Full wwPDB X-ray Structure Validation Report (i)

Feb 28, 2014 – 01:40 PM GMT

PDB ID	:	2H21
Title	:	Structure of Rubisco LSMT bound to AdoMet
Authors	:	Couture, J.F.; Hauk, G.; Trievel, R.C.
Deposited on	:	2006-05-17
Resolution	:	2.45 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html

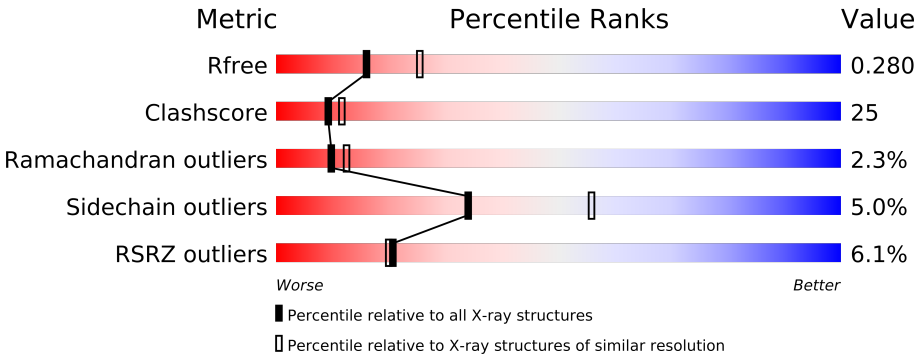
The following versions of software and data (see references) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.45 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}	66092	3566 (2.50-2.42)
Clashscore	79885	4471 (2.50-2.42)
Ramachandran outliers	78287	4383 (2.50-2.42)
Sidechain outliers	78261	4385 (2.50-2.42)
RSRZ outliers	66119	3568 (2.50-2.42)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	440	
1	B	440	
1	C	440	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11121 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

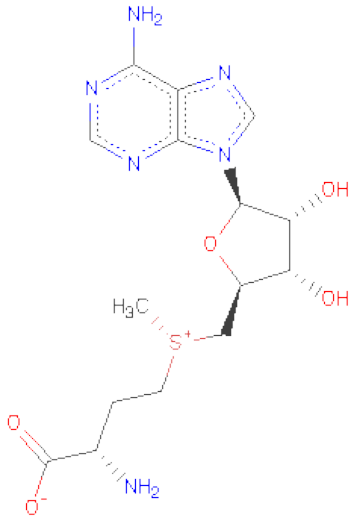
- Molecule 1 is a protein called Ribulose-1,5 bisphosphate carboxylase/oxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	0	0	0
			3413	2189	562	655	7			
1	B	440	Total	C	N	O	S	0	0	0
			3542	2270	585	680	7			
1	C	438	Total	C	N	O	S	0	0	0
			3526	2262	582	675	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	483	GLU	-	CLONING ARTIFACT	UNP Q43088
A	484	ASN	-	CLONING ARTIFACT	UNP Q43088
A	485	LEU	-	CLONING ARTIFACT	UNP Q43088
A	486	TYR	-	CLONING ARTIFACT	UNP Q43088
A	487	PHE	-	CLONING ARTIFACT	UNP Q43088
A	488	GLN	-	CLONING ARTIFACT	UNP Q43088
B	483	GLU	-	CLONING ARTIFACT	UNP Q43088
B	484	ASN	-	CLONING ARTIFACT	UNP Q43088
B	485	LEU	-	CLONING ARTIFACT	UNP Q43088
B	486	TYR	-	CLONING ARTIFACT	UNP Q43088
B	487	PHE	-	CLONING ARTIFACT	UNP Q43088
B	488	GLN	-	CLONING ARTIFACT	UNP Q43088
C	483	GLU	-	CLONING ARTIFACT	UNP Q43088
C	484	ASN	-	CLONING ARTIFACT	UNP Q43088
C	485	LEU	-	CLONING ARTIFACT	UNP Q43088
C	486	TYR	-	CLONING ARTIFACT	UNP Q43088
C	487	PHE	-	CLONING ARTIFACT	UNP Q43088
C	488	GLN	-	CLONING ARTIFACT	UNP Q43088

- Molecule 2 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
2	C	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

- Molecule 3 is water.

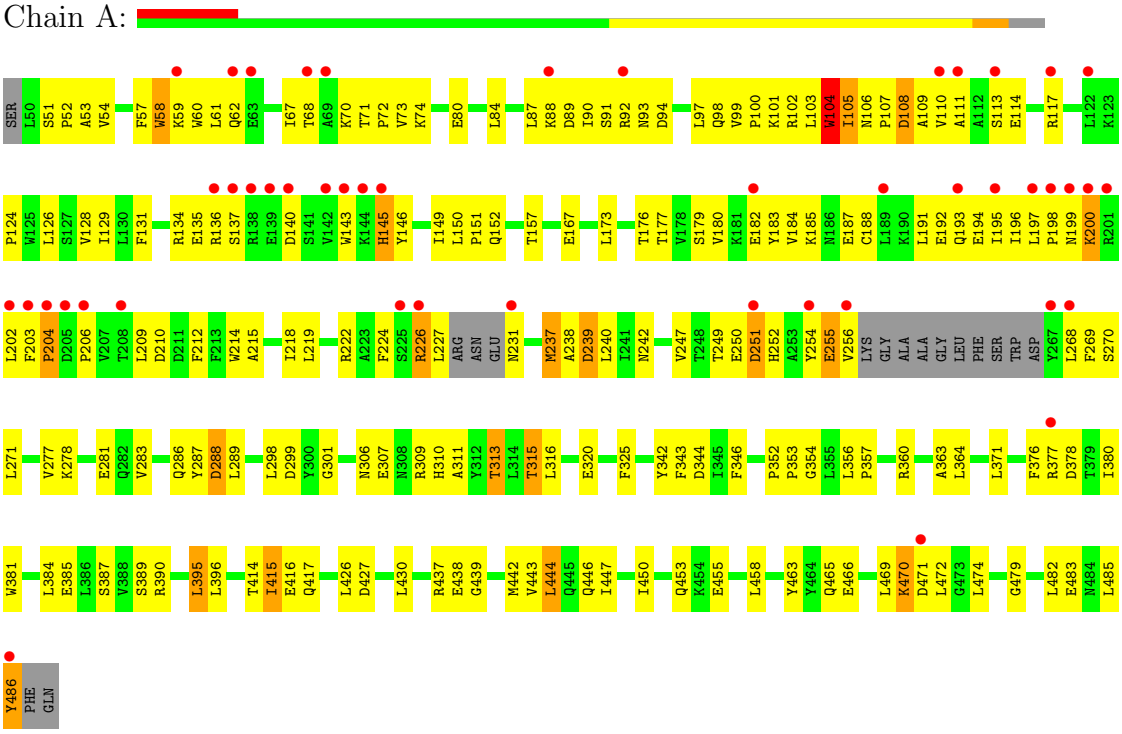
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	183	Total	O	0	0
			183	183		
3	B	186	Total	O	0	0
			186	186		
3	C	190	Total	O	0	0
			190	190		

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.

