION TAG	UNP P32140

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O S 15 8 2 4 1	0	0
2	B	1	Total C N O S 15 8 2 4 1	0	0
2	C	1	Total C N O S 15 8 2 4 1	0	0
2	D	1	Total C N O S 15 8 2 4 1	0	0
2	E	1	Total C N O S 15 8 2 4 1	0	0
2	F	1	Total C N O S 15 8 2 4 1	0	0

- Molecule 3 is water.

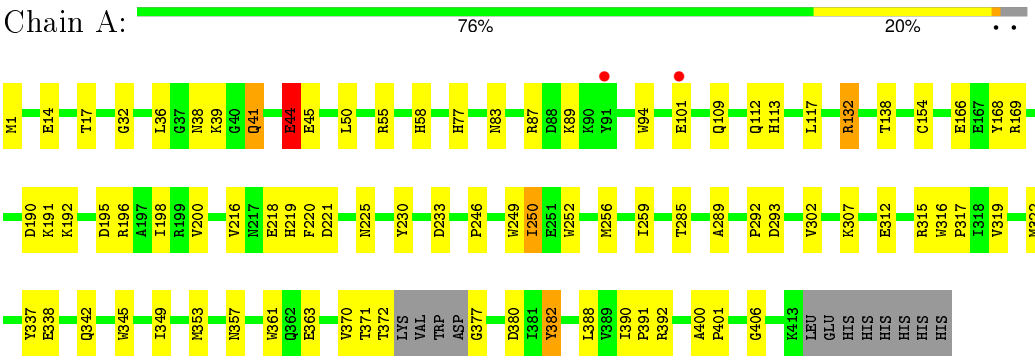
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	247	Total O 247 247	0	0
3	B	213	Total O 213 213	0	0
3	C	214	Total O 214 214	0	0
3	D	244	Total O 244 244	0	0
3	E	224	Total O 224 224	0	0
3	F	243	Total O 243 243	0	0

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.

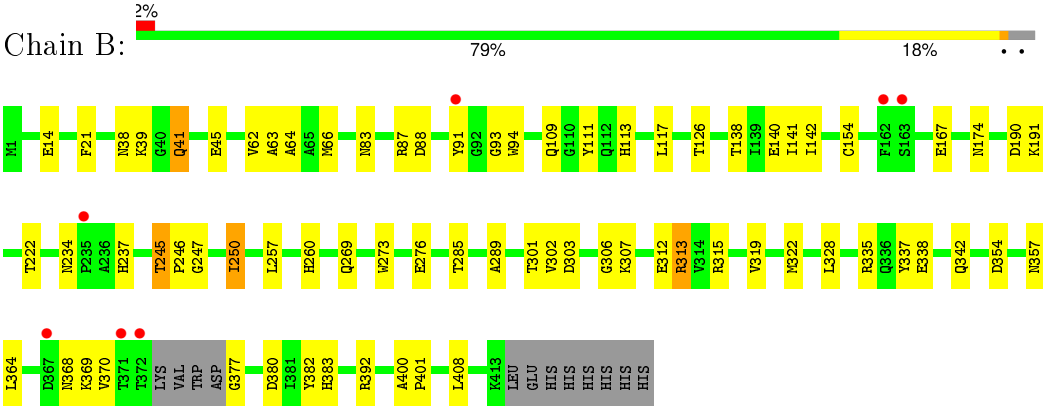
- Molecule 1: Uncharacterized sugar isomerase yihS

Chain A:



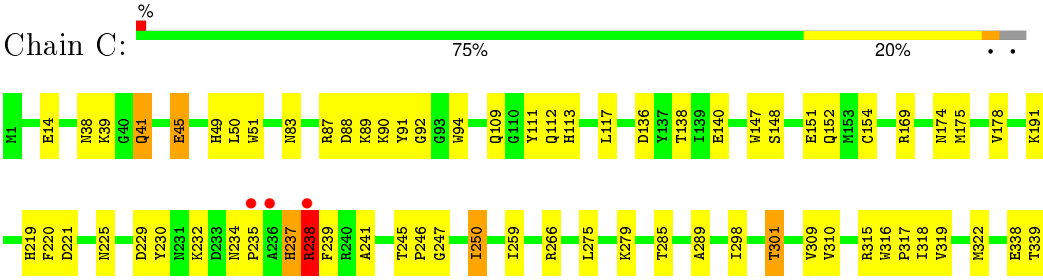
- Molecule 1: Uncharacterized sugar isomerase yihS

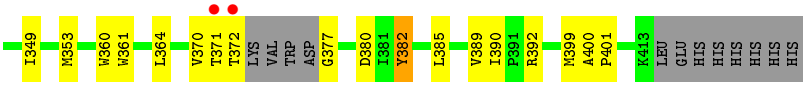
Chain B:



- Molecule 1: Uncharacterized sugar isomerase yihS

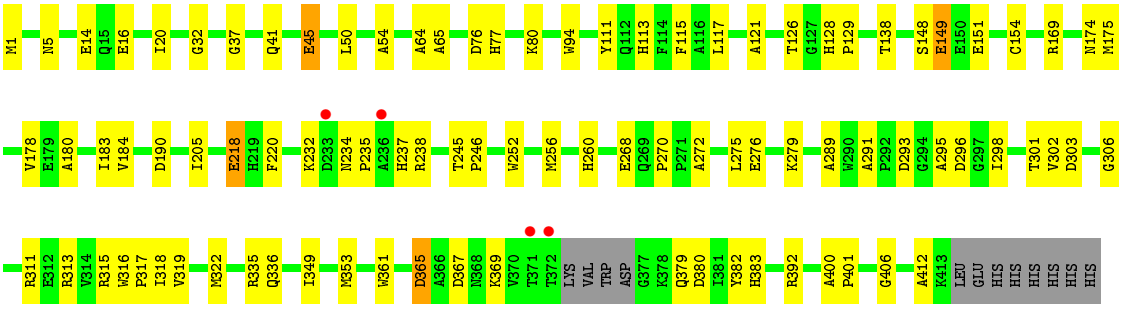
Chain C:





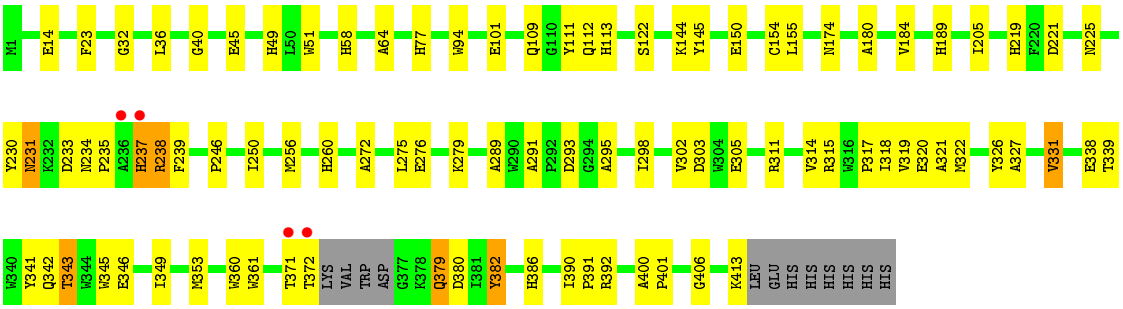
• Molecule 1: Uncharacterized sugar isomerase yihS

