Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:41 AM GMT

PDB ID	:	3BRY
Title	:	Crystal structure of the Ralstonia pickettii toluene transporter TbuX
Authors	:	Hearn, E.M.; Patel, D.R.; van den Berg, B.
Deposited on	:	2007-12-21
Resolution	:	3.20 Å(reported)

The following versions of software and data (see references (i)) 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
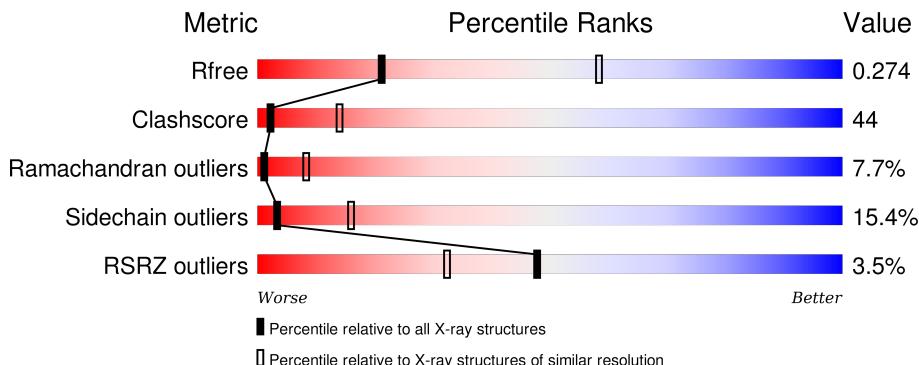
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
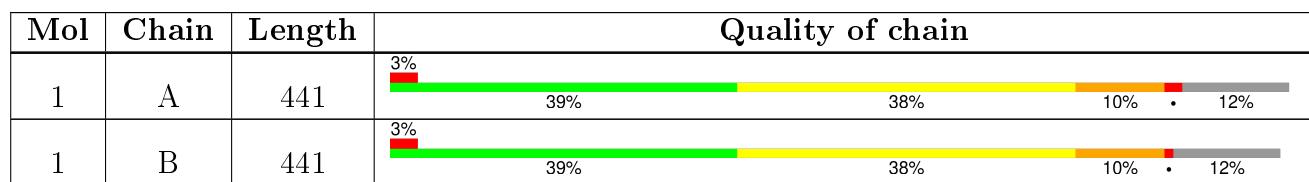
The reported resolution of this entry is 3.20 Å.

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	Percentile Ranks	Value
Rfree		0.274
Clashscore		44
Ramachandran outliers		7.7%
Sidechain outliers		15.4%
RSRZ outliers		3.5%

Worse .... *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	441	3% 39% 38% 10% • 12%
1	B	441	3% 39% 38% 10% • 12%

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	C8E	A	502	-	-	-	X
2	C8E	B	501	-	-	-	X

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5708 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 TbuX.
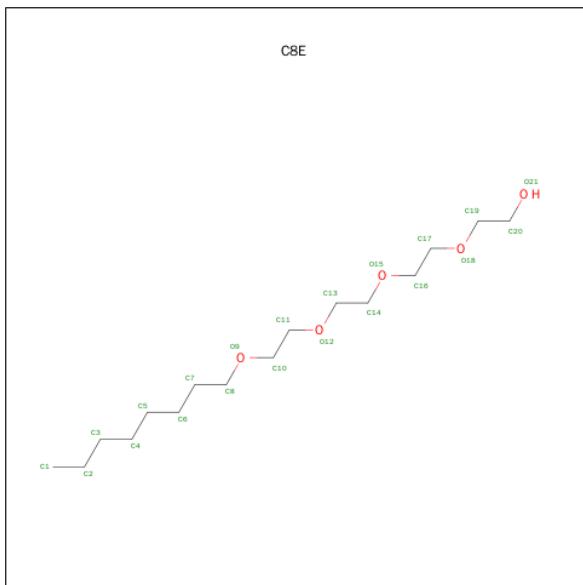
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total 2833	C 1779	N 501	O 546	S 7	0	0	0
1	B	389	Total 2833	C 1779	N 501	O 546	S 7	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	EXPRESSION TAG	UNP Q9RBW8
A	2	GLY	-	EXPRESSION TAG	UNP Q9RBW8
A	436	HIS	-	EXPRESSION TAG	UNP Q9RBW8
A	437	HIS	-	EXPRESSION TAG	UNP Q9RBW8
A	438	HIS	-	EXPRESSION TAG	UNP Q9RBW8
A	439	HIS	-	EXPRESSION TAG	UNP Q9RBW8
A	440	HIS	-	EXPRESSION TAG	UNP Q9RBW8
A	441	HIS	-	EXPRESSION TAG	UNP Q9RBW8
B	1	ALA	-	EXPRESSION TAG	UNP Q9RBW8
B	2	GLY	-	EXPRESSION TAG	UNP Q9RBW8
B	436	HIS	-	EXPRESSION TAG	UNP Q9RBW8
B	437	HIS	-	EXPRESSION TAG	UNP Q9RBW8
B	438	HIS	-	EXPRESSION TAG	UNP Q9RBW8
B	439	HIS	-	EXPRESSION TAG	UNP Q9RBW8
B	440	HIS	-	EXPRESSION TAG	UNP Q9RBW8
B	441	HIS	-	EXPRESSION TAG	UNP Q9RBW8

- Molecule 2 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: $C_{16}H_{34}O_5$).