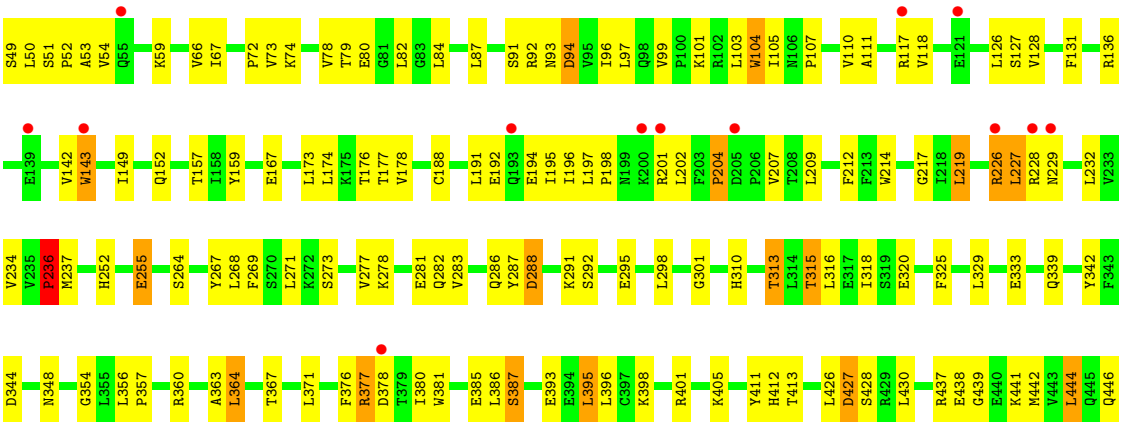
• Molecule 1: Ribulose-1,5 bisphosphate carboxylase/oxygenase

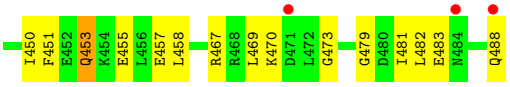
Chain A:



• Molecule 1: Ribulose-1,5 bisphosphate carboxylase/oxygenase

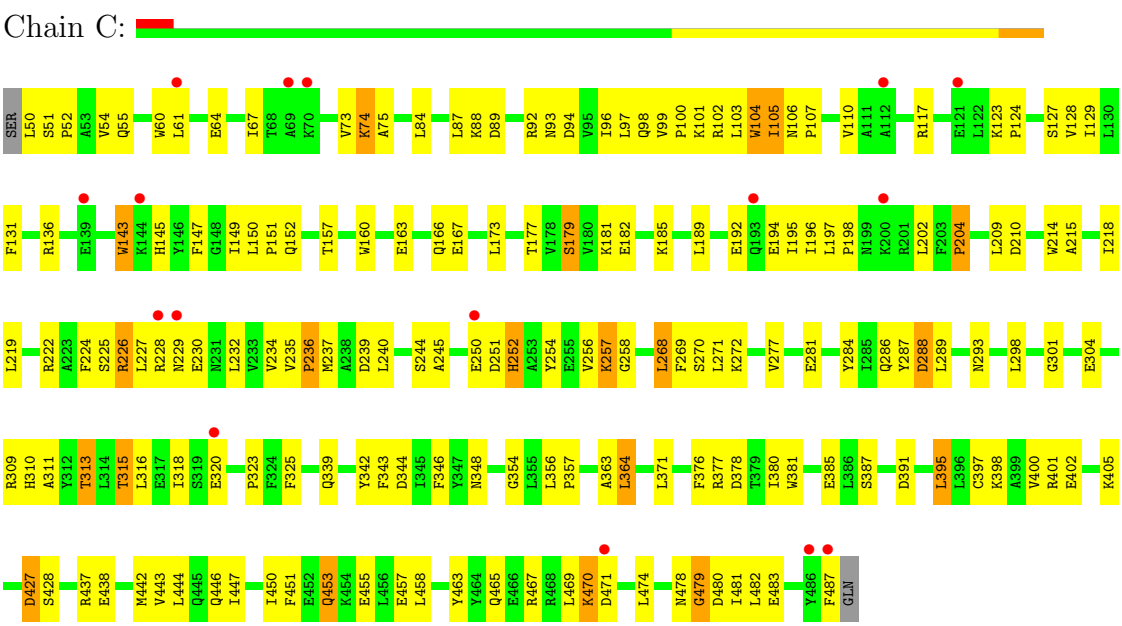
Chain B:





• Molecule 1: Ribulose-1,5 bisphosphate carboxylase/oxygenase

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	131.45Å 155.86Å 263.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.99 – 2.45 12.99 – 2.45	Depositor EDS
% Data completeness (in resolution range)	96.0 (12.99-2.45) 96.1 (12.99-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.65 (at 2.44Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.248 , 0.288 0.239 , 0.280	Depositor DCC
R_{free} test set	4049 reflections (5.09%)	DCC
Wilson B-factor (Å^2)	54.9	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 54.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	2 of 97807 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11121	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.39	0/3482	0.58	0/4723
1	B	0.41	0/3617	0.61	0/4906
1	C	0.39	0/3601	0.60	0/4886
All	All	0.40	0/10700	0.60	0/14515

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3413	0	3384	213	0
1	B	3542	0	3501	155	0
1	C	3526	0	3488	185	0
2	A	27	0	22	0	0
2	B	27	0	22	0	0
2	C	27	0	22	1	0
3	A	183	0	0	27	0
3	B	186	0	0	18	0
3	C	190	0	0	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11121	0	10439	522	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 25.