Chain D:



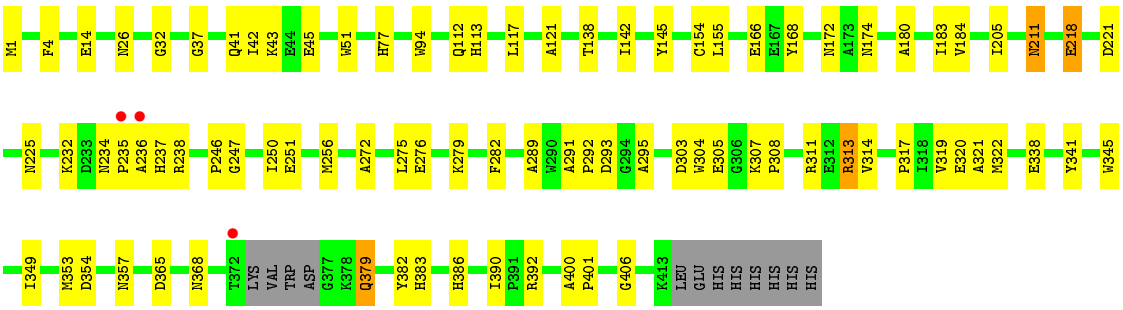
• Molecule 1: Uncharacterized sugar isomerase yihS

Chain E:



• Molecule 1: Uncharacterized sugar isomerase yihS

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	245.87Å 142.16Å 94.59Å 90.00° 107.61° 90.00°	Depositor
Resolution (Å)	14.97 – 2.50 48.66 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.5 (14.97-2.50) 96.6 (48.66-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	12.79 (at 2.51Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.180 , 0.236 0.180 , 0.236	Depositor DCC
R_{free} test set	10331 reflections (10.06%)	DCC
Wilson B-factor (Å^2)	18.6	Xtriage
Anisotropy	0.888	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 50.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 103226 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	21377	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.83% 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: 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	A	0.33	0/3421	0.57	0/4657
1	B	0.32	0/3421	0.56	0/4657
1	C	0.33	0/3421	0.57	0/4657
1	D	0.34	0/3421	0.58	0/4657
1	E	0.34	0/3421	0.58	0/4657
1	F	0.34	0/3421	0.57	0/4657
All	All	0.33	0/20526	0.57	0/27942

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

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	3317	0	3155	78	0
1	B	3317	0	3155	74	0
1	C	3317	0	3155	91	0
1	D	3317	0	3155	71	0
1	E	3317	0	3155	75	0
1	F	3317	0	3155	68	0
2	A	15	0	18	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	15	0	18	1	0
2	C	15	0	18	1	0
2	D	15	0	18	1	0
2	E	15	0	18	3	0
2	F	15	0	18	0	0
3	A	247	0	0	8	0
3	B	213	0	0	7	0
3	C	214	0	0	4	0
3	D	244	0	0	8	0
3	E	224	0	0	6	0
3	F	243	0	0	10	0
All	All	21377	0	19038	447	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 11.