C8E
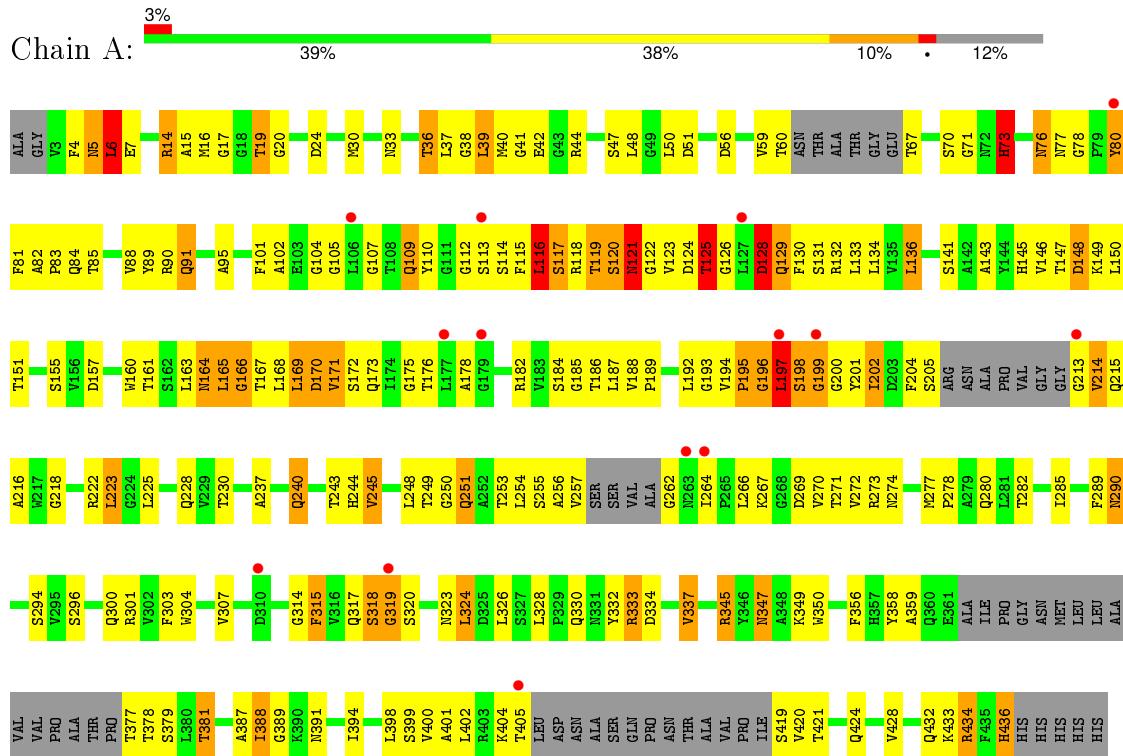
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			21	16	5		
2	A	1	Total	C	O	0	0
			21	16	5		
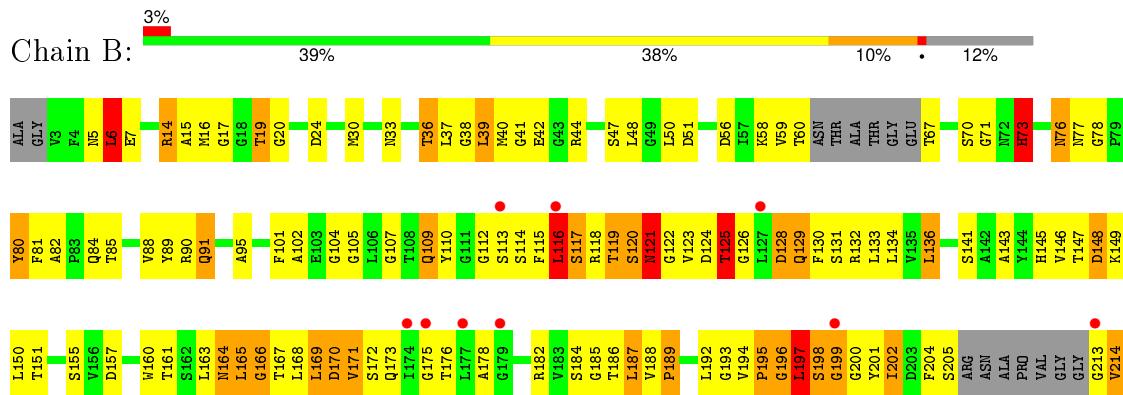
3 Residue-property plots ⓘ
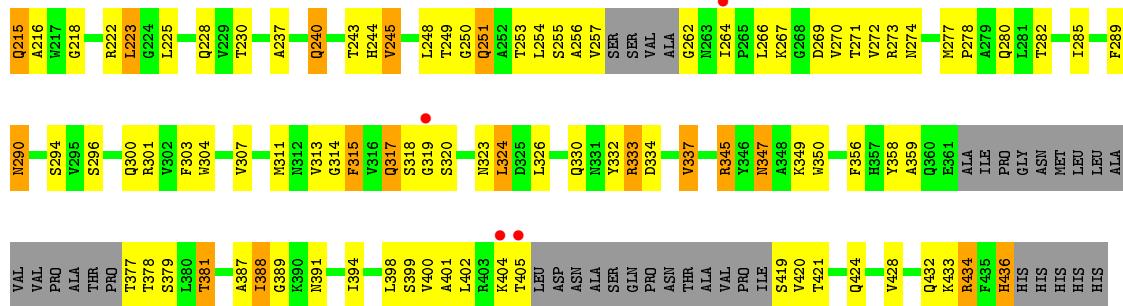
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: TbuX

- Molecule 1: TbuX

4 Data and refinement statistics (i)

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	125.29Å 125.24Å 269.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.20 31.92 – 2.74	Depositor EDS
% Data completeness (in resolution range)	98.4 (8.00-3.20) 98.2 (31.92-2.74)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.19 (at 2.76Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.268 , 0.280 0.258 , 0.274	Depositor DCC
R_{free} test set	1255 reflections (7.73%)	DCC
Wilson B-factor (Å^2)	56.9	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 32.4	EDS
Estimated twinning fraction	0.478 for -k,-h,-l	Xtriage
L-test for twinning[2]	$<\lvert L \rvert> = 0.50$, $<L^2> = 0.33$	Xtriage
Outliers	5 of 27405 reflections (0.018%)	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	5708	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $<\lvert L \rvert>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: C8E

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	0.35	0/2889	0.77	11/3903 (0.3%)
1	B	0.35	0/2889	0.80	11/3903 (0.3%)
All	All	0.35	0/5778	0.79	22/7806 (0.3%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	6	LEU	CA-CB-CG	-12.08	87.52	115.30
1	A	6	LEU	CA-CB-CG	-8.94	94.75	115.30
1	B	5	ASN	N-CA-C	-7.54	90.64	111.00
1	A	116	LEU	N-CA-C	-6.98	92.14	111.00
1	B	125	THR	N-CA-C	6.89	129.60	111.00
1	B	116	LEU	N-CA-C	-6.81	92.61	111.00
1	A	5	ASN	N-CA-C	-6.57	93.27	111.00
1	A	319	GLY	N-CA-C	-6.39	97.14	113.10
1	B	319	GLY	N-CA-C	-6.39	97.13	113.10
1	A	125	THR	N-CA-C	5.97	127.12	111.00
1	B	39	LEU	N-CA-C	-5.84	95.23	111.00
1	A	39	LEU	N-CA-C	-5.79	95.38	111.00
1	B	317	GLN	N-CA-C	5.62	126.17	111.00
1	A	317	GLN	N-CA-C	5.61	126.15	111.00
1	B	129	GLN	N-CA-C	5.36	125.47	111.00
1	A	129	GLN	N-CA-C	5.28	125.26	111.00
1	B	117	SER	N-CA-C	-5.23	96.88	111.00
1	A	117	SER	N-CA-C	-5.12	97.17	111.00
1	B	166	GLY	N-CA-C	-5.10	100.35	113.10
1	A	166	GLY	N-CA-C	-5.07	100.43	113.10
1	A	128	ASP	N-CA-C	5.04	124.59	111.00
1	B	5	ASN	CA-C-N	-5.00	106.20	117.20

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	2833	0	2677	248	0
1	B	2833	0	2677	245	0
2	A	21	0	34	5	0
2	B	21	0	34	5	0
All	All	5708	0	5422	493	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 44.