All (522) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:106:ASN:HD21	1:A:108:ASP:HB2	1.20	1.03
1:B:395:LEU:HD22	1:C:469:LEU:HD12	1.41	1.03
1:B:438:GLU:HG2	1:B:442:MET:HE2	1.42	0.97
1:C:50:LEU:HD22	1:C:54:VAL:HG11	1.49	0.94
1:A:395:LEU:HD22	1:B:469:LEU:HD12	1.51	0.93
1:B:286:GLN:HE21	1:B:288:ASP:H	0.98	0.92
1:C:470:LYS:HA	1:C:470:LYS:HE2	1.50	0.92
1:C:348:ASN:H	1:C:446:GLN:HE22	1.00	0.90
1:A:106:ASN:ND2	1:A:108:ASP:HB2	1.87	0.88
1:B:99:VAL:O	1:B:104:TRP:HH2	1.55	0.88
1:B:286:GLN:NE2	1:B:288:ASP:H	1.73	0.87
1:A:469:LEU:HD12	1:C:395:LEU:HD22	1.56	0.87
1:C:286:GLN:HE21	1:C:288:ASP:H	1.21	0.87
1:B:78:VAL:HG11	1:B:282:GLN:HE22	1.39	0.86
3:A:802:HOH:O	1:C:315:THR:HG22	1.75	0.86
1:B:286:GLN:HE21	1:B:288:ASP:N	1.74	0.84
1:C:97:LEU:HB2	1:C:237:MET:HE1	1.60	0.82
1:A:251:ASP:HA	3:A:808:HOH:O	1.80	0.81
1:C:348:ASN:H	1:C:446:GLN:NE2	1.78	0.81
1:B:173:LEU:O	1:B:177:THR:HG23	1.80	0.80
1:A:482:LEU:HD11	1:C:179:SER:HB3	1.61	0.80
1:A:197:LEU:HB2	1:A:198:PRO:HD3	1.63	0.80
1:B:395:LEU:CD2	1:C:469:LEU:HD12	2.11	0.78
1:B:99:VAL:O	1:B:104:TRP:CH2	2.36	0.77
1:B:96:ILE:HD11	1:B:273:SER:HB2	1.67	0.77
1:A:226:ARG:HH22	1:A:250:GLU:HG2	1.50	0.76
1:C:99:VAL:O	1:C:104:TRP:HH2	1.67	0.76
1:A:472:LEU:HD13	1:A:474:LEU:HD21	1.68	0.76
1:C:286:GLN:NE2	1:C:288:ASP:H	1.83	0.75
1:A:177:THR:HG22	1:A:298:LEU:HD12	1.67	0.75
1:C:136:ARG:HH22	1:C:152:GLN:HE22	1.34	0.75
1:A:94:ASP:HB3	3:A:850:HOH:O	1.85	0.75
1:A:191:LEU:O	1:A:196:ILE:HG13	1.88	0.74
1:A:192:GLU:HA	1:A:196:ILE:HB	1.67	0.74
1:A:439:GLY:HA2	1:A:442:MET:HE3	1.69	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:222:ARG:NH1	1:A:239:ASP:OD2	2.20	0.74
1:C:74:LYS:HG2	1:C:87:LEU:HD21	1.70	0.74
1:B:226:ARG:HA	3:B:813:HOH:O	1.89	0.73
1:C:348:ASN:N	1:C:446:GLN:HE22	1.83	0.73
1:B:315:THR:HG22	3:C:805:HOH:O	1.88	0.73
1:A:196:ILE:HA	1:A:203:PHE:CD1	2.25	0.72
1:A:438:GLU:HG2	1:A:442:MET:HE2	1.70	0.72
1:A:113:SER:HA	3:A:805:HOH:O	1.89	0.72
1:C:286:GLN:HE21	1:C:288:ASP:N	1.86	0.72
1:A:124:PRO:O	1:A:128:VAL:HG23	1.89	0.71
1:C:99:VAL:O	1:C:104:TRP:CH2	2.42	0.71
1:A:101:LYS:HA	1:A:104:TRP:CD2	2.25	0.71
1:B:197:LEU:HB2	1:B:198:PRO:HD3	1.72	0.71
1:C:104:TRP:HH2	1:C:269:PHE:H	1.38	0.71
1:C:73:VAL:HG21	1:C:84:LEU:HB3	1.72	0.69
1:A:315:THR:HG22	3:A:803:HOH:O	1.91	0.69
1:B:176:THR:HG21	1:C:481:ILE:HD12	1.75	0.69
1:A:110:VAL:N	3:A:812:HOH:O	2.26	0.69
1:C:371:LEU:HB3	1:C:380:ILE:HD13	1.76	0.68
1:C:67:ILE:HD11	1:C:237:MET:SD	2.33	0.68
1:C:250:GLU:HG2	1:C:289:LEU:HD12	1.74	0.68
1:A:194:GLU:C	1:A:195:ILE:HD12	2.13	0.68
1:A:200:LYS:HB3	3:A:927:HOH:O	1.93	0.68
1:C:177:THR:HG22	1:C:298:LEU:HD13	1.76	0.68
1:B:117:ARG:HB2	3:B:917:HOH:O	1.94	0.67
1:A:479:GLY:HA3	1:C:342:TYR:CE2	2.29	0.67
1:A:73:VAL:HG21	1:A:84:LEU:HB3	1.75	0.67
1:A:97:LEU:HD22	1:A:237:MET:HG3	1.76	0.67
1:A:188:CYS:HB3	1:A:212:PHE:CD1	2.30	0.67
1:A:136:ARG:HH22	1:A:152:GLN:HE22	1.43	0.67
1:A:395:LEU:CD2	1:B:469:LEU:HD12	2.25	0.67
1:A:286:GLN:HE21	1:A:288:ASP:H	1.43	0.66
1:A:104:TRP:O	1:A:105:ILE:HG13	1.96	0.66
1:A:167:GLU:HG3	1:A:437:ARG:NH1	2.10	0.66
1:B:439:GLY:HA2	1:B:442:MET:HE3	1.78	0.65
1:C:214:TRP:O	1:C:218:ILE:HG12	1.97	0.65
1:C:173:LEU:O	1:C:177:THR:HG23	1.97	0.64
1:B:49:SER:O	1:B:52:PRO:HG2	1.96	0.64
1:B:67:ILE:HD11	1:B:237:MET:SD	2.38	0.64
1:A:479:GLY:HA3	1:C:342:TYR:CZ	2.32	0.64
1:C:277:VAL:HG13	1:C:281:GLU:HB2	1.79	0.64
1:C:455:GLU:O	1:C:458:LEU:HB2	1.97	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:129:ILE:HG23	1:A:215:ALA:HB3	1.80	0.64
1:A:167:GLU:HG3	1:A:437:ARG:HH12	1.63	0.63
1:A:226:ARG:C	1:A:227:LEU:HD22	2.19	0.63
1:A:97:LEU:HD11	1:A:238:ALA:HB2	1.81	0.63
1:B:49:SER:C	1:B:52:PRO:HD2	2.19	0.63
1:A:249:THR:HA	3:A:925:HOH:O	1.99	0.63
1:C:149:ILE:HG22	3:C:861:HOH:O	1.98	0.63
1:A:104:TRP:HH2	1:A:269:PHE:H	1.46	0.63
1:B:104:TRP:NE1	3:B:821:HOH:O	2.29	0.63
1:A:99:VAL:O	1:A:104:TRP:HH2	1.81	0.63
1:A:313:THR:HB	1:A:344:ASP:OD1	1.99	0.63
1:A:99:VAL:HG12	1:A:104:TRP:HZ3	1.62	0.63
1:B:313:THR:HG21	1:C:478:ASN:CG	2.19	0.63
1:C:88:LYS:HD2	1:C:89:ASP:O	1.99	0.63
1:A:214:TRP:O	1:A:218:ILE:HG12	1.99	0.62
1:B:329:LEU:O	1:B:333:GLU:HG3	1.99	0.62
1:A:59:LYS:HD3	1:A:62:GLN:OE1	2.00	0.62
1:B:101:LYS:HA	1:B:104:TRP:CD2	2.35	0.62
1:C:250:GLU:O	1:C:250:GLU:HG3	2.00	0.62
1:B:401:ARG:O	1:B:405:LYS:HG3	1.99	0.62
1:A:286:GLN:HE21	1:A:288:ASP:C	2.03	0.61
1:C:250:GLU:C	1:C:252:HIS:H	2.04	0.61
1:C:405:LYS:HG2	3:C:846:HOH:O	2.01	0.61
1:A:140:ASP:HA	3:A:838:HOH:O	2.00	0.61
1:C:192:GLU:HA	1:C:196:ILE:HB	1.82	0.61
1:B:320:GLU:HA	1:B:325:PHE:CD1	2.35	0.61
1:B:78:VAL:HG11	1:B:282:GLN:NE2	2.12	0.60
1:C:286:GLN:HE21	1:C:288:ASP:C	2.04	0.60
1:C:52:PRO:HA	1:C:55:GLN:HE21	1.66	0.60
1:A:110:VAL:HG12	1:A:131:PHE:CG	2.36	0.60
1:A:455:GLU:O	1:A:458:LEU:HB2	2.01	0.60
1:B:99:VAL:HG12	1:B:104:TRP:HZ3	1.66	0.60
1:C:104:TRP:CH2	1:C:269:PHE:HB2	2.37	0.59
1:C:381:TRP:O	1:C:385:GLU:HG3	2.01	0.59
1:A:92:ARG:NH1	1:A:93:ASN:HD22	1.99	0.59
1:C:124:PRO:O	1:C:128:VAL:HG23	2.02	0.59
1:C:222:ARG:NH1	1:C:239:ASP:CG	2.56	0.59
1:B:196:ILE:HD13	1:B:207:VAL:HG21	1.84	0.59
1:A:286:GLN:NE2	1:A:288:ASP:H	1.99	0.59
1:C:257:LYS:HD2	1:C:268:LEU:HD11	1.85	0.59
1:B:381:TRP:O	1:B:385:GLU:HG3	2.03	0.58
1:A:111:ALA:N	3:A:812:HOH:O	2.30	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:110:VAL:HG12	1:B:131:PHE:CG	2.37	0.58
1:A:202:LEU:HA	3:A:918:HOH:O	2.02	0.58
1:B:78:VAL:HG12	1:B:79:THR:N	2.18	0.58
1:A:109:ALA:N	3:A:812:HOH:O	2.36	0.58
1:A:100:PRO:HA	1:A:268:LEU:HD12	1.86	0.58
1:C:194:GLU:C	1:C:195:ILE:HD12	2.24	0.58
1:A:307:GLU:HB3	3:A:964:HOH:O	2.03	0.58
1:C:301:GLY:HA3	3:C:819:HOH:O	2.04	0.57
1:A:226:ARG:NH2	1:A:250:GLU:HG2	2.18	0.57
1:A:173:LEU:O	1:A:177:THR:HG23	2.03	0.57