All (447) 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:371:THR:HG22	1:A:372:THR:H	1.28	0.99
1:E:379:GLN:NE2	1:E:379:GLN:H	1.62	0.97
1:E:154:CYS:H	1:E:174:ASN:HD21	1.14	0.94
1:B:154:CYS:H	1:B:174:ASN:HD21	1.13	0.93
1:E:379:GLN:HE21	1:E:379:GLN:H	1.17	0.92
1:C:301:THR:HG22	1:C:309:VAL:HB	1.51	0.92
1:A:154:CYS:H	1:A:174:ASN:HD21	1.13	0.91
1:A:41:GLN:H	1:A:41:GLN:NE2	1.70	0.89
1:A:41:GLN:H	1:A:41:GLN:HE21	1.21	0.88
1:F:379:GLN:H	1:F:379:GLN:NE2	1.71	0.88
1:B:319:VAL:HA	1:B:322:MET:HE3	1.55	0.87
1:C:154:CYS:H	1:C:174:ASN:HD21	1.22	0.86
1:F:250:ILE:HG12	1:F:321:ALA:HA	1.58	0.86
1:C:339:THR:O	1:C:343:THR:HG22	1.80	0.82
1:C:194:LEU:O	1:C:198:ILE:HD13	1.78	0.82
1:C:41:GLN:H	1:C:41:GLN:NE2	1.80	0.80
1:D:154:CYS:H	1:D:174:ASN:HD21	1.30	0.80
1:D:349:ILE:HB	1:D:353:MET:HE3	1.65	0.78
1:C:301:THR:HG21	3:C:3029:HOH:O	1.82	0.78
1:C:246:PRO:HG2	1:C:289:ALA:HB2	1.66	0.77
1:E:349:ILE:HB	1:E:353:MET:HE3	1.66	0.77
1:A:371:THR:HG22	1:A:372:THR:N	2.00	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:349:ILE:HB	1:F:353:MET:HE3	1.68	0.75
1:C:250:ILE:HD12	1:C:285:THR:HG21	1.69	0.75
1:C:198:ILE:HD11	1:C:259:ILE:HG23	1.68	0.75
1:B:41:GLN:NE2	1:B:41:GLN:H	1.83	0.75
1:B:246:PRO:HG2	1:B:289:ALA:HB2	1.69	0.74
1:E:238:ARG:HH11	1:E:238:ARG:HG2	1.53	0.74
1:D:37:GLY:HA3	1:D:41:GLN:NE2	2.01	0.74
1:D:293:ASP:HB2	1:D:311:ARG:NH1	2.03	0.74
1:E:150:GLU:HG2	3:E:3216:HOH:O	1.87	0.74
1:F:37:GLY:HA3	1:F:41:GLN:HE22	1.53	0.73
1:A:400:ALA:HB3	1:A:401:PRO:HD3	1.69	0.73
1:B:39:LYS:H	1:B:41:GLN:HE22	1.37	0.72
1:F:293:ASP:OD2	1:F:311:ARG:HD2	1.88	0.72
1:C:221:ASP:OD1	1:C:225:ASN:HB2	1.89	0.72
1:E:400:ALA:HB3	1:E:401:PRO:HD3	1.70	0.72
1:F:154:CYS:H	1:F:174:ASN:HD21	1.37	0.72
1:A:198:ILE:HD11	1:A:259:ILE:HG21	1.73	0.71
1:B:315:ARG:HD3	1:B:361:TRP:O	1.90	0.71
1:A:39:LYS:H	1:A:41:GLN:HE22	1.38	0.69
1:C:198:ILE:HD11	1:C:259:ILE:CG2	2.22	0.69
1:E:320:GLU:OE2	1:E:386:HIS:HD2	1.76	0.69
1:E:339:THR:O	1:E:343:THR:HG22	1.93	0.69
1:A:349:ILE:CA	1:A:353:MET:HE3	2.22	0.69
1:E:154:CYS:H	1:E:174:ASN:ND2	1.87	0.68
1:F:379:GLN:H	1:F:379:GLN:HE21	1.37	0.68
1:A:1:MET:HE1	1:B:64:ALA:HB1	1.75	0.68
1:C:349:ILE:CA	1:C:353:MET:HE3	2.23	0.68
1:D:293:ASP:HB2	1:D:311:ARG:HH11	1.58	0.68
1:D:37:GLY:HA3	1:D:41:GLN:HE22	1.58	0.68
1:C:39:LYS:H	1:C:41:GLN:HE22	1.42	0.68
1:A:1:MET:CE	1:B:64:ALA:HB1	2.24	0.67
1:D:245:THR:HG22	1:D:301:THR:HG22	1.77	0.67
1:C:315:ARG:HD3	1:C:361:TRP:O	1.94	0.67
1:D:293:ASP:CB	1:D:311:ARG:HH11	2.07	0.67
1:F:400:ALA:HB3	1:F:401:PRO:HD3	1.77	0.67
1:E:272:ALA:O	1:E:276:GLU:HG3	1.95	0.67
1:C:238:ARG:HH11	1:C:241:ALA:H	1.41	0.66
1:A:38:ASN:ND2	1:A:377:GLY:HA2	2.10	0.66
1:A:41:GLN:N	1:A:41:GLN:HE21	1.94	0.66
1:F:232:LYS:HE2	3:F:3039:HOH:O	1.94	0.65
1:B:154:CYS:H	1:B:174:ASN:ND2	1.91	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:VAL:HA	1:C:322:MET:HE3	1.78	0.65
1:C:371:THR:HG22	1:C:372:THR:N	2.11	0.65
1:E:379:GLN:HE21	1:E:379:GLN:N	1.91	0.65
1:A:349:ILE:HA	1:A:353:MET:HE3	1.78	0.65
1:E:94:TRP:H	1:E:113:HIS:CE1	2.15	0.64
1:A:371:THR:CG2	1:A:372:THR:H	2.09	0.64
1:A:38:ASN:HD21	1:A:377:GLY:HA2	1.62	0.64
1:B:400:ALA:HB3	1:B:401:PRO:HD3	1.79	0.64
1:E:406:GLY:HA2	3:E:3033:HOH:O	1.96	0.64
1:B:245:THR:HG21	3:B:3144:HOH:O	1.95	0.64
1:C:234:ASN:HB3	1:C:237:HIS:CG	2.33	0.64
1:C:245:THR:HG23	3:C:3010:HOH:O	1.96	0.64
1:A:218:GLU:HG2	3:A:3054:HOH:O	1.97	0.64
1:A:198:ILE:CD1	1:A:259:ILE:HG21	2.28	0.64
1:A:83:ASN:ND2	1:A:87:ARG:NH2	2.45	0.63
1:F:37:GLY:HA3	1:F:41:GLN:NE2	2.13	0.63
1:A:319:VAL:HA	1:A:322:MET:HE3	1.79	0.63
1:D:64:ALA:HB1	1:F:1:MET:CE	2.29	0.63
1:D:246:PRO:HG2	1:D:289:ALA:HB2	1.80	0.63
1:B:234:ASN:HB3	1:B:237:HIS:ND1	2.14	0.63
1:C:349:ILE:HB	1:C:353:MET:HE3	1.81	0.63
1:D:64:ALA:HB1	1:F:1:MET:HE1	1.81	0.63
1:C:38:ASN:OD1	1:C:377:GLY:HA2	1.99	0.62
1:D:94:TRP:H	1:D:113:HIS:CE1	2.18	0.62
1:C:49:HIS:HD2	3:C:3037:HOH:O	1.82	0.62
1:D:149:GLU:HB2	3:D:3110:HOH:O	1.98	0.62
1:B:109:GLN:O	1:B:113:HIS:HD2	1.82	0.62
1:A:154:CYS:H	1:A:174:ASN:ND2	1.92	0.62
1:E:315:ARG:HD3	1:E:361:TRP:O	2.00	0.62
1:A:250:ILE:HD12	1:A:285:THR:HG21	1.82	0.62
1:F:349:ILE:CB	1:F:353:MET:HE3	2.30	0.62
1:E:293:ASP:OD2	1:E:311:ARG:HD2	2.00	0.61
1:C:41:GLN:H	1:C:41:GLN:HE21	1.48	0.61
1:F:383:HIS:HB2	3:F:3105:HOH:O	2.01	0.61
1:A:87:ARG:O	1:A:89:LYS:HD2	2.01	0.60
1:C:298:ILE:N	1:C:298:ILE:HD12	2.16	0.60
1:A:198:ILE:HD11	1:A:259:ILE:CG2	2.31	0.60
1:E:94:TRP:H	1:E:113:HIS:HE1	1.49	0.60
1:B:302:VAL:HG11	1:B:306:GLY:HA2	1.83	0.60
1:C:349:ILE:CB	1:C:353:MET:HE3	2.31	0.60
1:A:315:ARG:HD3	1:A:361:TRP:O	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:389:VAL:HB	1:C:399:MET:HE1	1.83	0.60
1:F:246:PRO:HG2	1:F:289:ALA:HB2	1.83	0.60
1:D:335:ARG:HH21	1:D:335:ARG:HG2	1.66	0.59
1:E:315:ARG:HD2	1:E:360:TRP:HB2	1.84	0.59
1:A:94:TRP:H	1:A:113:HIS:HE1	1.50	0.59
1:D:245:THR:HG23	3:D:3071:HOH:O	2.02	0.59
1:E:315:ARG:NH2	1:E:380:ASP:O	2.35	0.59
1:F:314:VAL:O	1:F:317:PRO:HD2	2.02	0.59
1:B:302:VAL:HG12	1:B:303:ASP:O	2.03	0.59
1:E:32:GLY:O	1:E:77:HIS:HE1	1.85	0.59
1:D:365:ASP:HB3	1:D:367:ASP:H	1.66	0.59
1:A:132:ARG:HH21	1:A:132:ARG:HG3	1.67	0.59
1:C:245:THR:HG21	3:C:3209:HOH:O	2.03	0.58
1:C:390:ILE:HG13	1:C:399:MET:HE3	1.85	0.58
1:A:94:TRP:H	1:A:113:HIS:CE1	2.21	0.58
1:B:369:LYS:HD2	3:B:3188:HOH:O	2.03	0.58
1:C:238:ARG:NE	1:C:239:PHE:H	2.01	0.58
1:D:111:TYR:OH	2:D:3004:EPE:H32	2.03	0.58
1:E:246:PRO:HG2	1:E:289:ALA:HB2	1.87	0.57
1:C:400:ALA:HB3	1:C:401:PRO:HD3	1.84	0.57
1:C:340:TRP:HA	1:C:343:THR:CG2	2.33	0.57
1:E:293:ASP:HB2	1:E:311:ARG:NH1	2.19	0.57
1:B:319:VAL:HA	1:B:322:MET:CE	2.30	0.57
1:E:293:ASP:HB2	1:E:311:ARG:HH11	1.70	0.57
1:D:319:VAL:HA	1:D:322:MET:HE3	1.86	0.57
1:D:315:ARG:HD3	1:D:361:TRP:O	2.03	0.57
1:D:349:ILE:CB	1:D:353:MET:HE3	2.33	0.57
1:D:45:GLU:H	1:D:45:GLU:CD	2.08	0.57
1:B:335:ARG:NH1	1:B:338:GLU:OE1	2.38	0.56
1:B:14:GLU:HB2	1:B:392:ARG:NH1	2.20	0.56
1:F:218:GLU:HG3	3:F:3076:HOH:O	2.04	0.56
1:C:390:ILE:HG13	1:C:399:MET:CE	2.35	0.56
1:B:111:TYR:OH	2:B:3002:EPE:H82	2.06	0.56
1:E:293:ASP:CB	1:E:311:ARG:HH11	2.19	0.56
1:C:371:THR:HG22	1:C:372:THR:H	1.71	0.56
1:D:272:ALA:O	1:D:276:GLU:HG3	2.06	0.56
1:E:14:GLU:HB2	1:E:392:ARG:NH1	2.21	0.56
1:E:260:HIS:HE1	3:E:3092:HOH:O	1.89	0.56
1:F:379:GLN:N	1:F:379:GLN:HE21	2.05	0.55
1:F:247:GLY:O	1:F:250:ILE:HG22	2.07	0.55
1:D:400:ALA:HB3	1:D:401:PRO:HD3	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:TRP:HZ2	1:C:152:GLN:NE2	2.04	0.55
1:F:205:ILE:HG21	1:F:256:MET:CE	2.36	0.55
1:F:250:ILE:HD11	1:F:282:PHE:CD1	2.41	0.55
1:B:39:LYS:N	1:B:41:GLN:HE22	2.02	0.55
1:C:38:ASN:HD22	1:C:361:TRP:HZ3	1.54	0.55