All (493) 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:6:LEU:HD11	1:B:300:GLN:HE22	1.04	1.15
1:B:114:SER:O	1:B:117:SER:HB2	1.53	1.09
1:A:114:SER:O	1:A:117:SER:HB2	1.54	1.08
1:A:6:LEU:HD11	1:A:300:GLN:HE22	1.12	1.06
1:B:141:SER:HB3	1:B:155:SER:HB3	1.38	1.05
1:B:6:LEU:CD1	1:B:300:GLN:HE22	1.71	1.04
1:B:112:GLY:HA2	1:B:128:ASP:OD2	1.58	1.03
1:A:112:GLY:HA2	1:A:128:ASP:OD2	1.57	1.03
1:A:141:SER:HB3	1:A:155:SER:HB3	1.38	1.01
1:A:6:LEU:HD11	1:A:300:GLN:NE2	1.75	1.00
1:A:80:TYR:HD2	1:A:81:PHE:N	1.60	0.99
1:B:77:ASN:HB3	1:B:109:GLN:HB3	1.44	0.96
1:B:80:TYR:HD2	1:B:81:PHE:N	1.61	0.96
1:A:77:ASN:HB3	1:A:109:GLN:HB3	1.45	0.94
1:B:6:LEU:CD1	1:B:300:GLN:NE2	2.33	0.90
1:B:141:SER:HB3	1:B:155:SER:CB	2.03	0.89
1:B:6:LEU:HD11	1:B:300:GLN:NE2	1.86	0.89
1:A:141:SER:HB3	1:A:155:SER:CB	2.03	0.88
1:A:77:ASN:HB3	1:A:109:GLN:CB	2.03	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:ASN:HB3	1:B:109:GLN:CB	2.03	0.88
1:B:222:ARG:HE	1:B:240:GLN:NE2	1.73	0.86
1:A:48:LEU:HD12	1:A:85:THR:HG22	1.58	0.86
1:A:14:ARG:HH11	1:A:14:ARG:HG3	1.40	0.86
1:A:222:ARG:HE	1:A:240:GLN:NE2	1.73	0.84
1:A:123:VAL:HG11	1:A:257:VAL:HG11	1.59	0.84
1:B:48:LEU:HD12	1:B:85:THR:HG22	1.58	0.84
1:B:14:ARG:HH11	1:B:14:ARG:HG3	1.40	0.83
1:A:38:GLY:HA2	1:A:90:ARG:NE	1.93	0.83
1:B:123:VAL:HG11	1:B:257:VAL:HG11	1.59	0.83
1:B:38:GLY:HA2	1:B:90:ARG:NE	1.93	0.83
1:A:169:LEU:HD22	1:A:202:ILE:HD11	1.61	0.82
1:A:121:ASN:ND2	1:A:122:GLY:H	1.78	0.81
1:B:257:VAL:HG13	1:B:262:GLY:O	1.80	0.81
1:A:73:HIS:H	1:A:77:ASN:HD21	1.29	0.81
1:A:300:GLN:HB3	1:A:337:VAL:HG13	1.62	0.81
1:A:257:VAL:HG13	1:A:262:GLY:O	1.80	0.81
1:B:300:GLN:HB3	1:B:337:VAL:HG13	1.62	0.80
1:B:121:ASN:ND2	1:B:122:GLY:H	1.78	0.80
1:B:294:SER:CB	1:B:345:ARG:HH22	1.94	0.80
1:A:294:SER:CB	1:A:345:ARG:HH22	1.94	0.80
1:B:294:SER:HB2	1:B:345:ARG:HH22	1.47	0.80
1:B:169:LEU:HD22	1:B:202:ILE:HD11	1.61	0.80
1:A:294:SER:HB2	1:A:345:ARG:HH22	1.47	0.78
1:A:6:LEU:CD1	1:A:300:GLN:HE22	1.96	0.78
1:B:73:HIS:H	1:B:77:ASN:HD21	1.29	0.78
1:A:115:PHE:C	1:A:117:SER:H	1.86	0.77
1:A:6:LEU:CD1	1:A:300:GLN:NE2	2.47	0.77
1:B:14:ARG:HH11	1:B:14:ARG:CG	1.97	0.77
1:B:82:ALA:HB1	1:B:102:ALA:HB3	1.67	0.77
1:B:19:THR:HG21	1:B:296:SER:HB2	1.67	0.76
1:A:82:ALA:HB1	1:A:102:ALA:HB3	1.67	0.76
1:A:14:ARG:HH11	1:A:14:ARG:CG	1.97	0.76
1:B:6:LEU:HD23	1:B:6:LEU:C	2.06	0.76
1:B:17:GLY:H	1:B:381:THR:HG21	1.51	0.76
1:A:202:ILE:HG12	2:A:502:C8E:H202	1.68	0.75
1:A:80:TYR:CD2	1:A:81:PHE:N	2.52	0.75
1:B:347:ASN:HD22	1:B:347:ASN:C	1.90	0.75
1:B:80:TYR:CD2	1:B:81:PHE:N	2.53	0.75
1:A:19:THR:HG21	1:A:296:SER:HB2	1.67	0.75
1:A:121:ASN:HD22	1:A:122:GLY:H	1.33	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:GLY:H	1:A:381:THR:HG21	1.51	0.74
1:A:326:LEU:HD23	2:A:502:C8E:H191	1.70	0.74
1:B:147:THR:HG22	1:B:149:LYS:H	1.51	0.74
1:B:123:VAL:HG22	1:B:124:ASP:H	1.51	0.74
1:B:378:THR:HG22	1:B:402:LEU:HD23	1.70	0.74
1:B:115:PHE:C	1:B:117:SER:H	1.85	0.73
1:A:119:THR:HG21	1:A:123:VAL:HG12	1.69	0.73
1:B:121:ASN:HD22	1:B:122:GLY:H	1.33	0.73
1:A:378:THR:HG22	1:A:402:LEU:HD23	1.70	0.73
1:B:196:GLY:O	1:B:197:LEU:HB2	1.88	0.73
1:A:199:GLY:O	1:A:256:ALA:HA	1.88	0.73
1:A:147:THR:HG22	1:A:149:LYS:H	1.51	0.73
1:B:199:GLY:O	1:B:256:ALA:HA	1.88	0.73
1:A:347:ASN:C	1:A:347:ASN:HD22	1.90	0.73
1:A:123:VAL:HG22	1:A:124:ASP:H	1.52	0.72
1:B:119:THR:HG21	1:B:123:VAL:HG12	1.70	0.72
1:B:50:LEU:O	1:B:50:LEU:HD12	1.90	0.72
1:A:50:LEU:O	1:A:50:LEU:HD12	1.90	0.71
1:A:196:GLY:O	1:A:197:LEU:HB2	1.88	0.71
1:B:136:LEU:HB2	1:B:160:TRP:HB3	1.73	0.71
1:A:136:LEU:HB2	1:A:160:TRP:HB3	1.73	0.70
1:A:119:THR:CG2	1:A:123:VAL:HG12	2.20	0.70
1:B:119:THR:CG2	1:B:123:VAL:HG12	2.21	0.70
1:A:80:TYR:CD1	1:A:134:LEU:HD22	2.27	0.70
1:A:116:LEU:O	1:A:168:LEU:HD23	1.92	0.70
1:B:80:TYR:CD1	1:B:134:LEU:HD22	2.27	0.69
1:B:169:LEU:HD23	1:B:200:GLY:O	1.93	0.69
1:A:129:GLN:NE2	1:A:168:LEU:HD22	2.09	0.68
1:A:16:MET:O	1:A:19:THR:HB	1.93	0.68
1:B:89:TYR:OH	1:B:91:GLN:HG3	1.92	0.68
1:B:129:GLN:NE2	1:B:168:LEU:HD22	2.08	0.68
1:A:254:LEU:HB3	1:A:315:PHE:HE2	1.58	0.68
1:A:89:TYR:OH	1:A:91:GLN:HG3	1.92	0.68
1:B:95:ALA:HB3	1:B:143:ALA:HB3	1.76	0.68
1:A:95:ALA:HB3	1:A:143:ALA:HB3	1.75	0.68
1:A:170:ASP:CG	1:A:171:VAL:N	2.47	0.68
1:B:170:ASP:CG	1:B:171:VAL:N	2.47	0.68
1:A:169:LEU:HD23	1:A:200:GLY:O	1.93	0.68
1:B:170:ASP:CG	1:B:171:VAL:H	1.96	0.67
1:A:170:ASP:CG	1:A:171:VAL:H	1.96	0.67
1:B:202:ILE:HG12	2:B:501:C8E:H201	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:LEU:HB3	1:B:315:PHE:HE2	1.58	0.67
1:B:116:LEU:O	1:B:168:LEU:HD23	1.93	0.67
1:B:254:LEU:HD23	1:B:255:SER:N	2.10	0.67
1:A:80:TYR:HD2	1:A:81:PHE:H	1.41	0.67
1:B:16:MET:O	1:B:19:THR:HB	1.94	0.66
1:A:147:THR:HG22	1:A:148:ASP:N	2.10	0.66
1:B:333:ARG:HB3	1:B:333:ARG:HH11	1.59	0.66
1:A:301:ARG:NH2	1:A:334:ASP:HB2	2.11	0.66
1:B:147:THR:HG22	1:B:148:ASP:N	2.11	0.65
1:A:333:ARG:HH11	1:A:333:ARG:HB3	1.59	0.65
1:B:255:SER:HB2	1:B:264:ILE:O	1.96	0.65
1:A:214:VAL:HG12	1:A:250:GLY:HA3	1.79	0.65
1:A:115:PHE:O	1:A:116:LEU:HB2	1.96	0.65
1:A:254:LEU:HD23	1:A:255:SER:N	2.10	0.65
1:A:255:SER:HB2	1:A:264:ILE:O	1.96	0.65
1:B:301:ARG:NH2	1:B:334:ASP:HB2	2.12	0.65
1:B:121:ASN:ND2	1:B:122:GLY:N	2.45	0.64
1:A:251:GLN:HA	1:A:269:ASP:HA	1.79	0.64
1:B:251:GLN:HA	1:B:269:ASP:HA	1.79	0.64
1:B:80:TYR:HD2	1:B:81:PHE:H	1.42	0.64
1:B:214:VAL:HG12	1:B:250:GLY:HA3	1.79	0.64
1:A:119:THR:HG21	1:A:123:VAL:CG1	2.28	0.64