1:C:64:GLU:OE1	1:C:102:ARG:NH1	2.35	0.57
1:B:101:LYS:HA	1:B:104:TRP:CE2	2.39	0.57
1:A:227:LEU:HD12	1:A:255:GLU:OE2	2.04	0.57
1:A:180:VAL:O	1:A:184:VAL:HG23	2.04	0.57
1:A:110:VAL:HG23	1:A:111:ALA:N	2.19	0.57
1:A:157:THR:OG1	1:A:177:THR:HG21	2.05	0.57
1:A:101:LYS:HA	1:A:104:TRP:CE2	2.38	0.57
1:B:107:PRO:O	1:B:110:VAL:HG22	2.05	0.57
1:C:73:VAL:CG2	1:C:84:LEU:HB3	2.35	0.56
1:C:61:LEU:HB3	1:C:67:ILE:HG12	1.87	0.56
1:A:74:LYS:HB3	1:A:87:LEU:HD11	1.88	0.56
1:C:313:THR:HB	1:C:344:ASP:OD1	2.05	0.56
1:C:98:GLN:HA	1:C:269:PHE:O	2.05	0.56
1:A:117:ARG:HB2	3:A:819:HOH:O	2.05	0.56
1:A:247:VAL:HG11	3:A:859:HOH:O	2.05	0.56
1:A:100:PRO:C	1:A:102:ARG:H	2.09	0.56
1:A:363:ALA:HB1	1:A:395:LEU:HD13	1.86	0.56
1:A:192:GLU:HA	1:A:196:ILE:HD12	1.88	0.56
1:C:103:LEU:O	1:C:143:TRP:CZ3	2.59	0.56
1:C:54:VAL:HA	1:C:149:ILE:HD11	1.85	0.56
1:B:78:VAL:HG12	1:B:80:GLU:H	1.70	0.56
1:A:91:SER:O	1:A:94:ASP:HB2	2.06	0.56
1:B:177:THR:HG22	1:B:298:LEU:HD12	1.88	0.56
1:A:226:ARG:O	1:A:227:LEU:HD13	2.05	0.56
1:C:110:VAL:HG12	1:C:131:PHE:CG	2.41	0.56
1:C:97:LEU:HD22	1:C:237:MET:HE3	1.87	0.56
1:B:411:TYR:HB3	3:B:825:HOH:O	2.06	0.56
1:A:195:ILE:HG22	1:A:203:PHE:HE1	1.70	0.55
1:C:479:GLY:O	1:C:483:GLU:HG2	2.04	0.55
1:A:53:ALA:C	1:A:149:ILE:HD11	2.26	0.55
1:B:438:GLU:HG2	1:B:442:MET:CE	2.27	0.55
1:C:427:ASP:HA	3:C:893:HOH:O	2.06	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:463:TYR:HB2	3:A:972:HOH:O	2.06	0.55
1:C:254:TYR:HB3	1:C:271:LEU:HD13	1.88	0.55
1:A:354:GLY:HA2	1:A:357:PRO:HG2	1.89	0.55
1:A:376:PHE:O	1:A:378:ASP:N	2.37	0.55
1:A:395:LEU:HD22	1:B:469:LEU:CD1	2.31	0.55
1:A:103:LEU:HA	1:A:143:TRP:CH2	2.41	0.55
1:A:104:TRP:CH2	1:A:269:PHE:HB2	2.41	0.55
1:A:195:ILE:HG22	1:A:203:PHE:CE1	2.41	0.55
1:A:136:ARG:NH2	1:A:152:GLN:HE22	2.05	0.55
1:B:97:LEU:HD22	1:B:237:MET:HG2	1.88	0.55
1:A:102:ARG:HG2	1:A:102:ARG:O	2.06	0.55
1:B:174:LEU:O	1:B:178:VAL:HG23	2.06	0.55
1:A:167:GLU:HG2	1:A:430:LEU:CD1	2.37	0.54
1:B:136:ARG:HH22	1:B:152:GLN:HE22	1.55	0.54
1:B:110:VAL:HG21	1:B:127:SER:HB3	1.89	0.54
1:A:99:VAL:O	1:A:104:TRP:CH2	2.60	0.54
1:A:97:LEU:HD22	1:A:237:MET:CG	2.36	0.54
1:C:157:THR:OG1	1:C:177:THR:HG21	2.07	0.54
1:B:110:VAL:HG12	1:B:131:PHE:CB	2.38	0.54
1:A:192:GLU:HA	1:A:196:ILE:CB	2.37	0.54
1:A:197:LEU:HA	3:A:927:HOH:O	2.07	0.54
1:A:137:SER:HB2	3:A:901:HOH:O	2.06	0.54
1:C:318:ILE:O	1:C:339:GLN:NE2	2.40	0.54
1:A:108:ASP:C	3:A:812:HOH:O	2.46	0.54
1:C:101:LYS:HA	1:C:104:TRP:CD2	2.43	0.54
1:C:51:SER:O	1:C:55:GLN:HG3	2.08	0.54
1:A:106:ASN:HB2	1:A:107:PRO:CD	2.38	0.54
1:B:59:LYS:HB2	1:B:59:LYS:NZ	2.23	0.54
1:C:286:GLN:HE22	1:C:309:ARG:HH22	1.55	0.53
1:C:224:PHE:HD2	1:C:254:TYR:CE2	2.25	0.53
1:C:98:GLN:HG2	1:C:270:SER:HA	1.90	0.53
1:A:157:THR:OG1	1:A:177:THR:CG2	2.57	0.53
1:A:101:LYS:HA	1:A:104:TRP:CE3	2.43	0.53
1:B:142:VAL:HG23	3:B:918:HOH:O	2.08	0.53
1:B:97:LEU:HD13	1:B:237:MET:HE3	1.89	0.53
1:B:78:VAL:CG1	1:B:79:THR:N	2.71	0.53
1:C:354:GLY:HA2	1:C:357:PRO:HG2	1.90	0.53
1:B:451:PHE:O	1:B:455:GLU:HG3	2.08	0.53
1:C:185:LYS:O	1:C:189:LEU:HG	2.08	0.53
1:C:202:LEU:O	1:C:204:PRO:HD3	2.09	0.53
1:C:105:ILE:HB	1:C:234:VAL:HB	1.89	0.53
1:A:224:PHE:HZ	1:A:238:ALA:O	1.91	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:277:VAL:HG13	1:A:281:GLU:HB2	1.90	0.53
1:A:145:HIS:N	3:A:938:HOH:O	2.42	0.53
1:C:453:GLN:O	1:C:457:GLU:HG3	2.08	0.53
1:A:315:THR:HG23	1:B:473:GLY:O	2.08	0.52
1:C:446:GLN:O	1:C:450:ILE:HG13	2.09	0.52
1:A:182:GLU:O	1:A:185:LYS:HB3	2.10	0.52
1:B:446:GLN:O	1:B:450:ILE:HG13	2.09	0.52
1:B:104:TRP:CZ2	3:B:821:HOH:O	2.63	0.52
1:C:97:LEU:HB2	1:C:237:MET:CE	2.36	0.52
1:C:136:ARG:NH2	1:C:152:GLN:HE22	2.06	0.52
1:A:240:LEU:HD12	1:A:240:LEU:N	2.25	0.52
1:C:104:TRP:HH2	1:C:269:PHE:N	2.06	0.52
1:A:286:GLN:HE21	1:A:288:ASP:N	2.07	0.52
1:C:97:LEU:HD22	1:C:237:MET:CE	2.40	0.52
1:A:110:VAL:HG12	1:A:131:PHE:CB	2.40	0.52
1:C:74:LYS:HD3	1:C:75:ALA:O	2.09	0.52
1:A:206:PRO:HA	3:A:815:HOH:O	2.10	0.52
1:C:482:LEU:HG	3:C:947:HOH:O	2.10	0.52
1:B:136:ARG:HD2	1:B:214:TRP:CH2	2.45	0.51
1:A:238:ALA:HB1	1:A:271:LEU:HD22	1.93	0.51
1:C:167:GLU:HG3	1:C:437:ARG:NH1	2.26	0.51
1:B:287:TYR:O	1:B:288:ASP:HB2	2.10	0.51
1:C:316:LEU:HA	3:C:850:HOH:O	2.08	0.51
1:B:50:LEU:HD23	1:B:51:SER:N	2.25	0.51
1:B:277:VAL:HG13	1:B:281:GLU:HB2	1.92	0.51
1:A:380:ILE:O	1:A:384:LEU:HG	2.11	0.51
1:C:286:GLN:NE2	1:C:288:ASP:C	2.63	0.51
1:B:73:VAL:CG2	1:B:84:LEU:HB3	2.41	0.51
1:B:91:SER:O	1:B:94:ASP:HB2	2.11	0.51
1:A:469:LEU:C	1:A:471:ASP:H	2.14	0.50
1:B:313:THR:HB	1:B:344:ASP:OD1	2.11	0.50
1:A:278:LYS:HD2	3:A:866:HOH:O	2.11	0.50
1:A:104:TRP:HE3	1:A:104:TRP:N	2.10	0.50
1:B:363:ALA:O	1:B:364:LEU:C	2.50	0.50
1:B:92:ARG:O	1:B:93:ASN:HB2	2.11	0.50
1:C:287:TYR:O	1:C:288:ASP:HB2	2.10	0.50
1:B:236:PRO:O	1:B:237:MET:C	2.49	0.50
1:B:192:GLU:HA	1:B:196:ILE:HB	1.94	0.50
1:A:100:PRO:C	1:A:102:ARG:N	2.65	0.50
1:A:183:TYR:CE2	1:A:187:GLU:HG3	2.47	0.50
1:C:104:TRP:CH2	1:C:269:PHE:N	2.80	0.50
1:B:371:LEU:HB3	1:B:380:ILE:HD13	1.92	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:97:LEU:HD13	1:A:237:MET:HG2	1.93	0.50
1:C:117:ARG:HD2	3:C:888:HOH:O	2.11	0.50
1:A:301:GLY:HA3	3:A:810:HOH:O	2.11	0.50
1:A:88:LYS:HE2	1:A:89:ASP:HB2	1.93	0.50
1:A:415:ILE:HG22	1:A:416:GLU:OE2	2.12	0.50
1:A:167:GLU:HG2	1:A:430:LEU:HD12	1.94	0.49
1:C:401:ARG:O	1:C:405:LYS:HG3	2.12	0.49
1:B:380:ILE:HG23	1:B:381:TRP:N	2.27	0.49
1:B:92:ARG:CZ	1:B:92:ARG:HB2	2.42	0.49
1:A:443:VAL:O	1:A:447:ILE:HG13	2.12	0.49
1:B:278:LYS:HD2	3:B:942:HOH:O	2.12	0.49
1:A:105:ILE:HD11	1:A:143:TRP:CD2	2.47	0.49
1:B:277:VAL:CG1	1:B:281:GLU:HB2	2.42	0.49
1:A:286:GLN:HG2	1:A:289:LEU:HG	1.94	0.49
1:A:176:THR:HG21	1:B:481:ILE:HD12	1.92	0.49
1:A:131:PHE:CE2	1:A:135:GLU:HG3	2.48	0.49