1:D:218:GLU:HG3	3:D:3072:HOH:O	2.05	0.55
1:C:238:ARG:NH1	1:C:241:ALA:H	2.04	0.55
1:F:211:ASN:ND2	1:F:211:ASN:C	2.59	0.55
1:D:32:GLY:O	1:D:77:HIS:HE1	1.91	0.54
1:D:291:ALA:HA	1:D:295:ALA:O	2.07	0.54
1:C:349:ILE:HA	1:C:353:MET:HE3	1.89	0.54
1:F:345:TRP:CZ3	1:F:353:MET:HE1	2.42	0.54
1:C:94:TRP:H	1:C:113:HIS:CE1	2.25	0.54
1:B:245:THR:HG23	3:B:3051:HOH:O	2.08	0.54
1:B:303:ASP:OD2	1:B:307:LYS:HB2	2.08	0.54
1:F:236:ALA:HB3	3:F:3112:HOH:O	2.06	0.54
1:E:349:ILE:CB	1:E:353:MET:HE3	2.36	0.54
1:A:349:ILE:CB	1:A:353:MET:HE3	2.38	0.53
1:D:117:LEU:HA	1:D:138:THR:HG21	1.90	0.53
1:E:109:GLN:O	1:E:113:HIS:HD2	1.91	0.53
1:D:406:GLY:HA2	3:D:3016:HOH:O	2.09	0.53
1:C:14:GLU:HB2	1:C:392:ARG:NH1	2.24	0.53
1:D:175:MET:HB2	1:D:252:TRP:CZ2	2.44	0.53
1:F:319:VAL:HA	1:F:322:MET:HE3	1.89	0.53
1:B:302:VAL:HG13	1:B:306:GLY:C	2.30	0.53
1:E:221:ASP:OD2	1:E:225:ASN:HB2	2.08	0.53
1:E:49:HIS:HD2	3:E:3146:HOH:O	1.92	0.53
1:E:205:ILE:HG21	1:E:256:MET:HE1	1.90	0.52
1:A:132:ARG:CG	1:A:132:ARG:HH21	2.22	0.52
1:C:315:ARG:NH2	1:C:380:ASP:O	2.43	0.52
1:B:313:ARG:HG3	1:B:368:ASN:OD1	2.09	0.52
1:B:190:ASP:OD1	1:B:192:LYS:HG2	2.10	0.52
1:B:83:ASN:ND2	1:B:87:ARG:NH2	2.58	0.52
1:C:380:ASP:OD1	1:C:382:TYR:HB3	2.10	0.52
1:F:234:ASN:N	1:F:235:PRO:HD3	2.24	0.52
1:A:190:ASP:OD1	1:A:192:LYS:HG2	2.10	0.52
1:E:314:VAL:O	1:E:317:PRO:HD2	2.09	0.52
1:B:269:GLN:HA	1:B:269:GLN:NE2	2.25	0.52
1:C:109:GLN:O	1:C:113:HIS:HD2	1.93	0.51
1:A:246:PRO:HG2	1:A:289:ALA:HB2	1.93	0.51
1:C:234:ASN:HA	1:C:237:HIS:CE1	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:ALA:O	1:D:184:VAL:HG23	2.10	0.51
1:A:326:TYR:CZ	1:A:391:PRO:HA	2.46	0.51
1:A:39:LYS:HE2	1:A:357:ASN:OD1	2.10	0.51
1:D:154:CYS:H	1:D:174:ASN:ND2	2.04	0.51
1:F:234:ASN:HB3	1:F:237:HIS:CD2	2.46	0.51
1:B:39:LYS:HB2	1:B:41:GLN:NE2	2.26	0.51
1:B:38:ASN:HD22	1:B:361:TRP:HZ3	1.57	0.51
1:B:94:TRP:H	1:B:113:HIS:CE1	2.28	0.51
1:F:406:GLY:HA2	3:F:3021:HOH:O	2.10	0.51
1:E:275:LEU:HG	1:E:279:LYS:HE3	1.91	0.51
1:B:62:VAL:HG12	1:B:66:MET:CE	2.40	0.51
1:A:319:VAL:HA	1:A:322:MET:CE	2.41	0.51
1:A:132:ARG:NH1	1:A:187:VAL:O	2.45	0.51
1:D:232:LYS:O	1:D:235:PRO:HD3	2.10	0.51
1:D:238:ARG:HD3	3:D:3079:HOH:O	2.11	0.50
1:F:303:ASP:OD2	1:F:307:LYS:HB3	2.11	0.50
1:E:36:LEU:HD22	1:E:40:GLY:O	2.11	0.50
1:C:266:ARG:HB3	1:E:189:HIS:CD2	2.47	0.50
1:C:154:CYS:H	1:C:174:ASN:ND2	1.99	0.50
1:E:380:ASP:OD1	1:E:382:TYR:HB3	2.12	0.50
1:A:390:ILE:HG23	3:A:3191:HOH:O	2.10	0.50
1:C:238:ARG:HA	1:C:238:ARG:HE	1.77	0.50
1:B:190:ASP:HB3	1:B:193:TRP:CD1	2.47	0.50
1:B:302:VAL:CG1	1:B:306:GLY:HA2	2.42	0.50
1:A:191:LYS:HE2	1:D:190:ASP:HB2	1.94	0.50
1:C:340:TRP:O	1:C:343:THR:HG23	2.12	0.50
1:A:41:GLN:N	1:A:41:GLN:NE2	2.51	0.50
1:A:83:ASN:HD22	1:A:87:ARG:NH2	2.10	0.50
1:A:196:ARG:O	1:A:200:VAL:HG23	2.11	0.50
1:C:301:THR:HB	1:C:310:VAL:HB	1.93	0.50
1:C:90:LYS:HD2	1:C:91:TYR:CE2	2.47	0.50
1:B:191:LYS:HG2	1:B:195:ASP:OD2	2.12	0.49
1:C:83:ASN:ND2	1:C:87:ARG:NH2	2.61	0.49
1:E:291:ALA:HA	1:E:295:ALA:O	2.12	0.49
1:C:338:GLU:O	1:C:342:GLN:HG3	2.11	0.49
1:F:43:LYS:HG2	3:F:3223:HOH:O	2.12	0.49
1:D:65:ALA:HB2	3:D:3022:HOH:O	2.12	0.49
1:D:94:TRP:H	1:D:113:HIS:HE1	1.57	0.49
1:E:289:ALA:O	1:E:298:ILE:HA	2.13	0.49
1:A:221:ASP:OD1	1:A:225:ASN:HB2	2.12	0.49
1:E:345:TRP:CZ3	1:E:353:MET:HE1	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:HIS:CE1	1:D:270:PRO:HG3	2.48	0.49
1:E:234:ASN:HB3	1:E:237:HIS:CE1	2.47	0.49
1:B:140:GLU:HA	3:B:3208:HOH:O	2.12	0.49
1:F:247:GLY:O	1:F:251:GLU:HG3	2.13	0.48
1:E:338:GLU:O	1:E:341:TYR:HB3	2.13	0.48
1:E:180:ALA:O	1:E:184:VAL:HG23	2.13	0.48
1:F:32:GLY:O	1:F:77:HIS:HE1	1.96	0.48
1:B:93:GLY:HA2	1:B:141:ILE:HD12	1.95	0.48
1:A:349:ILE:HB	1:A:353:MET:HE3	1.94	0.48
1:C:301:THR:CG2	1:C:309:VAL:HB	2.32	0.48
1:A:370:VAL:HG23	3:A:3227:HOH:O	2.12	0.48
1:C:238:ARG:O	1:C:239:PHE:HB3	2.14	0.47
1:B:335:ARG:HD2	3:B:3212:HOH:O	2.14	0.47
1:F:275:LEU:HD11	1:F:279:LYS:HE3	1.96	0.47
1:C:316:TRP:CG	1:C:317:PRO:HD3	2.49	0.47
1:A:166:GLU:HG2	1:A:168:TYR:HB3	1.94	0.47
1:A:132:ARG:NH2	3:A:3073:HOH:O	2.47	0.47
1:E:303:ASP:OD2	1:E:305:GLU:HG2	2.15	0.47
1:A:14:GLU:HB2	1:A:392:ARG:NH1	2.29	0.47
1:D:121:ALA:HB1	1:D:183:ILE:HG22	1.96	0.47
1:F:121:ALA:HB1	1:F:183:ILE:HG22	1.97	0.47
1:A:326:TYR:CE2	1:A:391:PRO:HA	2.48	0.47
1:B:328:LEU:HD13	1:B:337:TYR:CE2	2.49	0.47
1:C:198:ILE:HD12	1:C:259:ILE:HD13	1.97	0.47
1:C:39:LYS:N	1:C:41:GLN:HE22	2.11	0.47
1:A:1:MET:HE3	1:B:126:THR:HB	1.97	0.47
1:C:371:THR:CG2	1:C:372:THR:N	2.77	0.47
1:C:148:SER:OG	1:C:151:GLU:HB2	2.15	0.47
1:A:371:THR:O	1:A:372:THR:HG23	2.15	0.47
1:D:365:ASP:HB2	1:D:369:LYS:H	1.79	0.47
1:B:88:ASP:OD2	1:B:91:TYR:HB2	2.15	0.47
1:B:94:TRP:CH2	1:B:141:ILE:HD11	2.50	0.47
1:B:94:TRP:CZ3	1:B:141:ILE:HD11	2.50	0.46
1:E:315:ARG:HD2	1:E:360:TRP:CB	2.45	0.46
1:F:291:ALA:HA	1:F:295:ALA:O	2.15	0.46
1:D:316:TRP:CG	1:D:317:PRO:HD3	2.50	0.46
1:E:319:VAL:HA	1:E:322:MET:HE3	1.98	0.46
1:F:14:GLU:HB2	1:F:392:ARG:NH1	2.30	0.46
1:C:340:TRP:HA	1:C:343:THR:HG23	1.97	0.46
1:C:117:LEU:HA	1:C:138:THR:HG21	1.97	0.46
1:C:88:ASP:HB3	1:C:92:GLY:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:VAL:HG12	1:B:66:MET:HE2	1.98	0.46
1:B:315:ARG:NH2	1:B:380:ASP:O	2.47	0.46
1:C:298:ILE:HD13	1:C:318:ILE:HD12	1.97	0.46
1:C:385:LEU:O	1:C:399:MET:HE1	2.16	0.46
1:E:345:TRP:HZ3	1:E:353:MET:HE1	1.81	0.46
1:A:132:ARG:HH22	1:D:268:GLU:HA	1.81	0.46
1:D:319:VAL:HA	1:D:322:MET:CE	2.45	0.46
1:C:275:LEU:HG	1:C:279:LYS:HE3	1.97	0.46
1:F:221:ASP:OD2	1:F:225:ASN:HB2	2.15	0.46
1:F:94:TRP:H	1:F:113:HIS:CE1	2.34	0.46
1:D:175:MET:HB2	1:D:252:TRP:CE2	2.50	0.46
1:A:191:LYS:HG2	1:A:195:ASP:OD2	2.15	0.46
1:F:145:TYR:O	1:F:155:LEU:HD12	2.16	0.46
1:B:41:GLN:NE2	1:B:41:GLN:N	2.59	0.46
1:B:312:GLU:HG2	1:B:363:GLU:OE2	2.16	0.46
1:F:272:ALA:O	1:F:276:GLU:HG3	2.14	0.46
1:A:39:LYS:N	1:A:41:GLN:HE22	2.11	0.45
1:C:315:ARG:HD2	1:C:360:TRP:CB	2.45	0.45
1:E:51:TRP:CZ3	2:E:3005:EPE:H92	2.51	0.45
1:A:44:GLU:N	1:A:44:GLU:CD	2.69	0.45
1:C:238:ARG:HH11	1:C:241:ALA:N	2.12	0.45
1:C:136:ASP:O	1:C:140:GLU:HG3	2.16	0.45
1:C:169:ARG:HB2	1:C:220:PHE:HB2	1.97	0.45
1:A:1:MET:HB2	1:B:126:THR:O	2.16	0.45
1:D:291:ALA:HB2	1:D:296:ASP:HA	1.98	0.45
1:F:26:ASN:O	1:F:42:ILE:HD11	2.17	0.45
1:D:303:ASP:HB2	3:D:3187:HOH:O	2.17	0.45
1:E:58:HIS:HD2	1:E:122:SER:OG	1.98	0.45
1:F:117:LEU:HA	1:F:138:THR:HG21	1.97	0.45
1:C:111:TYR:OH	2:C:3003:EPE:H32	2.16	0.45
1:A:175:MET:HB2	1:A:252:TRP:CZ2	2.52	0.45
1:B:354:ASP:OD2	1:B:357:ASN:HB2	2.17	0.45
1:E:219:HIS:CD2	1:E:230:TYR:HB3	2.52	0.45
1:F:205:ILE:HG21	1:F:256:MET:HE1	1.99	0.45
1:E:233:ASP:C	1:E:234:ASN:HD22	2.20	0.45
1:D:298:ILE:HD12	1:D:318:ILE:HA	1.99	0.45