1:A:243:THR:HB	1:A:277:MET:HB2	1.80	0.64
1:A:391:ASN:O	1:A:433:LYS:HA	1.98	0.63
1:B:119:THR:HG21	1:B:123:VAL:CG1	2.29	0.63
1:A:121:ASN:ND2	1:A:122:GLY:N	2.45	0.63
1:B:391:ASN:O	1:B:433:LYS:HA	1.98	0.63
1:A:4:PHE:HE1	1:A:277:MET:HG2	1.62	0.62
1:B:243:THR:HB	1:B:277:MET:HB2	1.81	0.62
1:B:115:PHE:O	1:B:116:LEU:HB2	1.99	0.62
1:B:6:LEU:HD13	1:B:300:GLN:NE2	2.15	0.62
1:B:15:ALA:HA	1:B:381:THR:HG23	1.82	0.62
1:B:121:ASN:N	1:B:121:ASN:HD22	1.99	0.61
1:B:168:LEU:HA	1:B:200:GLY:O	2.01	0.61
1:A:15:ALA:HA	1:A:381:THR:HG23	1.82	0.61
1:A:161:THR:HG21	1:A:245:VAL:CG1	2.30	0.61
1:B:117:SER:OG	1:B:128:ASP:OD2	2.19	0.61
1:A:202:ILE:HD13	2:A:502:C8E:H171	1.82	0.60
1:B:89:TYR:CE2	1:B:91:GLN:HB2	2.37	0.60
1:A:168:LEU:HA	1:A:200:GLY:O	2.01	0.60
1:B:77:ASN:CB	1:B:109:GLN:HB3	2.27	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:TYR:HD1	1:B:134:LEU:HD22	1.65	0.60
1:B:14:ARG:HE	1:B:428:VAL:CG2	2.14	0.60
1:B:161:THR:HG21	1:B:245:VAL:CG1	2.30	0.60
1:A:89:TYR:CE2	1:A:91:GLN:HB2	2.37	0.60
1:B:7:GLU:OE1	1:B:399:SER:OG	2.19	0.60
1:A:121:ASN:N	1:A:121:ASN:HD22	1.98	0.60
1:A:301:ARG:HG2	1:A:303:PHE:CE2	2.37	0.60
1:B:301:ARG:HG2	1:B:303:PHE:CE2	2.36	0.60
1:A:14:ARG:HE	1:A:428:VAL:CG2	2.14	0.60
1:A:202:ILE:HD12	1:A:202:ILE:H	1.67	0.59
1:A:254:LEU:HB3	1:A:315:PHE:CE2	2.37	0.59
1:A:80:TYR:HD1	1:A:134:LEU:HD22	1.65	0.59
1:A:161:THR:HG21	1:A:245:VAL:HG11	1.82	0.59
1:B:202:ILE:H	1:B:202:ILE:HD12	1.68	0.59
1:B:121:ASN:HD22	1:B:122:GLY:N	2.01	0.59
1:B:124:ASP:C	1:B:125:THR:HG23	2.23	0.59
1:B:70:SER:HB2	1:B:109:GLN:H	1.67	0.59
1:A:82:ALA:HB1	1:A:102:ALA:CB	2.33	0.59
1:A:150:LEU:HD23	1:A:151:THR:N	2.17	0.59
1:A:70:SER:HB2	1:A:109:GLN:H	1.67	0.59
1:B:109:GLN:HE21	1:B:130:PHE:HB3	1.68	0.59
1:B:161:THR:HG21	1:B:245:VAL:HG11	1.83	0.59
1:B:150:LEU:HD23	1:B:151:THR:N	2.17	0.59
1:B:248:LEU:HB2	1:B:272:VAL:HB	1.84	0.58
1:A:77:ASN:CB	1:A:109:GLN:HB3	2.28	0.58
1:A:170:ASP:C	1:A:172:SER:N	2.56	0.58
1:A:248:LEU:HB2	1:A:272:VAL:HB	1.84	0.58
1:B:254:LEU:HB3	1:B:315:PHE:CE2	2.37	0.58
1:A:294:SER:HB2	1:A:345:ARG:NH2	2.18	0.57
1:A:117:SER:OG	1:A:128:ASP:OD2	2.21	0.57
1:A:124:ASP:C	1:A:125:THR:HG23	2.24	0.57
1:A:132:ARG:O	1:A:163:LEU:HA	2.04	0.57
1:A:109:GLN:HE21	1:A:130:PHE:HB3	1.68	0.57
1:B:37:LEU:HD23	1:B:40:MET:HE2	1.86	0.57
1:A:333:ARG:HH11	1:A:333:ARG:CB	2.17	0.57
1:A:147:THR:CG2	1:A:148:ASP:N	2.68	0.57
1:B:170:ASP:C	1:B:172:SER:N	2.56	0.57
1:B:333:ARG:CB	1:B:333:ARG:HH11	2.17	0.57
1:A:387:ALA:C	1:A:389:GLY:H	2.09	0.57
1:A:398:LEU:HD21	1:A:400:VAL:HG22	1.87	0.56
1:B:147:THR:CG2	1:B:148:ASP:N	2.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:ALA:C	1:B:389:GLY:H	2.09	0.56
1:A:37:LEU:HD23	1:A:40:MET:HE2	1.86	0.56
1:B:313:VAL:HG11	2:B:501:C8E:H202	1.87	0.56
1:B:132:ARG:O	1:B:163:LEU:HA	2.04	0.56
1:B:82:ALA:HB1	1:B:102:ALA:CB	2.34	0.56
1:B:164:ASN:HB2	1:B:204:PHE:O	2.06	0.56
1:A:7:GLU:OE1	1:A:399:SER:OG	2.15	0.56
1:A:59:VAL:HA	1:A:419:SER:O	2.06	0.56
1:A:257:VAL:HG12	1:A:257:VAL:O	2.06	0.56
1:A:129:GLN:HA	1:A:166:GLY:O	2.07	0.55
1:B:132:ARG:HD3	1:B:134:LEU:HD11	1.87	0.55
1:A:119:THR:OG1	1:A:121:ASN:ND2	2.39	0.55
1:A:125:THR:OG1	1:A:126:GLY:N	2.39	0.55
1:B:294:SER:HB2	1:B:345:ARG:NH2	2.18	0.55
1:A:132:ARG:HD3	1:A:134:LEU:HD11	1.87	0.55
1:A:121:ASN:HD22	1:A:122:GLY:N	2.01	0.55
1:B:59:VAL:HA	1:B:419:SER:O	2.06	0.55
1:B:19:THR:HG21	1:B:296:SER:CB	2.37	0.55
1:B:398:LEU:HD21	1:B:400:VAL:HG22	1.87	0.55
1:B:129:GLN:HA	1:B:166:GLY:O	2.07	0.55
1:B:119:THR:OG1	1:B:121:ASN:ND2	2.39	0.55
1:A:164:ASN:HB2	1:A:204:PHE:O	2.06	0.55
1:A:214:VAL:HG12	1:A:250:GLY:CA	2.37	0.55
1:B:84:GLN:HG2	1:B:101:PHE:HA	1.88	0.55
1:B:169:LEU:O	1:B:169:LEU:HG	2.07	0.55
1:A:169:LEU:O	1:A:169:LEU:HG	2.07	0.55
1:A:223:LEU:O	1:A:223:LEU:HD22	2.06	0.54
1:A:5:ASN:O	1:A:6:LEU:HB2	2.07	0.54
1:B:59:VAL:HG13	1:B:420:VAL:HG22	1.90	0.54
1:B:214:VAL:HG12	1:B:250:GLY:CA	2.37	0.54
1:A:14:ARG:CG	1:A:14:ARG:NH1	2.65	0.54
1:B:36:THR:O	1:B:39:LEU:HB2	2.08	0.54
1:A:41:GLY:HA3	1:A:434:ARG:NH2	2.22	0.54
1:A:59:VAL:HG13	1:A:420:VAL:HG22	1.90	0.54
1:B:125:THR:OG1	1:B:126:GLY:N	2.39	0.54
1:A:36:THR:O	1:A:39:LEU:HB2	2.07	0.54
1:B:270:VAL:HG23	1:B:314:GLY:O	2.08	0.54
1:B:257:VAL:O	1:B:257:VAL:HG12	2.06	0.54
1:B:223:LEU:O	1:B:223:LEU:HD22	2.07	0.54
1:A:115:PHE:HA	1:A:118:ARG:H	1.73	0.53
1:B:41:GLY:HA3	1:B:434:ARG:NH2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:GLN:HG2	1:A:101:PHE:HA	1.89	0.53
1:B:378:THR:HG22	1:B:402:LEU:CD2	2.38	0.53
1:B:15:ALA:C	1:B:381:THR:CG2	2.77	0.53
1:A:270:VAL:HG23	1:A:314:GLY:O	2.08	0.53
1:B:115:PHE:HA	1:B:118:ARG:H	1.73	0.53
1:A:240:GLN:HB3	1:A:280:GLN:HB3	1.90	0.53
1:A:15:ALA:C	1:A:381:THR:CG2	2.77	0.53
1:A:222:ARG:HE	1:A:240:GLN:HE21	1.55	0.53
1:B:388:ILE:O	1:B:388:ILE:HG22	2.08	0.53
1:A:6:LEU:O	1:A:6:LEU:HD23	2.08	0.53
1:B:240:GLN:HB3	1:B:280:GLN:HB3	1.90	0.52
1:B:170:ASP:OD1	1:B:171:VAL:N	2.42	0.52
1:A:255:SER:CB	1:A:264:ILE:O	2.57	0.52
1:A:347:ASN:C	1:A:347:ASN:ND2	2.62	0.52
1:B:168:LEU:HD13	1:B:201:TYR:HD1	1.75	0.52
1:B:213:GLY:O	1:B:214:VAL:HG13	2.10	0.52
1:A:388:ILE:O	1:A:388:ILE:HG22	2.08	0.52
1:B:56:ASP:HA	1:B:71:GLY:HA3	1.91	0.52
1:B:255:SER:CB	1:B:264:ILE:O	2.57	0.52
1:A:56:ASP:HA	1:A:71:GLY:CA	2.40	0.52
1:A:168:LEU:HD13	1:A:201:TYR:HD1	1.74	0.52
1:A:170:ASP:OD1	1:A:171:VAL:N	2.42	0.52
1:A:163:LEU:O	1:A:164:ASN:HB3	2.10	0.52
1:A:213:GLY:O	1:A:214:VAL:HG13	2.10	0.52