1:B:227:LEU:HD11	1:B:269:PHE:HD1	1.77	0.49
1:B:110:VAL:HG12	1:B:131:PHE:HB2	1.94	0.49
1:B:167:GLU:HG2	1:B:430:LEU:HD12	1.94	0.49
1:A:110:VAL:CG2	1:A:111:ALA:N	2.76	0.49
1:A:226:ARG:HG2	1:A:226:ARG:HH21	1.78	0.49
1:B:288:ASP:CG	1:B:291:LYS:HD3	2.33	0.49
1:B:446:GLN:HA	3:B:927:HOH:O	2.12	0.49
1:B:105:ILE:HD11	1:B:143:TRP:CD2	2.48	0.49
1:B:149:ILE:O	1:B:149:ILE:HG22	2.11	0.49
1:C:97:LEU:HD22	1:C:237:MET:SD	2.53	0.49
1:A:222:ARG:HD3	1:A:239:ASP:OD2	2.13	0.49
1:C:245:ALA:HB2	1:C:304:GLU:OE2	2.12	0.49
1:C:251:ASP:O	1:C:252:HIS:O	2.31	0.48
1:A:80:GLU:HG3	1:A:242:ASN:ND2	2.27	0.48
1:B:441:LYS:NZ	3:B:825:HOH:O	2.45	0.48
1:A:126:LEU:HD22	1:A:191:LEU:HD11	1.95	0.48
1:A:356:LEU:N	1:A:357:PRO:HD2	2.28	0.48
1:B:376:PHE:C	1:B:378:ASP:H	2.16	0.48
1:B:386:LEU:O	1:B:387:SER:CB	2.60	0.48
1:C:463:TYR:O	1:C:467:ARG:HG3	2.13	0.48
1:C:438:GLU:HG2	1:C:442:MET:HE2	1.96	0.48
1:B:194:GLU:C	1:B:195:ILE:HD12	2.34	0.48
1:A:51:SER:HB3	1:A:54:VAL:CG2	2.42	0.48
1:B:376:PHE:O	1:B:378:ASP:N	2.46	0.48
1:A:104:TRP:O	1:A:105:ILE:CG1	2.62	0.48
1:A:114:GLU:HB2	3:A:980:HOH:O	2.12	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:192:GLU:HA	1:A:196:ILE:CG1	2.44	0.48
1:B:313:THR:HG21	1:C:478:ASN:ND2	2.28	0.48
1:A:376:PHE:C	1:A:378:ASP:H	2.16	0.48
1:B:367:THR:HB	3:B:904:HOH:O	2.13	0.48
1:B:301:GLY:HA3	3:B:817:HOH:O	2.13	0.48
1:C:371:LEU:HB3	1:C:380:ILE:CD1	2.42	0.48
1:A:277:VAL:HG21	1:A:283:VAL:HA	1.96	0.47
1:A:482:LEU:HD11	1:C:179:SER:CB	2.38	0.47
1:C:227:LEU:HD11	1:C:256:VAL:HG23	1.94	0.47
1:A:465:GLN:HB3	1:C:395:LEU:HD11	1.95	0.47
1:B:103:LEU:O	1:B:143:TRP:CZ3	2.67	0.47
1:B:159:TYR:OH	1:B:217:GLY:HA3	2.14	0.47
1:B:255:GLU:HA	1:B:268:LEU:O	2.14	0.47
1:A:67:ILE:HG13	1:A:71:THR:HG21	1.97	0.47
1:A:192:GLU:HB3	3:A:854:HOH:O	2.14	0.47
1:B:348:ASN:H	1:B:446:GLN:HE22	1.63	0.47
1:B:73:VAL:HG21	1:B:84:LEU:HB3	1.97	0.47
1:B:292:SER:OG	1:B:295:GLU:HG3	2.14	0.47
1:C:103:LEU:O	1:C:143:TRP:HZ3	1.97	0.47
1:C:147:PHE:HD2	1:C:150:LEU:HD12	1.80	0.47
1:A:254:TYR:CE1	1:A:256:VAL:HG22	2.49	0.47
1:B:277:VAL:HG21	1:B:283:VAL:HG12	1.96	0.47
1:A:98:GLN:HA	1:A:269:PHE:O	2.14	0.47
1:B:118:VAL:HG13	3:B:917:HOH:O	2.14	0.47
1:A:149:ILE:HG22	3:A:848:HOH:O	2.13	0.47
1:C:427:ASP:OD2	1:C:428:SER:N	2.48	0.47
1:C:380:ILE:HG23	1:C:381:TRP:N	2.29	0.47
1:B:488:GLN:HB3	3:B:968:HOH:O	2.15	0.47
1:A:150:LEU:HD13	1:A:218:ILE:HD12	1.96	0.47
1:B:126:LEU:HD22	1:B:191:LEU:HD11	1.97	0.47
1:A:134:ARG:HH11	1:A:134:ARG:HG2	1.79	0.47
1:C:293:ASN:HD22	1:C:310:HIS:CD2	2.33	0.47
1:A:192:GLU:O	1:A:197:LEU:HG	2.16	0.46
1:C:478:ASN:O	1:C:480:ASP:N	2.47	0.46
1:A:202:LEU:O	1:A:204:PRO:HD3	2.15	0.46
1:B:201:ARG:HB3	3:B:878:HOH:O	2.14	0.46
1:A:117:ARG:HD2	3:A:849:HOH:O	2.14	0.46
1:C:225:SER:O	1:C:227:LEU:N	2.48	0.46
1:A:68:THR:OG1	1:A:70:LYS:HB3	2.15	0.46
1:A:469:LEU:CD1	1:C:395:LEU:HD22	2.37	0.46
1:A:179:SER:HB3	1:B:482:LEU:HD12	1.97	0.46
1:C:226:ARG:HG2	1:C:252:HIS:CD2	2.50	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:438:GLU:CD	1:C:442:MET:HE2	2.35	0.46
1:C:471:ASP:N	3:C:833:HOH:O	2.48	0.46
1:C:97:LEU:HD13	1:C:237:MET:HE3	1.98	0.46
1:A:103:LEU:HA	1:A:143:TRP:HH2	1.78	0.46
1:A:58:TRP:CE3	1:A:58:TRP:HA	2.51	0.46
1:C:110:VAL:HG21	1:C:127:SER:HB3	1.97	0.46
1:C:438:GLU:HG2	1:C:442:MET:CE	2.46	0.46
1:B:264:SER:HA	1:B:267:TYR:CZ	2.51	0.46
1:B:318:ILE:O	1:B:339:GLN:NE2	2.48	0.46
1:A:376:PHE:CZ	1:C:323:PRO:HB3	2.50	0.46
1:A:197:LEU:HB2	1:A:198:PRO:CD	2.42	0.46
1:A:157:THR:CB	1:A:177:THR:HG21	2.46	0.46
1:A:188:CYS:HB3	1:A:212:PHE:CE1	2.51	0.46
1:C:438:GLU:OE2	1:C:442:MET:HE2	2.16	0.46
1:C:96:ILE:HD12	1:C:271:LEU:HG	1.98	0.46
1:A:104:TRP:CE3	1:A:104:TRP:N	2.83	0.46
1:B:103:LEU:HA	1:B:143:TRP:CH2	2.51	0.46
1:A:316:LEU:HD12	1:A:343:PHE:CE1	2.51	0.45
1:C:226:ARG:HG2	1:C:252:HIS:NE2	2.31	0.45
1:C:250:GLU:C	1:C:252:HIS:N	2.70	0.45
1:A:218:ILE:O	1:A:222:ARG:HB2	2.15	0.45
1:A:100:PRO:O	1:A:102:ARG:N	2.49	0.45
1:B:342:TYR:CZ	1:C:479:GLY:HA3	2.51	0.45
1:B:395:LEU:HD11	1:C:465:GLN:HB3	1.96	0.45
1:B:96:ILE:HD13	1:B:283:VAL:HG21	1.98	0.45
1:A:98:GLN:HE21	1:A:270:SER:HB2	1.81	0.45
1:A:152:GLN:NE2	1:A:152:GLN:HA	2.31	0.45
1:A:371:LEU:HB3	1:A:380:ILE:HD13	1.99	0.45
1:A:287:TYR:O	1:A:288:ASP:HB2	2.17	0.45
1:A:286:GLN:HE22	1:A:309:ARG:HH22	1.64	0.45
1:A:389:SER:HA	1:A:463:TYR:CG	2.51	0.45
1:B:54:VAL:HA	1:B:149:ILE:HD11	1.99	0.45
1:C:100:PRO:HA	1:C:268:LEU:HB3	1.99	0.45
1:C:286:GLN:HE21	1:C:288:ASP:CA	2.30	0.45
1:C:400:VAL:HG11	1:C:451:PHE:CD1	2.51	0.45
1:A:469:LEU:HD12	1:C:395:LEU:CD2	2.36	0.45
1:A:474:LEU:HD22	1:C:316:LEU:CD2	2.47	0.45
1:A:54:VAL:N	1:A:149:ILE:HD11	2.32	0.45
1:B:482:LEU:O	1:B:482:LEU:HD23	2.16	0.45
1:A:57:PHE:CE1	1:A:146:TYR:HA	2.51	0.45
1:A:474:LEU:HD22	1:C:316:LEU:HD23	1.99	0.45
1:C:97:LEU:C	1:C:97:LEU:HD12	2.36	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:455:GLU:O	1:B:458:LEU:HB2	2.17	0.45
1:A:106:ASN:HB2	1:A:107:PRO:HD2	1.99	0.44
1:C:157:THR:OG1	1:C:177:THR:CG2	2.64	0.44
1:B:110:VAL:HG23	1:B:111:ALA:N	2.31	0.44
1:C:167:GLU:HG3	1:C:437:ARG:HH12	1.82	0.44
1:C:197:LEU:N	1:C:198:PRO:HD2	2.32	0.44
1:B:188:CYS:HB3	1:B:212:PHE:CD1	2.52	0.44
1:B:128:VAL:HG11	1:B:219:LEU:HD11	1.98	0.44
1:C:446:GLN:NE2	3:C:971:HOH:O	2.49	0.44
1:A:98:GLN:HE21	1:A:270:SER:CB	2.31	0.44
1:B:117:ARG:HA	3:B:891:HOH:O	2.17	0.44
1:A:61:LEU:C	1:A:67:ILE:HG22	2.37	0.44
1:C:107:PRO:O	1:C:110:VAL:HG22	2.17	0.44
1:C:244:SER:HB2	1:C:284:TYR:CD2	2.52	0.44
1:B:360:ARG:HG2	1:B:396:LEU:CD2	2.48	0.44
1:B:467:ARG:HA	1:B:470:LYS:HG2	1.98	0.44
1:A:105:ILE:O	1:A:105:ILE:HG22	2.18	0.44
1:C:286:GLN:HG2	1:C:289:LEU:HG	1.98	0.44
1:A:92:ARG:HH11	1:A:93:ASN:HD22	1.62	0.44
1:B:202:LEU:O	1:B:204:PRO:HD3	2.18	0.44
