Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:50 PM GMT

PDB ID	:	3V8F
Title	:	Crystal structure of crosslinked GltPh V216C-M385C mutant
Authors	:	Verdon, G.; Boudker, O.
Deposited on	:	2011-12-22
Resolution	:	3.80 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:

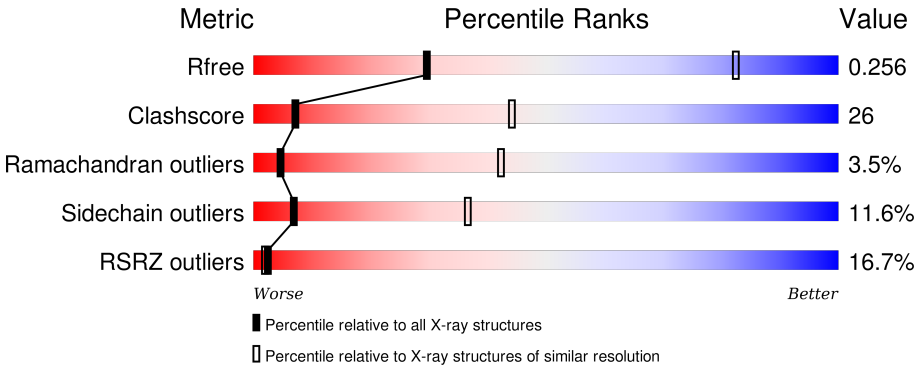
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.80 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	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

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	422	23% 48% 43% 6% •
1	B	422	16% 50% 41% 6% •
1	C	422	10% 48% 42% 6% • •

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	ASP	A	901	-	-	-	X
2	ASP	B	901	-	-	-	X
2	ASP	C	901	-	-	X	X
3	NA	A	902	-	-	-	X
3	NA	B	902	-	-	-	X
3	NA	C	902	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9155 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 sodium-coupled L-aspartate transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	0	0	0
			3038	1999	490	532	17			
1	B	411	Total	C	N	O	S	0	0	0
			3043	2002	491	533	17			
1	C	410	Total	C	N	O	S	0	0	0
			3038	1999	490	532	17			

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	HIS	ASP	engineered mutation	UNP O59010
A	40	HIS	LYS	engineered mutation	UNP O59010
A	125	HIS	LYS	engineered mutation	UNP O59010
A	132	HIS	LYS	engineered mutation	UNP O59010
A	216	CYS	VAL	engineered mutation	UNP O59010
A	223	HIS	LYS	engineered mutation	UNP O59010
A	264	HIS	LYS	engineered mutation	UNP O59010
A	321	ALA	CYS	engineered mutation	UNP O59010
A	368	HIS	GLU	engineered mutation	UNP O59010
A	385	CYS	MET	engineered mutation	UNP O59010
A	418	THR	-	EXPRESSION TAG	UNP O59010
A	419	LEU	-	EXPRESSION TAG	UNP O59010
A	420	VAL	-	EXPRESSION TAG	UNP O59010
A	421	PRO	-	EXPRESSION TAG	UNP O59010
A	422	ARG	-	EXPRESSION TAG	UNP O59010
B	37	HIS	ASP	engineered mutation	UNP O59010
B	40	HIS	LYS	engineered mutation	UNP O59010
B	125	HIS	LYS	engineered mutation	UNP O59010
B	132	HIS	LYS	engineered mutation	UNP O59010
B	216	CYS	VAL	engineered mutation	UNP O59010
B	223	HIS	LYS	engineered mutation	UNP O59010
B	264	HIS	LYS	engineered mutation	UNP O59010
B	321	ALA	CYS	engineered mutation	UNP O59010