1:A:56:ASP:HA	1:A:71:GLY:HA3	1.92	0.52
1:B:163:LEU:O	1:B:164:ASN:HB3	2.10	0.52
1:B:15:ALA:O	1:B:381:THR:CG2	2.58	0.52
1:A:199:GLY:HA3	1:A:257:VAL:HB	1.92	0.51
1:B:56:ASP:HA	1:B:71:GLY:CA	2.40	0.51
1:B:199:GLY:HA3	1:B:257:VAL:HB	1.92	0.51
1:B:379:SER:HB3	1:B:401:ALA:HA	1.93	0.51
1:B:273:ARG:O	1:B:274:ASN:HB2	2.11	0.51
1:B:133:LEU:CD1	1:B:163:LEU:HB3	2.41	0.51
1:B:38:GLY:HA2	1:B:90:ARG:CD	2.40	0.51
1:A:19:THR:HG21	1:A:296:SER:CB	2.37	0.51
1:A:379:SER:HB3	1:A:401:ALA:HA	1.93	0.51
1:B:214:VAL:CG1	1:B:250:GLY:HA3	2.40	0.51
1:A:38:GLY:HA2	1:A:90:ARG:CD	2.40	0.51
1:A:119:THR:CG2	1:A:123:VAL:CG1	2.87	0.51
1:A:133:LEU:CD1	1:A:163:LEU:HB3	2.41	0.51
1:A:214:VAL:CG1	1:A:250:GLY:HA3	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ALA:O	1:A:381:THR:CG2	2.58	0.51
1:A:273:ARG:O	1:A:274:ASN:HB2	2.11	0.51
1:B:60:THR:HG22	1:B:67:THR:HA	1.91	0.51
1:B:225:LEU:C	1:B:225:LEU:HD12	2.31	0.51
1:A:225:LEU:C	1:A:225:LEU:HD12	2.31	0.50
1:A:60:THR:HG22	1:A:67:THR:HA	1.92	0.50
1:B:80:TYR:HD1	1:B:134:LEU:CD2	2.25	0.50
1:B:82:ALA:CB	1:B:102:ALA:HB3	2.40	0.50
1:B:359:ALA:O	1:B:377:THR:HB	2.11	0.50
1:B:131:SER:HA	1:B:165:LEU:HA	1.94	0.50
1:B:347:ASN:C	1:B:347:ASN:ND2	2.62	0.50
1:A:77:ASN:CB	1:A:109:GLN:CB	2.86	0.50
1:A:398:LEU:C	1:A:398:LEU:HD23	2.32	0.50
1:A:30:MET:HG2	1:A:141:SER:OG	2.12	0.50
1:B:133:LEU:HD13	1:B:163:LEU:HB3	1.94	0.50
1:B:38:GLY:O	1:B:145:HIS:HE1	1.95	0.50
1:B:398:LEU:C	1:B:398:LEU:HD23	2.32	0.50
1:A:133:LEU:HD13	1:A:163:LEU:HB3	1.94	0.49
1:A:80:TYR:HD1	1:A:134:LEU:CD2	2.24	0.49
1:A:131:SER:HA	1:A:165:LEU:HA	1.94	0.49
1:A:280:GLN:NE2	1:A:300:GLN:OE1	2.45	0.49
1:A:67:THR:HG23	1:A:67:THR:O	2.12	0.49
1:A:359:ALA:O	1:A:377:THR:HB	2.11	0.49
1:B:222:ARG:HE	1:B:240:GLN:HE21	1.55	0.49
1:A:204:PHE:O	1:A:205:SER:HB2	2.12	0.49
1:A:378:THR:HG22	1:A:402:LEU:CD2	2.38	0.49
1:B:254:LEU:O	1:B:266:LEU:HB2	2.12	0.49
1:A:254:LEU:O	1:A:266:LEU:HB2	2.12	0.49
1:A:186:THR:H	1:A:323:ASN:HB2	1.78	0.49
1:B:30:MET:HG2	1:B:141:SER:OG	2.12	0.49
1:B:204:PHE:O	1:B:205:SER:HB2	2.12	0.49
1:B:218:GLY:HA3	1:B:245:VAL:HA	1.95	0.49
1:A:14:ARG:NE	1:A:428:VAL:CG2	2.76	0.48
1:B:186:THR:H	1:B:323:ASN:HB2	1.78	0.48
1:B:280:GLN:NE2	1:B:300:GLN:OE1	2.47	0.48
1:B:163:LEU:CD2	1:B:248:LEU:HD13	2.43	0.48
1:A:164:ASN:HB3	1:A:213:GLY:N	2.28	0.48
1:B:67:THR:O	1:B:67:THR:HG23	2.12	0.48
1:A:289:PHE:O	1:A:290:ASN:HB3	2.14	0.48
1:B:129:GLN:HE22	1:B:168:LEU:HD22	1.79	0.48
1:A:38:GLY:O	1:A:145:HIS:HE1	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:PHE:O	1:B:290:ASN:HB3	2.14	0.48
1:B:278:PRO:HD3	1:B:304:TRP:CZ3	2.49	0.48
1:B:347:ASN:ND2	1:B:349:LYS:H	2.12	0.48
1:A:163:LEU:CD2	1:A:248:LEU:HD13	2.43	0.48
1:A:80:TYR:C	1:A:80:TYR:CD2	2.86	0.48
1:B:14:ARG:NE	1:B:428:VAL:CG2	2.76	0.48
1:B:14:ARG:CG	1:B:14:ARG:NH1	2.65	0.48
1:A:347:ASN:ND2	1:A:349:LYS:H	2.12	0.48
1:B:237:ALA:HA	1:B:282:THR:O	2.14	0.48
1:A:169:LEU:CD2	1:A:202:ILE:HD11	2.38	0.47
1:B:164:ASN:HB3	1:B:213:GLY:N	2.28	0.47
1:A:301:ARG:HH21	1:A:334:ASP:HB2	1.78	0.47
1:A:237:ALA:HA	1:A:282:THR:O	2.14	0.47
1:A:218:GLY:HA3	1:A:245:VAL:HA	1.95	0.47
1:A:278:PRO:HD3	1:A:304:TRP:CZ3	2.49	0.47
1:B:330:GLN:HG2	1:B:332:TYR:OH	2.14	0.47
1:B:301:ARG:HH21	1:B:334:ASP:HB2	1.79	0.47
1:B:169:LEU:CD2	1:B:202:ILE:HD11	2.39	0.47
1:A:80:TYR:C	1:A:80:TYR:HD2	2.17	0.47
1:A:77:ASN:HB3	1:A:109:GLN:HB2	1.91	0.47
1:A:119:THR:HG23	1:A:123:VAL:HG12	1.96	0.47
1:A:347:ASN:ND2	1:A:350:TRP:H	2.12	0.47
1:B:165:LEU:HD23	1:B:167:THR:HG22	1.97	0.47
1:B:196:GLY:O	1:B:197:LEU:CB	2.61	0.47
1:A:214:VAL:HG12	1:A:250:GLY:N	2.30	0.47
1:A:82:ALA:CB	1:A:102:ALA:HB3	2.40	0.47
1:A:89:TYR:CZ	1:A:91:GLN:HG3	2.49	0.47
1:A:129:GLN:HE22	1:A:168:LEU:HD22	1.79	0.47
1:B:347:ASN:ND2	1:B:350:TRP:H	2.12	0.47
1:B:89:TYR:CZ	1:B:91:GLN:HG3	2.49	0.47
1:B:24:ASP:HA	1:B:36:THR:HG23	1.97	0.47
1:A:330:GLN:HG2	1:A:332:TYR:OH	2.15	0.47
1:B:119:THR:CG2	1:B:123:VAL:CG1	2.88	0.46
1:B:70:SER:HB3	1:B:110:TYR:CD1	2.50	0.46
1:A:42:GLU:HA	1:A:90:ARG:HB3	1.98	0.46
1:A:163:LEU:HD23	1:A:214:VAL:HG23	1.97	0.46
1:B:80:TYR:CE1	1:B:134:LEU:HD22	2.50	0.46
1:B:42:GLU:HA	1:B:90:ARG:HB3	1.98	0.46
1:B:214:VAL:HG12	1:B:250:GLY:N	2.30	0.46
1:A:14:ARG:NH1	1:A:14:ARG:HB2	2.31	0.46
1:A:147:THR:CG2	1:A:148:ASP:H	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:TYR:CE1	1:A:134:LEU:HD22	2.50	0.46
1:A:146:VAL:CG2	1:A:150:LEU:HD22	2.46	0.46
1:A:4:PHE:CE1	1:A:277:MET:HG2	2.49	0.46
1:B:398:LEU:HD23	1:B:399:SER:N	2.31	0.46
1:A:216:ALA:CB	1:A:248:LEU:HD23	2.46	0.46
1:B:77:ASN:HB3	1:B:109:GLN:HB2	1.91	0.45
1:B:163:LEU:HD23	1:B:214:VAL:HG23	1.97	0.45
1:B:119:THR:HG23	1:B:123:VAL:HG12	1.97	0.45
1:B:77:ASN:CB	1:B:109:GLN:CB	2.85	0.45
1:B:120:SER:O	1:B:121:ASN:HB3	2.17	0.45
1:B:146:VAL:CG2	1:B:150:LEU:HD22	2.46	0.45
1:A:115:PHE:CD1	1:A:115:PHE:C	2.90	0.45
1:A:405:THR:CB	1:A:421:THR:HG22	2.46	0.45
1:A:70:SER:HB3	1:A:110:TYR:CD1	2.50	0.45
1:A:196:GLY:HA3	1:A:257:VAL:C	2.37	0.45
1:A:398:LEU:HD23	1:A:399:SER:N	2.31	0.45
1:A:24:ASP:HA	1:A:36:THR:HG23	1.97	0.45
1:A:165:LEU:HD23	1:A:167:THR:HG22	1.97	0.45
1:B:307:VAL:O	1:B:307:VAL:HG12	2.16	0.45
1:A:196:GLY:O	1:A:197:LEU:CB	2.61	0.45
1:B:147:THR:CG2	1:B:148:ASP:H	2.29	0.45
1:B:434:ARG:NH1	1:B:436:HIS:CE1	2.85	0.45
1:B:216:ALA:CB	1:B:248:LEU:HD23	2.46	0.45
1:A:434:ARG:NH1	1:A:436:HIS:CE1	2.85	0.45
1:B:405:THR:CB	1:B:421:THR:HG22	2.46	0.45
1:B:121:ASN:N	1:B:121:ASN:ND2	2.65	0.45