1:B:104:TRP:CE2	3:B:821:HOH:O	2.70	0.44
1:C:391:ASP:O	1:C:395:LEU:HB2	2.17	0.44
1:B:176:THR:CG2	1:C:481:ILE:HD12	2.46	0.44
1:B:412:HIS:CD2	1:B:413:THR:HG23	2.53	0.44
1:A:389:SER:HA	1:A:463:TYR:HB3	2.00	0.44
1:C:163:GLU:O	1:C:166:GLN:HB2	2.18	0.44
1:B:104:TRP:N	1:B:104:TRP:CE3	2.87	0.43
1:B:356:LEU:O	1:B:360:ARG:HG3	2.17	0.43
1:A:466:GLU:O	1:A:470:LYS:HG2	2.17	0.43
1:A:360:ARG:HG2	1:A:396:LEU:CD2	2.49	0.43
1:B:310:HIS:CD2	1:B:439:GLY:HA3	2.53	0.43
1:A:60:TRP:HB2	1:A:145:HIS:HD2	1.83	0.43
1:C:98:GLN:HE21	1:C:270:SER:HB2	1.83	0.43
1:B:97:LEU:HB2	1:B:237:MET:CE	2.47	0.43
1:B:219:LEU:HG	1:B:232:LEU:HD11	2.00	0.43
1:A:444:LEU:HD12	1:A:444:LEU:HA	1.79	0.43
1:A:320:GLU:HA	1:A:325:PHE:CD1	2.54	0.43
1:C:465:GLN:HA	1:C:465:GLN:OE1	2.18	0.43
1:C:50:LEU:N	3:C:953:HOH:O	2.51	0.43
1:C:240:LEU:HD23	1:C:240:LEU:HA	1.87	0.43
1:A:222:ARG:HH11	1:A:239:ASP:CG	2.15	0.43
1:B:97:LEU:C	1:B:97:LEU:HD12	2.39	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:397:CYS:O	1:C:401:ARG:HG3	2.19	0.43
1:C:222:ARG:NH1	1:C:239:ASP:OD2	2.50	0.43
1:A:354:GLY:HA2	1:A:357:PRO:CG	2.48	0.43
1:A:485:LEU:O	1:A:486:TYR:HB3	2.19	0.43
1:A:131:PHE:O	1:A:135:GLU:HG2	2.19	0.43
1:B:395:LEU:HD22	1:C:469:LEU:CD1	2.28	0.43
1:B:66:VAL:HA	3:B:983:HOH:O	2.18	0.43
1:C:363:ALA:HB1	1:C:395:LEU:HD13	2.01	0.42
1:A:194:GLU:CB	1:A:195:ILE:HD12	2.49	0.42
1:C:74:LYS:HG2	1:C:87:LEU:CD2	2.44	0.42
1:A:286:GLN:NE2	1:A:288:ASP:C	2.71	0.42
1:C:227:LEU:HB3	1:C:230:GLU:O	2.19	0.42
1:C:60:TRP:HB2	1:C:145:HIS:HD2	1.84	0.42
1:C:157:THR:HA	1:C:160:TRP:CD1	2.54	0.42
1:C:222:ARG:NH2	2:C:803:SAM:OXT	2.51	0.42
1:A:88:LYS:O	1:A:90:ILE:HG13	2.19	0.42
1:C:151:PRO:HG3	3:C:827:HOH:O	2.19	0.42
1:C:252:HIS:N	1:C:252:HIS:CD2	2.86	0.42
1:C:104:TRP:HE3	1:C:104:TRP:N	2.18	0.42
1:B:380:ILE:HG23	1:B:381:TRP:H	1.83	0.42
1:A:483:GLU:C	1:A:485:LEU:H	2.23	0.42
1:A:311:ALA:HB2	1:A:346:PHE:CD2	2.54	0.42
1:B:195:ILE:HD12	1:B:195:ILE:N	2.34	0.42
1:C:364:LEU:HD12	1:C:364:LEU:HA	1.87	0.42
1:A:88:LYS:HE2	1:A:89:ASP:CB	2.49	0.42
1:B:453:GLN:NE2	1:B:457:GLU:OE2	2.52	0.42
1:A:98:GLN:HG2	1:A:270:SER:HA	2.01	0.42
1:C:443:VAL:O	1:C:447:ILE:HG13	2.18	0.42
1:A:226:ARG:HG2	1:A:226:ARG:NH2	2.35	0.42
1:C:103:LEU:HA	1:C:143:TRP:CH2	2.55	0.42
1:C:106:ASN:HB2	1:C:107:PRO:HD2	2.01	0.42
1:B:202:LEU:C	1:B:204:PRO:HD3	2.40	0.42
1:C:470:LYS:HA	1:C:470:LYS:CE	2.33	0.42
1:C:254:TYR:HA	1:C:270:SER:O	2.20	0.42
1:C:316:LEU:HD12	1:C:343:PHE:CE1	2.55	0.42
1:A:384:LEU:HD23	1:A:384:LEU:HA	1.91	0.42
1:C:244:SER:HB2	1:C:284:TYR:CG	2.55	0.42
1:A:252:HIS:ND1	1:A:252:HIS:N	2.67	0.42
1:C:376:PHE:C	1:C:378:ASP:H	2.23	0.42
1:A:150:LEU:HA	1:A:151:PRO:HD3	1.89	0.42
1:C:257:LYS:O	1:C:268:LEU:HD12	2.19	0.42
1:B:393:GLU:O	1:B:396:LEU:HG	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:486:TYR:HB3	1:C:123:LYS:NZ	2.35	0.42
1:B:398:LYS:HD2	3:B:865:HOH:O	2.19	0.42
1:B:157:THR:OG1	1:B:177:THR:HG21	2.20	0.41
1:C:74:LYS:HB3	1:C:87:LEU:HD11	2.02	0.41
1:B:364:LEU:HD12	1:B:364:LEU:HA	1.71	0.41
1:B:427:ASP:OD2	1:B:428:SER:N	2.52	0.41
1:A:414:THR:OG1	1:A:417:GLN:HG3	2.19	0.41
1:C:235:VAL:HG21	1:C:269:PHE:CD1	2.56	0.41
1:A:479:GLY:CA	1:C:342:TYR:CE2	3.02	0.41
1:A:197:LEU:O	1:A:199:ASN:N	2.53	0.41
1:C:105:ILE:HD11	1:C:143:TRP:CD2	2.55	0.41
1:C:222:ARG:NH1	1:C:239:ASP:OD1	2.53	0.41
1:B:50:LEU:HD23	1:B:50:LEU:C	2.41	0.41
1:B:356:LEU:N	1:B:357:PRO:HD2	2.35	0.41
1:C:94:ASP:O	1:C:272:LYS:HB2	2.19	0.41
1:B:377:ARG:HD3	1:B:377:ARG:HA	1.82	0.41
1:C:181:LYS:HE2	1:C:181:LYS:HB3	1.92	0.41
1:C:129:ILE:HG23	1:C:215:ALA:HB3	2.02	0.41
1:B:78:VAL:CG1	1:B:80:GLU:OE2	2.69	0.41
1:C:182:GLU:O	1:C:185:LYS:HB3	2.21	0.41
1:A:352:PRO:HA	1:A:353:PRO:HD3	1.90	0.41
1:C:92:ARG:O	1:C:93:ASN:HB2	2.20	0.41
1:C:311:ALA:HB2	1:C:346:PHE:CD2	2.55	0.41
1:B:227:LEU:HD11	1:B:269:PHE:CD1	2.54	0.41
1:A:310:HIS:CG	1:A:439:GLY:HA3	2.56	0.41
1:A:58:TRP:O	1:A:62:GLN:HG3	2.20	0.41
1:A:376:PHE:HZ	1:C:323:PRO:HB3	1.86	0.41
1:B:167:GLU:HG3	1:B:437:ARG:NH1	2.36	0.41
1:B:354:GLY:O	1:B:357:PRO:HG2	2.20	0.41
1:B:82:LEU:HA	1:B:82:LEU:HD23	1.87	0.41
1:C:398:LYS:O	1:C:402:GLU:HG2	2.20	0.41
1:C:104:TRP:O	1:C:143:TRP:CH2	2.74	0.41
1:B:167:GLU:HG2	1:B:430:LEU:CD1	2.50	0.41
1:C:356:LEU:HD23	1:C:356:LEU:HA	1.86	0.41
1:A:255:GLU:N	1:A:255:GLU:OE1	2.45	0.41
1:B:444:LEU:HA	1:B:444:LEU:HD12	1.84	0.41
1:B:316:LEU:HD23	1:C:474:LEU:CD2	2.50	0.41
1:B:104:TRP:CH2	1:B:269:PHE:HB2	2.56	0.41
1:A:298:LEU:HD23	1:A:298:LEU:C	2.41	0.41
1:A:58:TRP:CZ2	1:A:74:LYS:HA	2.56	0.41
1:A:390:ARG:HA	1:A:463:TYR:CZ	2.56	0.41
1:B:252:HIS:O	1:B:271:LEU:HA	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:104:TRP:CE3	1:C:104:TRP:N	2.88	0.41
1:C:481:ILE:HD11	3:C:946:HOH:O	2.19	0.41
1:A:88:LYS:HE2	1:A:89:ASP:H	1.86	0.41
1:C:363:ALA:O	1:C:364:LEU:C	2.59	0.41
1:A:192:GLU:HA	1:A:196:ILE:CD1	2.51	0.41
1:C:101:LYS:HA	1:C:104:TRP:CE3	2.55	0.41
1:A:470:LYS:HE2	1:A:470:LYS:HA	2.02	0.41
1:B:74:LYS:HB3	1:B:87:LEU:HD21	2.02	0.41
1:B:228:ARG:O	1:B:229:ASN:HB2	2.21	0.41
1:B:348:ASN:N	1:B:446:GLN:HE22	2.19	0.40
1:A:101:LYS:HG2	1:A:101:LYS:O	2.21	0.40
1:C:257:LYS:HD3	1:C:258:GLY:O	2.20	0.40
1:B:105:ILE:HB	1:B:234:VAL:HB	2.04	0.40
1:C:320:GLU:HA	1:C:325:PHE:CD1	2.56	0.40
1:A:381:TRP:O	1:A:385:GLU:HG3	2.21	0.40
1:B:104:TRP:N	1:B:104:TRP:HE3	2.18	0.40
1:C:376:PHE:O	1:C:378:ASP:N	2.53	0.40
1:C:228:ARG:HG2	1:C:229:ASN:ND2	2.36	0.40
1:A:193:GLN:HA	1:A:197:LEU:HD12	2.03	0.40
1:B:53:ALA:C	1:B:149:ILE:HD11	2.42	0.40
1:B:219:LEU:HA	1:B:219:LEU:HD12	1.87	0.40
1:A:342:TYR:CZ	1:B:479:GLY:HA3	2.55	0.40
1:C:487:PHE:HB3	3:C:832:HOH:O	2.21	0.40
1:A:187:GLU:O	1:A:191:LEU:HG	2.21	0.40
1:A:446:GLN:O	1:A:450:ILE:HG13	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