1:A:32:GLY:O	1:A:77:HIS:HE1	1.99	0.45
1:B:21:PHE:CZ	1:B:63:ALA:HB2	2.52	0.45
1:A:406:GLY:HA2	3:A:3072:HOH:O	2.16	0.45
1:A:316:TRP:CG	1:A:317:PRO:HD3	2.51	0.45
2:A:3001:EPE:H61	3:A:3124:HOH:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:ASP:OD2	1:D:311:ARG:HD2	2.18	0.45
1:E:289:ALA:HB1	1:E:298:ILE:HG23	1.99	0.45
1:B:364:LEU:HD23	1:B:370:VAL:HA	1.99	0.45
1:B:167:GLU:HA	1:B:222:THR:CG2	2.47	0.45
1:B:41:GLN:HE21	1:B:41:GLN:H	1.64	0.44
1:B:338:GLU:O	1:B:342:GLN:HG3	2.17	0.44
1:B:21:PHE:CE1	1:B:63:ALA:HB2	2.52	0.44
1:A:50:LEU:HB3	1:A:112:GLN:OE1	2.17	0.44
1:F:238:ARG:NE	3:F:3208:HOH:O	2.50	0.44
1:C:87:ARG:O	1:C:89:LYS:HD2	2.17	0.44
1:F:238:ARG:NH2	3:F:3036:HOH:O	2.50	0.44
1:B:83:ASN:HD22	1:B:87:ARG:CZ	2.31	0.44
1:D:234:ASN:HB3	1:D:237:HIS:CE1	2.52	0.44
1:B:383:HIS:HB2	3:B:3164:HOH:O	2.18	0.44
1:D:126:THR:HB	1:F:1:MET:HE3	2.00	0.44
1:E:342:GLN:O	1:E:346:GLU:HG2	2.18	0.44
1:F:4:PHE:HA	3:F:3060:HOH:O	2.18	0.44
1:F:313:ARG:HD2	1:F:368:ASN:OD1	2.18	0.43
1:C:50:LEU:HD23	1:C:112:GLN:HB3	2.00	0.43
1:D:148:SER:OG	1:D:151:GLU:HB2	2.18	0.43
1:F:293:ASP:HB2	1:F:311:ARG:NH1	2.33	0.43
1:B:38:ASN:OD1	1:B:377:GLY:HA2	2.18	0.43
1:E:386:HIS:O	1:E:390:ILE:HB	2.19	0.43
1:D:302:VAL:HG11	1:D:306:GLY:HA2	2.00	0.43
1:D:128:HIS:HA	1:D:129:PRO:HD3	1.90	0.43
1:B:250:ILE:HD12	1:B:285:THR:HG21	1.99	0.43
1:A:338:GLU:O	1:A:342:GLN:HG3	2.18	0.43
1:C:298:ILE:N	1:C:298:ILE:CD1	2.81	0.43
1:A:312:GLU:HG2	1:A:363:GLU:OE1	2.19	0.43
1:D:16:GLU:O	1:D:20:ILE:HG12	2.19	0.43
1:D:275:LEU:HG	1:D:279:LYS:HE3	2.00	0.43
1:E:298:ILE:HD12	1:E:318:ILE:HA	1.99	0.43
1:C:89:LYS:N	1:C:89:LYS:HD2	2.33	0.43
1:E:51:TRP:HB3	1:E:112:GLN:HG2	2.01	0.43
1:D:302:VAL:CG1	1:D:306:GLY:HA2	2.48	0.43
1:E:111:TYR:OH	2:E:3005:EPE:H32	2.18	0.43
1:E:250:ILE:HD13	1:E:321:ALA:HA	2.01	0.43
1:A:233:ASP:HB2	3:A:3229:HOH:O	2.18	0.43
1:F:386:HIS:HA	1:F:390:ILE:HD12	2.01	0.43
1:C:45:GLU:CD	1:C:45:GLU:H	2.21	0.43
1:A:169:ARG:HB2	1:A:220:PHE:HB2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:LEU:HD22	1:D:94:TRP:HB2	2.00	0.43
1:C:229:ASP:OD1	1:C:232:LYS:HD2	2.19	0.43
1:B:273:TRP:HA	1:B:276:GLU:HB2	2.00	0.43
1:D:379:GLN:CD	1:D:379:GLN:H	2.23	0.43
1:C:250:ILE:HD12	1:C:285:THR:CG2	2.46	0.42
1:C:371:THR:CG2	1:C:372:THR:H	2.32	0.42
1:E:231:ASN:HD22	1:E:231:ASN:HA	1.62	0.42
1:B:138:THR:O	1:B:142:ILE:HG12	2.18	0.42
1:C:198:ILE:HD12	1:C:198:ILE:N	2.34	0.42
1:F:345:TRP:HZ3	1:F:353:MET:HE1	1.85	0.42
2:A:3001:EPE:H31	3:A:3050:HOH:O	2.19	0.42
1:E:145:TYR:O	1:E:155:LEU:HD12	2.20	0.42
1:C:41:GLN:HE21	1:C:41:GLN:N	2.14	0.42
1:C:51:TRP:HD1	1:C:112:GLN:OE1	2.02	0.42
1:D:76:ASP:O	1:D:80:LYS:HG2	2.20	0.42
1:D:32:GLY:O	1:D:77:HIS:CE1	2.72	0.42
1:E:144:LYS:HD2	1:E:145:TYR:CE2	2.54	0.42
1:D:1:MET:SD	1:E:64:ALA:HB1	2.60	0.42
1:E:379:GLN:NE2	1:E:379:GLN:N	2.46	0.42
1:C:38:ASN:ND2	1:C:361:TRP:HZ3	2.17	0.42
1:F:172:ASN:N	1:F:218:GLU:OE1	2.50	0.42
1:B:269:GLN:HA	1:B:269:GLN:HE21	1.85	0.42
1:A:117:LEU:HA	1:A:138:THR:HG21	2.01	0.42
1:F:365:ASP:HB2	3:F:3204:HOH:O	2.20	0.42
1:E:23:PHE:CZ	1:E:40:GLY:HA2	2.55	0.42
1:F:180:ALA:O	1:F:184:VAL:HG23	2.20	0.42
1:B:94:TRP:H	1:B:113:HIS:HE1	1.66	0.42
1:B:190:ASP:HB3	1:B:193:TRP:HD1	1.82	0.42
1:F:138:THR:O	1:F:142:ILE:HG12	2.18	0.42
1:B:257:LEU:O	1:B:260:HIS:HB3	2.19	0.42
1:F:304:TRP:HA	1:F:304:TRP:CE3	2.55	0.42
1:E:371:THR:HG22	1:E:372:THR:N	2.35	0.42
1:A:17:THR:HA	1:A:388:LEU:HD13	2.02	0.42
1:E:239:PHE:HD1	2:E:3005:EPE:HO8	1.68	0.42
1:D:148:SER:CB	1:D:151:GLU:HB2	2.50	0.42
1:C:234:ASN:HB3	1:C:237:HIS:CD2	2.54	0.41
1:C:175:MET:O	1:C:178:VAL:HB	2.20	0.41
1:E:386:HIS:HA	1:E:390:ILE:HG13	2.00	0.41
1:D:5:ASN:O	1:D:412:ALA:HA	2.20	0.41
1:E:315:ARG:O	1:E:319:VAL:HG23	2.20	0.41
1:E:246:PRO:CG	1:E:289:ALA:HB2	2.49	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:GLN:CA	1:B:269:GLN:HE21	2.33	0.41
1:B:117:LEU:HA	1:B:138:THR:HG21	2.01	0.41
1:A:101:GLU:N	1:A:101:GLU:OE2	2.53	0.41
1:C:94:TRP:H	1:C:113:HIS:HE1	1.65	0.41
1:F:293:ASP:OD2	1:F:313:ARG:NH2	2.54	0.41
1:B:234:ASN:HB3	1:B:237:HIS:CG	2.56	0.41
1:A:109:GLN:O	1:A:113:HIS:HD2	2.02	0.41
1:A:219:HIS:CD2	1:A:230:TYR:HB3	2.55	0.41
1:E:233:ASP:C	1:E:235:PRO:HD3	2.41	0.41
1:F:338:GLU:O	1:F:341:TYR:HB3	2.20	0.41
1:D:335:ARG:HG2	1:D:335:ARG:NH2	2.35	0.41
1:C:50:LEU:HB3	1:C:112:GLN:OE1	2.21	0.41
1:D:169:ARG:HB2	1:D:220:PHE:HB2	2.02	0.41
1:D:54:ALA:HB1	1:D:115:PHE:O	2.21	0.41
1:A:1:MET:HE2	1:B:64:ALA:HB1	2.00	0.41
1:D:315:ARG:NH2	1:D:380:ASP:O	2.52	0.41
1:F:307:LYS:HA	1:F:308:PRO:HD3	1.91	0.41
1:A:293:ASP:OD1	1:A:293:ASP:N	2.53	0.41
1:C:198:ILE:HD11	1:C:259:ILE:HG21	2.03	0.41
1:C:247:GLY:O	1:C:250:ILE:HG22	2.21	0.41
1:D:175:MET:O	1:D:178:VAL:HB	2.21	0.41
1:A:216:VAL:HB	1:A:249:TRP:CD1	2.56	0.41
1:B:247:GLY:O	1:B:250:ILE:HG22	2.20	0.41
1:F:51:TRP:HB3	1:F:112:GLN:HG2	2.01	0.41
1:A:55:ARG:O	1:A:58:HIS:HB3	2.21	0.41
1:D:383:HIS:HB2	3:D:3045:HOH:O	2.21	0.41
1:D:293:ASP:CB	1:D:311:ARG:NH1	2.74	0.41
1:F:211:ASN:HD22	1:F:211:ASN:C	2.23	0.41
1:B:62:VAL:O	1:B:66:MET:HG3	2.22	0.41
1:E:338:GLU:O	1:E:342:GLN:HG3	2.21	0.41
1:F:291:ALA:N	1:F:292:PRO:CD	2.84	0.41
1:E:327:ALA:O	1:E:331:VAL:HG12	2.20	0.41
1:E:413:LYS:HE2	1:E:413:LYS:HB3	1.88	0.41
1:B:109:GLN:O	1:B:113:HIS:CD2	2.70	0.40
1:E:326:TYR:CZ	1:E:391:PRO:HA	2.56	0.40
1:B:245:THR:HG22	1:B:301:THR:HG22	2.03	0.40
1:E:189:HIS:HE1	3:E:3073:HOH:O	2.04	0.40
1:F:275:LEU:CD1	1:F:279:LYS:HE3	2.52	0.40
1:D:205:ILE:HG21	1:D:256:MET:HE1	2.03	0.40
1:D:14:GLU:HB2	1:D:392:ARG:NH1	2.36	0.40
1:F:251:GLU:HG2	1:F:320:GLU:HG3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:ARG:CZ	1:C:239:PHE:H	2.34	0.40
1:B:408:LEU:HB2	3:B:3084:HOH:O	2.21	0.40
1:F:379:GLN:N	1:F:379:GLN:NE2	2.54	0.40
1:F:154:CYS:H	1:F:174:ASN:ND2	2.11	0.40
1:A:345:TRP:HZ3	1:A:353:MET:HE2	1.86	0.40
1:A:246:PRO:HA	1:A:249:TRP:CD2	2.56	0.40
1:E:58:HIS:HE1	3:E:3011:HOH:O	2.04	0.40
1:C:219:HIS:CD2	1:C:230:TYR:HB3	2.56	0.40
1:A:380:ASP:OD1	1:A:382:TYR:HB3	2.22	0.40
1:C:364:LEU:HD23	1:C:370:VAL:HA	2.03	0.40
1:F:166:GLU:HG2	1:F:168:TYR:HB3	2.02	0.40
1:C:315:ARG:HD2	1:C:360:TRP:HB2	2.03	0.40
1:A:252:TRP:O	1:A:256:MET:HG3	2.20	0.40
1:A:328:LEU:HD13	1:A:337:TYR:CE2	2.56	0.40
1:F:354:ASP:OD2	1:F:357:ASN:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	405/421 (96%)	390 (96%)	14 (4%)	1 (0%)	52 75
1	B	405/421 (96%)	388 (96%)	17 (4%)	0	100 100
1	C	405/421 (96%)	388 (96%)	13 (3%)	4 (1%)	19 34
1	D	405/421 (96%)	392 (97%)	13 (3%)	0	100 100
1	E	405/421 (96%)	393 (97%)	12 (3%)	0	100 100
1	F	405/421 (96%)	393 (97%)	12 (3%)	0	100 100
All	All	2430/2526 (96%)	2344 (96%)	81 (3%)	5 (0%)	52 75