1:A:270:VAL:CG2	1:A:271:THR:N	2.79	0.45
1:B:196:GLY:HA3	1:B:257:VAL:C	2.37	0.44
1:A:256:ALA:O	1:A:264:ILE:N	2.49	0.44
1:B:14:ARG:NE	1:B:428:VAL:HG21	2.32	0.44
1:B:270:VAL:CG2	1:B:271:THR:N	2.79	0.44
1:A:40:MET:HE1	1:A:88:VAL:HG21	1.99	0.44
1:A:115:PHE:C	1:A:117:SER:N	2.56	0.44
1:A:254:LEU:HD23	1:A:254:LEU:C	2.37	0.44
1:B:14:ARG:NH1	1:B:14:ARG:HB2	2.32	0.44
1:B:40:MET:HE1	1:B:88:VAL:HG21	1.99	0.44
1:B:215:GLN:HE21	1:B:215:GLN:HB3	1.54	0.44
1:A:202:ILE:HG12	2:A:502:C8E:C20	2.42	0.44
1:B:89:TYR:HE2	1:B:91:GLN:HB2	1.80	0.44
1:B:278:PRO:HG3	1:B:304:TRP:CE2	2.53	0.44
1:B:124:ASP:HB3	1:B:125:THR:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:ARG:NE	1:A:428:VAL:HG21	2.32	0.44
1:A:121:ASN:N	1:A:121:ASN:ND2	2.65	0.44
1:A:356:PHE:CE2	1:A:358:TYR:HB2	2.53	0.44
1:A:307:VAL:HG12	1:A:307:VAL:O	2.16	0.44
1:B:243:THR:HG22	1:B:244:HIS:N	2.33	0.43
1:B:115:PHE:CD1	1:B:115:PHE:C	2.91	0.43
1:B:255:SER:CA	1:B:264:ILE:O	2.67	0.43
1:A:278:PRO:HG3	1:A:304:TRP:CE2	2.53	0.43
1:B:185:GLY:HA3	1:B:324:LEU:HA	2.01	0.43
1:B:193:GLY:O	1:B:195:PRO:N	2.51	0.43
1:B:254:LEU:C	1:B:254:LEU:HD23	2.38	0.43
1:A:170:ASP:C	1:A:172:SER:H	2.22	0.43
1:A:214:VAL:HA	1:A:249:THR:O	2.19	0.43
1:A:120:SER:O	1:A:121:ASN:HB3	2.17	0.43
1:A:89:TYR:HE2	1:A:91:GLN:HB2	1.80	0.43
1:B:253:THR:HG22	1:B:267:LYS:HG3	2.00	0.43
1:A:328:LEU:HD11	2:A:502:C8E:H142	2.01	0.43
1:A:123:VAL:HG22	1:A:124:ASP:N	2.26	0.43
1:A:123:VAL:C	1:A:124:ASP:OD2	2.57	0.43
1:B:47:SER:O	1:B:85:THR:HA	2.18	0.43
1:A:173:GLN:O	1:A:175:GLY:N	2.46	0.43
1:B:356:PHE:CE2	1:B:358:TYR:HB2	2.53	0.43
1:A:197:LEU:O	1:A:198:SER:HB2	2.19	0.43
1:A:253:THR:HG22	1:A:267:LYS:HG3	2.00	0.43
1:B:173:GLN:O	1:B:175:GLY:N	2.46	0.43
1:B:123:VAL:HG22	1:B:124:ASP:N	2.25	0.43
1:B:256:ALA:O	1:B:264:ILE:N	2.49	0.43
1:B:123:VAL:C	1:B:124:ASP:OD2	2.57	0.43
1:A:280:GLN:NE2	1:A:300:GLN:CD	2.73	0.43
1:A:255:SER:CA	1:A:264:ILE:O	2.67	0.43
1:A:303:PHE:HA	1:A:334:ASP:OD1	2.19	0.43
1:A:193:GLY:O	1:A:195:PRO:N	2.51	0.43
1:A:15:ALA:O	1:A:381:THR:HG22	2.19	0.42
1:B:197:LEU:O	1:B:198:SER:HB2	2.18	0.42
1:A:6:LEU:HD23	1:A:6:LEU:C	2.39	0.42
1:B:223:LEU:C	1:B:223:LEU:HD22	2.39	0.42
1:B:254:LEU:CB	1:B:315:PHE:HE2	2.30	0.42
1:B:303:PHE:HA	1:B:334:ASP:OD1	2.19	0.42
1:B:387:ALA:C	1:B:389:GLY:N	2.72	0.42
1:A:47:SER:O	1:A:85:THR:HA	2.18	0.42
1:A:161:THR:HG21	1:A:245:VAL:HG12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:MET:CE	2:B:501:C8E:H131	2.49	0.42
1:B:214:VAL:HA	1:B:249:THR:O	2.19	0.42
1:B:274:ASN:N	1:B:274:ASN:HD22	2.16	0.42
1:A:274:ASN:HD22	1:A:274:ASN:N	2.16	0.42
1:A:243:THR:HG22	1:A:244:HIS:N	2.33	0.42
1:B:280:GLN:NE2	1:B:300:GLN:CD	2.73	0.42
1:A:124:ASP:HB3	1:A:125:THR:HG22	2.01	0.42
1:A:254:LEU:CB	1:A:315:PHE:HE2	2.30	0.42
1:A:185:GLY:HA3	1:A:324:LEU:HA	2.01	0.42
1:A:186:THR:N	1:A:323:ASN:HB2	2.35	0.42
1:B:15:ALA:O	1:B:381:THR:HG22	2.20	0.42
1:A:141:SER:CB	1:A:155:SER:HB3	2.28	0.42
1:B:161:THR:HG21	1:B:245:VAL:HG12	2.00	0.42
1:B:14:ARG:CB	1:B:14:ARG:NH1	2.83	0.41
1:B:150:LEU:C	1:B:150:LEU:HD23	2.40	0.41
1:A:387:ALA:C	1:A:389:GLY:N	2.72	0.41
1:A:223:LEU:C	1:A:223:LEU:HD22	2.39	0.41
1:A:404:LYS:O	1:A:421:THR:HA	2.20	0.41
1:B:311:MET:HE3	2:B:501:C8E:O12	2.20	0.41
1:A:82:ALA:HA	1:A:83:PRO:HD3	1.92	0.41
1:A:14:ARG:NH1	1:A:14:ARG:CB	2.83	0.41
1:A:150:LEU:HD23	1:A:150:LEU:C	2.40	0.41
1:B:125:THR:O	1:B:128:ASP:OD1	2.38	0.41
1:A:129:GLN:OE1	1:A:167:THR:HA	2.21	0.41
1:B:161:THR:CG2	1:B:245:VAL:CG1	2.96	0.41
1:B:404:LYS:O	1:B:421:THR:HA	2.20	0.41
1:B:161:THR:HG23	1:B:161:THR:O	2.21	0.41
1:A:70:SER:HB3	1:A:110:TYR:CG	2.56	0.41
1:A:119:THR:O	1:A:121:ASN:N	2.52	0.41
1:B:37:LEU:CD2	1:B:40:MET:CE	2.99	0.41
1:A:37:LEU:CD2	1:A:40:MET:CE	2.99	0.41
1:A:228:GLN:NE2	1:A:230:THR:O	2.53	0.41
1:B:228:GLN:NE2	1:B:230:THR:O	2.54	0.41
1:A:161:THR:CG2	1:A:245:VAL:CG1	2.96	0.41
1:B:37:LEU:HD23	1:B:40:MET:CE	2.51	0.41
1:B:186:THR:N	1:B:323:ASN:HB2	2.35	0.41
1:B:129:GLN:OE1	1:B:167:THR:HA	2.21	0.41
1:A:44:ARG:O	1:A:434:ARG:HA	2.21	0.41
1:B:240:GLN:HE21	1:B:240:GLN:HB2	1.62	0.41
1:B:107:GLY:HA2	1:B:131:SER:O	2.20	0.41
1:A:107:GLY:HA2	1:A:131:SER:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ARG:NE	1:A:240:GLN:NE2	2.56	0.41
1:A:5:ASN:HB3	1:A:6:LEU:H	1.52	0.41
1:B:141:SER:CB	1:B:155:SER:HB3	2.28	0.41
1:B:70:SER:HB3	1:B:110:TYR:CG	2.56	0.41
1:B:14:ARG:HE	1:B:428:VAL:HG23	1.85	0.41
1:B:398:LEU:HD21	1:B:400:VAL:CG2	2.51	0.41
1:B:44:ARG:O	1:B:434:ARG:HA	2.21	0.41
1:B:58:LYS:HB2	1:B:58:LYS:HE3	1.87	0.41
1:B:161:THR:HG23	1:B:248:LEU:HD21	2.03	0.41
1:A:318:SER:HB3	1:A:319:GLY:H	1.65	0.41
1:A:146:VAL:HG22	1:A:150:LEU:HB3	2.03	0.40
1:B:315:PHE:CE1	1:B:317:GLN:HG2	2.57	0.40
1:A:165:LEU:HD13	1:A:165:LEU:H	1.87	0.40
1:A:161:THR:HG23	1:A:161:THR:O	2.21	0.40
1:B:326:LEU:HD23	2:B:501:C8E:H191	2.03	0.40
1:B:80:TYR:CD2	1:B:80:TYR:C	2.87	0.40
1:B:165:LEU:H	1:B:165:LEU:HD13	1.87	0.40
1:B:187:LEU:C	1:B:189:PRO:N	2.75	0.40
1:B:115:PHE:C	1:B:117:SER:N	2.55	0.40
1:B:119:THR:O	1:B:121:ASN:N	2.53	0.40
1:A:164:ASN:CB	1:A:213:GLY:N	2.84	0.40
1:A:14:ARG:HH11	1:A:14:ARG:CB	2.33	0.40
1:A:398:LEU:HD21	1:A:400:VAL:CG2	2.51	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	377/441 (86%)	296 (78%)	52 (14%)	29 (8%)	1	8
1	B	377/441 (86%)	295 (78%)	53 (14%)	29 (8%)	1	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	754/882 (86%)	591 (78%)	105 (14%)	58 (8%)	1 8