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	418/440 (95%)	369 (88%)	38 (9%)	11 (3%)	8 10
1	B	438/440 (100%)	400 (91%)	31 (7%)	7 (2%)	14 21
1	C	436/440 (99%)	398 (91%)	26 (6%)	12 (3%)	8 9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1292/1320 (98%)	1167 (90%)	95 (7%)	30 (2%)	10 12

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	105	ILE
1	A	204	PRO
1	A	364	LEU
1	B	236	PRO
1	B	364	LEU
1	C	226	ARG
1	C	364	LEU
1	A	377	ARG
1	B	288	ASP
1	B	377	ARG
1	B	387	SER
1	C	252	HIS
1	C	479	GLY
1	A	104	TRP
1	A	288	ASP
1	C	204	PRO
1	C	288	ASP
1	C	377	ARG
1	C	470	LYS
1	C	387	SER
1	A	52	PRO
1	A	200	LYS
1	A	306	ASN
1	A	387	SER
1	A	470	LYS
1	B	227	LEU
1	C	105	ILE
1	C	232	LEU
1	C	236	PRO
1	B	204	PRO

5.3.2 Protein sidechains

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	374/386 (97%)	350 (94%)	24 (6%)	25	41
1	B	386/386 (100%)	369 (96%)	17 (4%)	39	62
1	C	384/386 (100%)	368 (96%)	16 (4%)	40	64
All	All	1144/1158 (99%)	1087 (95%)	57 (5%)	34	56