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	GLU
1	C	191	LYS
1	C	235	PRO
1	C	237	HIS
1	C	238	ARG

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	335/347 (96%)	325 (97%)	10 (3%)	48	76
1	B	335/347 (96%)	329 (98%)	6 (2%)	66	88
1	C	335/347 (96%)	328 (98%)	7 (2%)	61	85
1	D	335/347 (96%)	328 (98%)	7 (2%)	61	85
1	E	335/347 (96%)	325 (97%)	10 (3%)	48	76
1	F	335/347 (96%)	328 (98%)	7 (2%)	61	85
All	All	2010/2082 (96%)	1963 (98%)	47 (2%)	58	83

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	41	GLN
1	A	44	GLU
1	A	45	GLU
1	A	132	ARG
1	A	250	ILE
1	A	292	PRO
1	A	302	VAL
1	A	307	LYS
1	A	382	TYR
1	B	41	GLN
1	B	45	GLU
1	B	245	THR
1	B	250	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	313	ARG
1	B	382	TYR
1	C	41	GLN
1	C	45	GLU
1	C	238	ARG
1	C	250	ILE
1	C	301	THR
1	C	343	THR
1	C	382	TYR
1	D	45	GLU
1	D	149	GLU
1	D	218	GLU
1	D	313	ARG
1	D	336	GLN
1	D	365	ASP
1	D	382	TYR
1	E	45	GLU
1	E	101	GLU
1	E	231	ASN
1	E	237	HIS
1	E	238	ARG
1	E	302	VAL
1	E	331	VAL
1	E	343	THR
1	E	379	GLN
1	E	382	TYR
1	F	45	GLU
1	F	211	ASN
1	F	218	GLU
1	F	305	GLU
1	F	313	ARG
1	F	379	GLN
1	F	382	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	41	GLN
1	A	49	HIS
1	A	77	HIS
1	A	83	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	113	HIS
1	A	172	ASN
1	A	174	ASN
1	A	189	HIS
1	A	217	ASN
1	A	223	GLN
1	A	231	ASN
1	A	269	GLN
1	B	41	GLN
1	B	49	HIS
1	B	77	HIS
1	B	83	ASN
1	B	113	HIS
1	B	152	GLN
1	B	172	ASN
1	B	174	ASN
1	B	217	ASN
1	B	231	ASN
1	B	269	GLN
1	B	336	GLN
1	C	41	GLN
1	C	49	HIS
1	C	77	HIS
1	C	83	ASN
1	C	113	HIS
1	C	152	GLN
1	C	172	ASN
1	C	174	ASN
1	C	231	ASN
1	C	269	GLN
1	C	283	ASN
1	D	15	GLN
1	D	49	HIS
1	D	77	HIS
1	D	83	ASN
1	D	113	HIS
1	D	174	ASN
1	D	212	ASN
1	D	217	ASN
1	D	237	HIS
1	D	336	GLN
1	E	26	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	38	ASN
1	E	49	HIS
1	E	58	HIS
1	E	77	HIS
1	E	113	HIS
1	E	174	ASN
1	E	189	HIS
1	E	212	ASN
1	E	217	ASN
1	E	231	ASN
1	E	234	ASN
1	E	260	HIS
1	E	269	GLN
1	E	336	GLN
1	E	379	GLN
1	E	386	HIS
1	F	49	HIS
1	F	77	HIS
1	F	113	HIS
1	F	174	ASN
1	F	211	ASN
1	F	212	ASN
1	F	217	ASN
1	F	260	HIS
1	F	269	GLN
1	F	336	GLN
1	F	379	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 (i)