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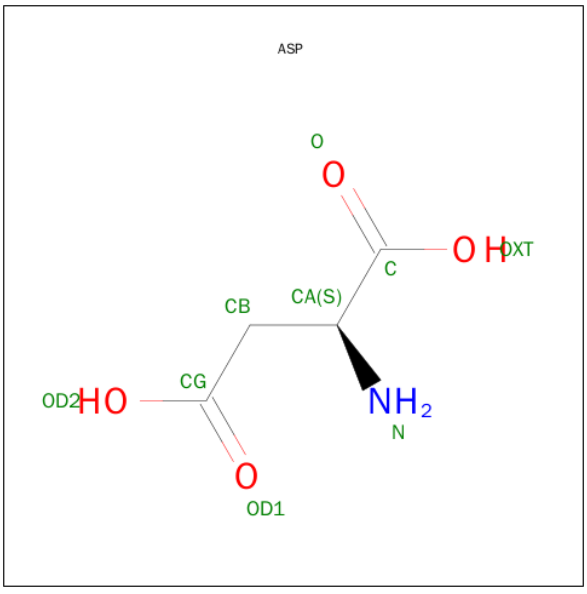
Chain	Residue	Modelled	Actual	Comment	Reference
B	368	HIS	GLU	engineered mutation	UNP O59010
B	385	CYS	MET	engineered mutation	UNP O59010
B	418	THR	-	EXPRESSION TAG	UNP O59010
B	419	LEU	-	EXPRESSION TAG	UNP O59010
B	420	VAL	-	EXPRESSION TAG	UNP O59010
B	421	PRO	-	EXPRESSION TAG	UNP O59010
B	422	ARG	-	EXPRESSION TAG	UNP O59010
C	37	HIS	ASP	engineered mutation	UNP O59010
C	40	HIS	LYS	engineered mutation	UNP O59010
C	125	HIS	LYS	engineered mutation	UNP O59010
C	132	HIS	LYS	engineered mutation	UNP O59010
C	216	CYS	VAL	engineered mutation	UNP O59010
C	223	HIS	LYS	engineered mutation	UNP O59010
C	264	HIS	LYS	engineered mutation	UNP O59010
C	321	ALA	CYS	engineered mutation	UNP O59010
C	368	HIS	GLU	engineered mutation	UNP O59010
C	385	CYS	MET	engineered mutation	UNP O59010
C	418	THR	-	EXPRESSION TAG	UNP O59010
C	419	LEU	-	EXPRESSION TAG	UNP O59010
C	420	VAL	-	EXPRESSION TAG	UNP O59010
C	421	PRO	-	EXPRESSION TAG	UNP O59010
C	422	ARG	-	EXPRESSION TAG	UNP O59010

- Molecule 2 is ASPARTIC ACID (three-letter code: ASP) (formula: $C_4H_7NO_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 9 4 1 4	0	0
2	B	1	Total C N O 9 4 1 4	0	0
2	C	1	Total C N O 9 4 1 4	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Na 2 2	0	0
3	A	2	Total Na 2 2	0	0
3	C	2	Total Na 2 2	0	0

- Molecule 4 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Hg 1 1	0	0
4	A	1	Total Hg 1 1	0	0
4	C	1	Total Hg 1 1	0	0

3 Residue-property plots (i)

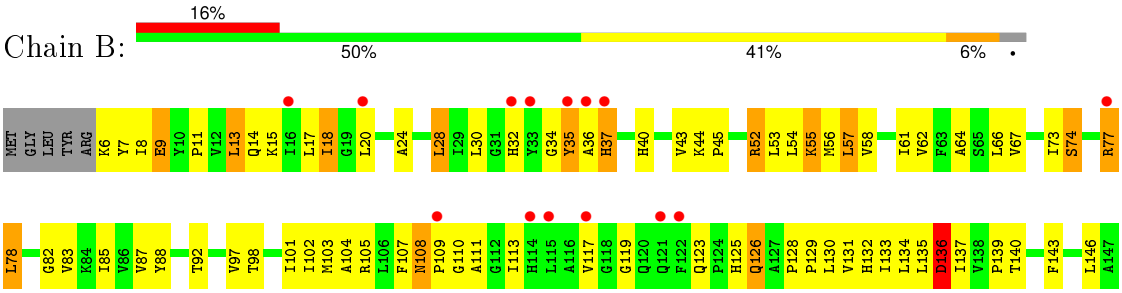
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

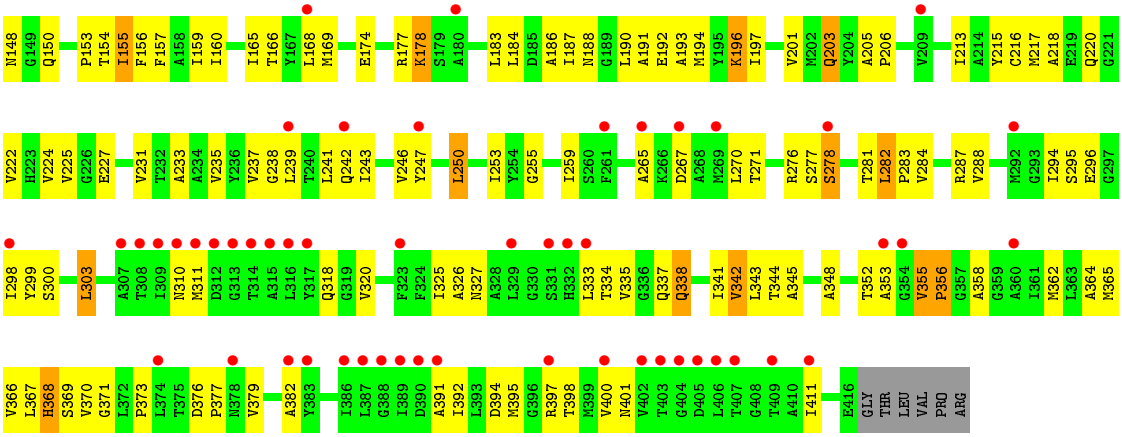
- Molecule 1: sodium-coupled L-aspartate transporter