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

Mol	Chain	Res	Type
1	A	58	TRP
1	A	72	PRO
1	A	104	TRP
1	A	108	ASP
1	A	145	HIS
1	A	209	LEU
1	A	210	ASP
1	A	219	LEU
1	A	226	ARG
1	A	231	ASN
1	A	237	MET
1	A	239	ASP
1	A	251	ASP
1	A	255	GLU
1	A	299	ASP
1	A	313	THR
1	A	315	THR
1	A	395	LEU
1	A	415	ILE
1	A	426	LEU
1	A	427	ASP
1	A	444	LEU
1	A	453	GLN
1	A	486	TYR
1	B	72	PRO
1	B	94	ASP
1	B	104	TRP
1	B	143	TRP
1	B	209	LEU
1	B	219	LEU
1	B	226	ARG
1	B	236	PRO
1	B	255	GLU
1	B	313	THR

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Mol	Chain	Res	Type
1	B	315	THR
1	B	395	LEU
1	B	426	LEU
1	B	427	ASP
1	B	444	LEU
1	B	453	GLN
1	B	483	GLU
1	C	74	LYS
1	C	104	TRP
1	C	143	TRP
1	C	179	SER
1	C	209	LEU
1	C	210	ASP
1	C	219	LEU
1	C	236	PRO
1	C	257	LYS
1	C	268	LEU
1	C	313	THR
1	C	315	THR
1	C	395	LEU
1	C	427	ASP
1	C	444	LEU
1	C	453	GLN

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

Mol	Chain	Res	Type
1	A	55	GLN
1	A	93	ASN
1	A	98	GLN
1	A	106	ASN
1	A	152	GLN
1	A	169	GLN
1	A	193	GLN
1	A	286	GLN
1	A	310	HIS
1	B	93	ASN
1	B	152	GLN
1	B	169	GLN
1	B	286	GLN
1	B	310	HIS
1	B	453	GLN

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Mol	Chain	Res	Type
1	B	460	GLN
1	B	488	GLN
1	C	55	GLN
1	C	98	GLN
1	C	145	HIS
1	C	152	GLN
1	C	169	GLN
1	C	229	ASN
1	C	286	GLN
1	C	310	HIS
1	C	446	GLN

5.3.3 RNA

There are no RNA chains 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

3 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	SAM	A	801	-	26,29,29	2.50	2 (7%)	38,42,42	1.05	4 (10%)
2	SAM	B	802	-	26,29,29	2.30	3 (11%)	38,42,42	0.96	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SAM	C	803	-	26,29,29	2.28	2 (7%)	38,42,42	0.96	2 (5%)

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	SAM	A	801	-	-	0/13/33/33	0/1/3/3
2	SAM	B	802	-	-	0/13/33/33	0/1/3/3
2	SAM	C	803	-	-	0/13/33/33	0/1/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	SAM	CG-SD	-12.08	1.57	1.80
2	C	803	SAM	CG-SD	-10.84	1.59	1.80
2	B	802	SAM	CG-SD	-10.71	1.59	1.80
2	B	802	SAM	C2-N3	2.34	1.36	1.32
2	A	801	SAM	C8-N9	2.06	1.39	1.36
2	C	803	SAM	C2-N3	2.06	1.36	1.32
2	B	802	SAM	C2-N1	2.04	1.37	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	803	SAM	CB-CG-SD	2.26	117.42	112.49
2	A	801	SAM	O4'-C1'-N9	2.23	110.51	108.44
2	B	802	SAM	CB-CG-SD	2.22	117.32	112.49
2	C	803	SAM	C8-N9-C4	-2.19	105.23	106.90
2	A	801	SAM	CG-CB-CA	2.11	115.33	112.22
2	A	801	SAM	C8-N9-C4	-2.08	105.31	106.90
2	A	801	SAM	C8-N9-C1'	2.05	130.43	126.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	424/440 (96%)	0.48	47 (11%)	6	5	43, 66, 117, 126	0
1	B	440/440 (100%)	0.03	16 (3%)	41	41	37, 61, 97, 115	0
1	C	438/440 (99%)	0.06	16 (3%)	39	40	39, 63, 97, 115	0
All	All	1302/1320 (98%)	0.19	79 (6%)	21	20	37, 63, 104, 126	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	197	LEU	9.8
1	C	487	PHE	7.7
1	A	198	PRO	7.7
1	A	267	TYR	6.8
1	A	140	ASP	6.7
1	C	229	ASN	6.1
1	C	250	GLU	5.7
1	A	111	ALA	5.7
1	A	193	GLN	5.3
1	A	137	SER	4.7
1	B	200	LYS	4.6
1	C	471	ASP	4.4
1	A	117	ARG	4.4
1	A	254	TYR	4.1
1	B	488	GLN	4.1
1	A	201	ARG	4.0
1	B	193	GLN	4.0
1	C	486	TYR	3.9
1	A	203	PHE	3.9
1	A	139	GLU	3.9
1	B	139	GLU	3.9
1	A	145	HIS	3.7
1	C	193	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	200	LYS	3.7
1	A	202	LEU	3.7
1	A	204	PRO	3.5
1	A	486	TYR	3.5
1	A	251	ASP	3.4
1	A	377	ARG	3.4
1	A	138	ARG	3.4
1	B	471	ASP	3.3
1	A	144	LYS	3.3
1	A	206	PRO	3.2
1	C	200	LYS	3.2
1	A	110	VAL	3.0
1	B	117	ARG	3.0
1	B	378	ASP	3.0
1	A	136	ARG	2.9
1	A	231	ASN	2.8
1	B	229	ASN	2.8
1	B	143	TRP	2.8
1	A	122	LEU	2.7
1	A	189	LEU	2.7
1	C	112	ALA	2.6
1	B	201	ARG	2.6
1	C	228	ARG	2.6
1	B	226	ARG	2.5
1	A	208	THR	2.5
1	B	121	GLU	2.5
1	A	226	ARG	2.4
1	A	195	ILE	2.4
1	A	63	GLU	2.4
1	B	484	ASN	2.4
1	A	68	THR	2.4
1	C	121	GLU	2.3
1	B	228	ARG	2.3
1	C	139	GLU	2.3
1	A	69	ALA	2.3
1	A	205	ASP	2.3
1	C	70	LYS	2.2
1	C	69	ALA	2.2
1	A	256	VAL	2.2
1	C	320	GLU	2.2
1	C	61	LEU	2.2
1	B	205	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	182	GLU	2.2
1	A	113	SER	2.1
1	A	59	LYS	2.1
1	A	225	SER	2.1
1	A	62	GLN	2.1
1	A	88	LYS	2.1
1	C	144	LYS	2.1
1	A	471	ASP	2.1
1	A	268	LEU	2.1
1	A	142	VAL	2.0
1	A	92	ARG	2.0
1	A	143	TRP	2.0
1	B	55	GLN	2.0
1	A	199	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	SAM	C	803	27/27	0.11	-0.18	43,55,57,59	0
2	SAM	A	801	27/27	0.12	-0.53	59,62,67,71	0
2	SAM	B	802	27/27	0.09	-0.82	34,42,46,49	0

6.5 Other polymers

There are no such residues in this entry.