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	76	ASN
1	A	121	ASN
1	A	176	THR
1	A	178	ALA
1	A	184	SER
1	A	188	VAL
1	A	194	VAL
1	A	195	PRO
1	B	6	LEU
1	B	76	ASN
1	B	121	ASN
1	B	176	THR
1	B	178	ALA
1	B	184	SER
1	B	188	VAL
1	B	194	VAL
1	B	195	PRO
1	A	104	GLY
1	A	164	ASN
1	A	199	GLY
1	A	214	VAL
1	A	290	ASN
1	A	324	LEU
1	A	388	ILE
1	B	104	GLY
1	B	164	ASN
1	B	199	GLY
1	B	214	VAL
1	B	290	ASN
1	B	324	LEU
1	B	388	ILE
1	A	73	HIS
1	A	197	LEU
1	B	73	HIS
1	B	120	SER
1	B	197	LEU

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Mol	Chain	Res	Type
1	A	20	GLY
1	A	78	GLY
1	A	120	SER
1	A	182	ARG
1	B	20	GLY
1	B	182	ARG
1	A	187	LEU
1	A	192	LEU
1	B	187	LEU
1	B	192	LEU
1	A	198	SER
1	B	198	SER
1	B	78	GLY
1	A	105	GLY
1	B	105	GLY
1	B	189	PRO
1	A	189	PRO
1	A	171	VAL
1	B	171	VAL
1	B	196	GLY
1	A	196	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	A	282/339 (83%)	238 (84%)	44 (16%)	3	15
1	B	282/339 (83%)	239 (85%)	43 (15%)	3	17
All	All	564/678 (83%)	477 (85%)	87 (15%)	3	16