6 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	$\#\|Z\| > 2$
2	EPE	A	3001	-	14,15,15	1.04	1 (7%)	18,20,20	2.05	3 (16%)
2	EPE	B	3002	-	14,15,15	0.93	1 (7%)	18,20,20	2.04	3 (16%)
2	EPE	C	3003	-	14,15,15	0.96	1 (7%)	18,20,20	1.71	4 (22%)
2	EPE	D	3004	-	14,15,15	1.00	1 (7%)	18,20,20	1.68	4 (22%)
2	EPE	E	3005	-	14,15,15	0.91	1 (7%)	18,20,20	1.65	3 (16%)
2	EPE	F	3006	-	14,15,15	0.96	1 (7%)	18,20,20	5.77	5 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EPE	A	3001	-	-	0/9/19/19	0/1/1/1
2	EPE	B	3002	-	-	0/9/19/19	0/1/1/1
2	EPE	C	3003	-	-	0/9/19/19	0/1/1/1
2	EPE	D	3004	-	-	0/9/19/19	0/1/1/1
2	EPE	E	3005	-	-	0/9/19/19	0/1/1/1
2	EPE	F	3006	-	-	0/9/19/19	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3002	EPE	O3S-S	2.05	1.51	1.46
2	D	3004	EPE	O3S-S	2.09	1.51	1.46
2	F	3006	EPE	O3S-S	2.11	1.51	1.46
2	A	3001	EPE	O3S-S	2.15	1.52	1.46
2	E	3005	EPE	O3S-S	2.21	1.52	1.46
2	C	3003	EPE	O3S-S	2.38	1.52	1.46