Chain A:

- Molecule 1: sodium-coupled L-aspartate transporter

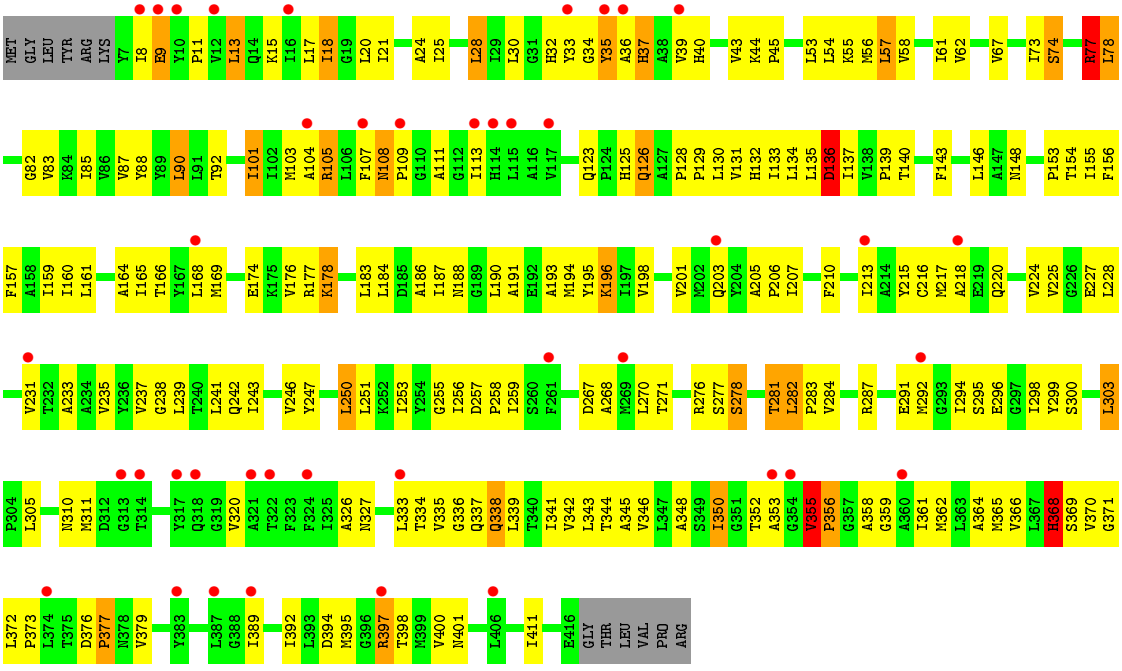
Chain B:





• Molecule 1: sodium-coupled L-aspartate transporter

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	124.30Å 199.81Å 111.25Å 90.00° 117.08° 90.00°	Depositor
Resolution (Å)	30.00 – 3.80 96.81 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-3.80) 99.5 (96.81-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.45 (at 3.78Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.243 , 0.255 0.239 , 0.256	Depositor DCC
R_{free} test set	1217 reflections (5.41%)	DCC
Wilson B-factor (Å^2)	152.4	Xtriage
Anisotropy	0.529	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 238.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	2 of 23745 reflections (0.008%)	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	9155	wwPDB-VP
Average B, all atoms (Å^2)	247.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% 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: NA, HG

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	0.53	0/3098	0.73	0/4227
1	B	0.66	0/3103	0.80	1/4234 (0.0%)
1	C	0.69	1/3098 (0.0%)	0.84	5/4227 (0.1%)
All	All	0.63	1/9299 (0.0%)	0.79	6/12688 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	136	ASP	CB-CG	5.03	1.62	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	77	ARG	NE-CZ-NH1	-8.81	115.89	120.30
1	C	77	ARG	NE-CZ-NH2	8.31	124.46	120.30
1	C	136	ASP	CB-CG-OD1	6.12	123.81	118.30
1	C	53	LEU	CA-CB-CG	-5.91	101.71	115.30
1	C	56	MET	CB-CG-SD	-5.72	95.25	112.40
1	B	56	MET	CB-CG-SD	-5.28	96.56	112.40

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	3038	0	3204	166	0
1	B	3043	0	3206	171	0
1	C	3038	0	3204	167	0
2	A	9	0	3	2	0
2	B	9	0	3	2	0
2	C	9	0	3	4	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
All	All	9155	0	9623	491	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 26.