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	14	ARG

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Mol	Chain	Res	Type
1	A	19	THR
1	A	33	ASN
1	A	36	THR
1	A	51	ASP
1	A	73	HIS
1	A	76	ASN
1	A	80	TYR
1	A	91	GLN
1	A	109	GLN
1	A	113	SER
1	A	116	LEU
1	A	119	THR
1	A	121	ASN
1	A	125	THR
1	A	128	ASP
1	A	136	LEU
1	A	148	ASP
1	A	157	ASP
1	A	165	LEU
1	A	169	LEU
1	A	170	ASP
1	A	197	LEU
1	A	202	ILE
1	A	215	GLN
1	A	223	LEU
1	A	240	GLN
1	A	245	VAL
1	A	251	GLN
1	A	285	ILE
1	A	315	PHE
1	A	318	SER
1	A	320	SER
1	A	333	ARG
1	A	337	VAL
1	A	345	ARG
1	A	347	ASN
1	A	381	THR
1	A	394	ILE
1	A	424	GLN
1	A	432	GLN
1	A	434	ARG
1	A	436	HIS

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Mol	Chain	Res	Type
1	B	14	ARG
1	B	19	THR
1	B	33	ASN
1	B	36	THR
1	B	51	ASP
1	B	73	HIS
1	B	76	ASN
1	B	80	TYR
1	B	91	GLN
1	B	109	GLN
1	B	113	SER
1	B	116	LEU
1	B	119	THR
1	B	121	ASN
1	B	125	THR
1	B	128	ASP
1	B	136	LEU
1	B	148	ASP
1	B	157	ASP
1	B	165	LEU
1	B	169	LEU
1	B	170	ASP
1	B	197	LEU
1	B	202	ILE
1	B	215	GLN
1	B	223	LEU
1	B	240	GLN
1	B	245	VAL
1	B	251	GLN
1	B	285	ILE
1	B	315	PHE
1	B	318	SER
1	B	320	SER
1	B	333	ARG
1	B	337	VAL
1	B	345	ARG
1	B	347	ASN
1	B	381	THR
1	B	394	ILE
1	B	424	GLN
1	B	432	GLN
1	B	434	ARG

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Mol	Chain	Res	Type
1	B	436	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	75	ASN
1	A	76	ASN
1	A	77	ASN
1	A	84	GLN
1	A	91	GLN
1	A	109	GLN
1	A	121	ASN
1	A	145	HIS
1	A	215	GLN
1	A	228	GLN
1	A	240	GLN
1	A	274	ASN
1	A	276	GLN
1	A	280	GLN
1	A	300	GLN
1	A	347	ASN
1	A	391	ASN
1	A	424	GLN
1	A	426	ASN
1	A	432	GLN
1	A	436	HIS
1	B	5	ASN
1	B	33	ASN
1	B	75	ASN
1	B	76	ASN
1	B	77	ASN
1	B	84	GLN
1	B	91	GLN
1	B	109	GLN
1	B	121	ASN
1	B	145	HIS
1	B	215	GLN
1	B	228	GLN
1	B	240	GLN
1	B	274	ASN
1	B	276	GLN

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Mol	Chain	Res	Type
1	B	280	GLN
1	B	300	GLN
1	B	347	ASN
1	B	391	ASN
1	B	424	GLN
1	B	426	ASN
1	B	432	GLN

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)

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	$\#|Z| > 2$
2	C8E	A	502	-	20,20,20	0.88	1 (5%)	19,19,19	2.11	6 (31%)
2	C8E	B	501	-	20,20,20	0.88	1 (5%)	19,19,19	2.02	7 (36%)

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	C8E	A	502	-	-	0/18/18/18	0/0/0/0
2	C8E	B	501	-	-	0/18/18/18	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	C8E	C19-C20	2.04	1.60	1.49
2	A	502	C8E	O12-C13	2.24	1.51	1.42

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	502	C8E	C7-C6-C5	-2.74	100.36	114.53
2	B	501	C8E	C7-C6-C5	-2.71	100.54	114.53
2	B	501	C8E	O9-C10-C11	-2.35	99.92	110.36
2	B	501	C8E	O18-C19-C20	2.10	120.12	110.43
2	A	502	C8E	O12-C13-C14	2.13	119.84	110.36
2	B	501	C8E	O15-C14-C13	2.16	119.96	110.36
2	B	501	C8E	C10-O9-C8	2.65	124.71	113.31
2	A	502	C8E	O18-C17-C16	2.86	123.07	110.36
2	A	502	C8E	O18-C19-C20	2.95	124.04	110.43
2	B	501	C8E	O12-C13-C14	3.91	127.76	110.36
2	A	502	C8E	O9-C8-C7	4.01	125.93	109.87
2	B	501	C8E	O9-C8-C7	4.63	128.40	109.87
2	A	502	C8E	O15-C14-C13	5.80	136.14	110.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	502	C8E	5	0
2	B	501	C8E	5	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	389/441 (88%)	-0.08	14 (3%)	46	31	18, 54, 119, 140	0
1	B	389/441 (88%)	-0.08	13 (3%)	50	35	19, 55, 119, 142	0
All	All	778/882 (88%)	-0.08	27 (3%)	48	32	18, 55, 119, 142	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	319	GLY	4.2
1	B	179	GLY	4.2
1	A	179	GLY	4.0
1	A	319	GLY	3.8
1	B	127	LEU	3.6
1	A	127	LEU	3.5
1	A	197	LEU	3.2
1	A	199	GLY	3.1
1	B	405	THR	3.0
1	A	310	ASP	2.9
1	B	174	ILE	2.8
1	B	404	LYS	2.8
1	A	264	ILE	2.8
1	B	213	GLY	2.7
1	A	213	GLY	2.6
1	A	113	SER	2.5
1	B	199	GLY	2.5
1	B	177	LEU	2.5
1	B	113	SER	2.4
1	B	175	GLY	2.3
1	A	80	TYR	2.3
1	B	264	ILE	2.2
1	A	177	LEU	2.2
1	A	405	THR	2.2

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Full wwPDB X-ray Structure Validation Report

Mol	Chain	Res	Type	RSRZ
1	A	106	LEU	2.0
1	A	263	ASN	2.0
1	B	116	LEU	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	C8E	B	501	21/21	0.40	1.03	13.02	86,98,102,102	0
2	C8E	A	502	21/21	0.43	0.84	9.57	88,96,97,97	0

6.5 Other polymers (i)

There are no such residues in this entry.