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	3006	EPE	O3S-S-O1S	-12.99	81.37	111.61
2	F	3006	EPE	O3S-S-O2S	-12.72	82.00	111.61
2	E	3005	EPE	O3S-S-O1S	-2.85	104.97	111.61
2	C	3003	EPE	O3S-S-O1S	-2.83	105.01	111.61
2	A	3001	EPE	O3S-S-O2S	-2.82	105.05	111.61
2	B	3002	EPE	O3S-S-O1S	-2.53	105.73	111.61
2	D	3004	EPE	O3S-S-O1S	-2.44	105.92	111.61
2	B	3002	EPE	O3S-S-O2S	-2.42	105.99	111.61
2	A	3001	EPE	O3S-S-O1S	-2.32	106.22	111.61
2	D	3004	EPE	O3S-S-O2S	-2.19	106.52	111.61
2	C	3003	EPE	O3S-S-O2S	-2.01	106.94	111.61
2	C	3003	EPE	O2S-S-C10	2.22	108.80	106.91
2	D	3004	EPE	O2S-S-C10	2.38	108.94	106.91
2	E	3005	EPE	O2S-S-C10	2.62	109.14	106.91
2	F	3006	EPE	O2S-S-O1S	2.77	123.57	113.48
2	E	3005	EPE	O1S-S-C10	3.96	110.28	106.91
2	C	3003	EPE	O1S-S-C10	4.65	110.87	106.91
2	D	3004	EPE	O1S-S-C10	4.75	110.96	106.91
2	F	3006	EPE	O2S-S-C10	5.89	111.93	106.91
2	B	3002	EPE	O1S-S-C10	6.75	112.67	106.91
2	A	3001	EPE	O1S-S-C10	6.94	112.83	106.91
2	F	3006	EPE	O1S-S-C10	14.57	119.34	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3001	EPE	2	0
2	B	3002	EPE	1	0
2	C	3003	EPE	1	0
2	D	3004	EPE	1	0
2	E	3005	EPE	3	0

5.7 Other polymers

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	409/421 (97%)	-0.27	2 (0%)	91 92	12, 19, 34, 47	0
1	B	409/421 (97%)	-0.06	7 (1%)	73 76	11, 20, 36, 56	0
1	C	409/421 (97%)	-0.20	5 (1%)	81 83	10, 19, 33, 70	0
1	D	409/421 (97%)	-0.23	4 (0%)	84 86	6, 16, 31, 52	0
1	E	409/421 (97%)	-0.15	4 (0%)	84 86	7, 16, 32, 50	0
1	F	409/421 (97%)	-0.28	3 (0%)	89 90	8, 17, 32, 47	0
All	All	2454/2526 (97%)	-0.20	25 (1%)	84 86	6, 18, 33, 70	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	235	PRO	4.8
1	D	372	THR	4.7
1	C	372	THR	4.3
1	C	236	ALA	4.0
1	C	238	ARG	3.6
1	B	91	TYR	3.3
1	E	236	ALA	3.1
1	B	163	SER	2.8
1	E	372	THR	2.8
1	B	235	PRO	2.8
1	C	371	THR	2.7
1	E	371	THR	2.7
1	D	233	ASP	2.6
1	D	371	THR	2.6
1	F	372	THR	2.6
1	D	236	ALA	2.5
1	E	237	HIS	2.4
1	F	235	PRO	2.3
1	A	91	TYR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	372	THR	2.2
1	F	236	ALA	2.2
1	B	371	THR	2.2
1	A	101	GLU	2.2
1	B	162	PHE	2.2
1	B	367	ASP	2.1

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
2	EPE	D	3004	15/15	0.96	0.24	10.38	25,38,44,48	0
2	EPE	B	3002	15/15	0.90	0.35	4.88	43,57,65,67	0
2	EPE	F	3006	15/15	0.93	0.27	4.78	29,39,48,52	0
2	EPE	E	3005	15/15	0.97	0.27	4.31	32,42,44,47	0
2	EPE	A	3001	15/15	0.92	0.23	2.10	40,42,49,51	0
2	EPE	C	3003	15/15	0.96	0.23	0.60	32,40,48,51	0

6.5 Other polymers (i)

There are no such residues in this entry.