All (491) 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:C:335:VAL:HA	1:C:338:GLN:HB2	1.44	0.97
1:A:335:VAL:HA	1:A:338:GLN:HB2	1.48	0.96
1:B:231:VAL:O	1:B:235:VAL:HG23	1.69	0.93
1:C:231:VAL:O	1:C:235:VAL:HG23	1.69	0.92
1:B:335:VAL:HA	1:B:338:GLN:HB2	1.52	0.91
1:B:128:PRO:HB2	1:B:129:PRO:HD2	1.55	0.87
1:A:61:ILE:CG2	1:A:194:MET:HB3	2.05	0.87
1:C:107:PHE:O	1:C:109:PRO:HD3	1.73	0.87
1:C:233:ALA:O	1:C:237:VAL:HG22	1.75	0.85
1:C:139:PRO:HB3	1:C:153:PRO:HB3	1.59	0.85
1:B:233:ALA:O	1:B:237:VAL:HG22	1.78	0.84
1:C:128:PRO:HB2	1:C:129:PRO:HD2	1.58	0.83
1:C:61:ILE:CG2	1:C:194:MET:HB3	2.09	0.82
1:C:334:THR:HG22	1:C:337:GLN:OE1	1.80	0.82
1:C:239:LEU:HD22	1:C:400:VAL:HG21	1.61	0.81
1:A:111:ALA:H	1:A:327:ASN:HB3	1.47	0.80
1:B:61:ILE:CG2	1:B:194:MET:HB3	2.11	0.80
1:A:231:VAL:O	1:A:235:VAL:HG23	1.81	0.80
1:A:107:PHE:O	1:A:109:PRO:HD3	1.82	0.80
1:A:139:PRO:HB3	1:A:153:PRO:HB3	1.62	0.79
1:C:111:ALA:H	1:C:327:ASN:HB3	1.46	0.79
1:A:355:VAL:HG22	1:A:356:PRO:HD2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:355:VAL:HG22	1:C:356:PRO:HD2	1.64	0.79
1:A:128:PRO:HB2	1:A:129:PRO:HD2	1.65	0.78
1:B:139:PRO:HB3	1:B:153:PRO:HB3	1.66	0.78
1:B:355:VAL:HG22	1:B:356:PRO:HD2	1.65	0.78
1:C:242:GLN:O	1:C:246:VAL:HB	1.84	0.77
1:B:107:PHE:O	1:B:109:PRO:HD3	1.83	0.77
1:C:155:ILE:HD11	1:C:365:MET:HG3	1.67	0.76
1:A:55:LYS:O	1:A:58:VAL:HG12	1.84	0.76
1:B:55:LYS:O	1:B:58:VAL:HG12	1.85	0.76
1:B:111:ALA:H	1:B:327:ASN:HB3	1.50	0.76
1:A:299:TYR:HB2	1:A:303:LEU:HD23	1.68	0.75
1:B:334:THR:HG22	1:B:337:GLN:OE1	1.85	0.75
1:A:157:PHE:HA	1:A:160:ILE:HG22	1.67	0.75
1:C:203:GLN:HE21	1:C:203:GLN:HA	1.52	0.75
1:A:169:MET:HA	1:A:177:ARG:HG3	1.68	0.75
1:B:128:PRO:CB	1:B:129:PRO:HD2	2.17	0.75
1:A:233:ALA:O	1:A:237:VAL:HG22	1.87	0.74
1:B:157:PHE:HA	1:B:160:ILE:HG22	1.68	0.74
1:A:326:ALA:HB2	1:A:333:LEU:HD13	1.69	0.74
1:C:326:ALA:HB2	1:C:333:LEU:HD13	1.68	0.74
1:B:165:ILE:HG21	1:B:184:LEU:HB2	1.70	0.74
1:C:345:ALA:HA	1:C:348:ALA:HB3	1.69	0.74
1:B:299:TYR:HB2	1:B:303:LEU:HD23	1.70	0.73
1:B:203:GLN:HA	1:B:203:GLN:HE21	1.53	0.73
1:C:299:TYR:HB2	1:C:303:LEU:HD23	1.70	0.73
1:C:128:PRO:CB	1:C:129:PRO:HD2	2.17	0.73
1:C:61:ILE:HG22	1:C:194:MET:HB3	1.70	0.73
1:B:284:VAL:HG13	1:B:287:ARG:HH21	1.53	0.72
1:C:157:PHE:HA	1:C:160:ILE:HG22	1.70	0.72
1:A:334:THR:HG22	1:A:337:GLN:OE1	1.89	0.72
1:C:123:GLN:HA	1:C:123:GLN:OE1	1.89	0.72
1:B:326:ALA:HB2	1:B:333:LEU:HD13	1.70	0.71
1:B:88:TYR:CZ	1:B:92:THR:HG21	2.25	0.71
1:A:61:ILE:HG22	1:A:194:MET:HB3	1.73	0.71
1:A:128:PRO:CB	1:A:129:PRO:HD2	2.21	0.70
1:B:113:ILE:HD11	1:B:224:VAL:HG23	1.73	0.70
1:A:203:GLN:HE21	1:A:203:GLN:HA	1.56	0.69
1:B:193:ALA:HB2	1:C:168:LEU:HD11	1.74	0.69
1:C:88:TYR:CZ	1:C:92:THR:HG21	2.28	0.69
1:A:61:ILE:HG22	1:A:194:MET:CB	2.23	0.69
1:C:15:LYS:O	1:C:18:ILE:HG22	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:GLN:OE1	1:B:123:GLN:HA	1.94	0.68
1:C:113:ILE:HD11	1:C:224:VAL:HG23	1.75	0.68
1:B:15:LYS:O	1:B:18:ILE:HG22	1.92	0.68
1:C:55:LYS:O	1:C:58:VAL:HG12	1.92	0.68
1:B:242:GLN:O	1:B:246:VAL:HB	1.94	0.68
1:A:88:TYR:CZ	1:A:92:THR:HG21	2.29	0.68
1:B:126:GLN:O	1:B:126:GLN:HG2	1.93	0.68
1:A:284:VAL:HG13	1:A:287:ARG:HH21	1.58	0.67
1:C:126:GLN:HG2	1:C:126:GLN:O	1.95	0.67
1:C:169:MET:HA	1:C:177:ARG:HG3	1.76	0.67
1:A:15:LYS:O	1:A:18:ILE:HG22	1.95	0.67
1:C:284:VAL:HG13	1:C:287:ARG:HH21	1.60	0.67
1:A:113:ILE:HD11	1:A:224:VAL:HG23	1.77	0.67
1:A:54:LEU:HD12	1:A:201:VAL:HG11	1.76	0.67
1:A:67:VAL:HG11	1:A:187:ILE:HD12	1.78	0.66
1:B:134:LEU:O	1:B:137:ILE:HG12	1.97	0.65
1:A:334:THR:O	1:A:337:GLN:HG2	1.96	0.65
1:B:345:ALA:HA	1:B:348:ALA:HB3	1.77	0.65
1:B:13:LEU:HD23	1:B:276:ARG:HD3	1.79	0.65
1:A:168:LEU:HD11	1:C:193:ALA:HB2	1.79	0.65
1:A:35:TYR:N	1:A:35:TYR:CD2	2.65	0.65
1:B:344:THR:HB	1:B:366:VAL:HG23	1.80	0.64
1:A:345:ALA:HA	1:A:348:ALA:HB3	1.80	0.64
1:B:61:ILE:HG22	1:B:194:MET:HB3	1.79	0.64
1:C:61:ILE:HG22	1:C:194:MET:CB	2.27	0.64
1:B:371:GLY:O	1:B:373:PRO:HD3	1.98	0.64
1:C:35:TYR:N	1:C:35:TYR:CD2	2.65	0.64
1:B:205:ALA:N	1:B:206:PRO:HD2	2.13	0.64
1:A:123:GLN:HA	1:A:123:GLN:OE1	1.96	0.64
1:A:111:ALA:N	1:A:327:ASN:HB3	2.12	0.63
1:A:217:MET:SD	1:A:225:VAL:HG22	2.37	0.63
1:B:186:ALA:O	1:B:188:ASN:O	2.17	0.63
1:A:242:GLN:O	1:A:246:VAL:HB	1.98	0.63
1:C:344:THR:HB	1:C:366:VAL:HG23	1.81	0.63
1:C:111:ALA:N	1:C:327:ASN:HB3	2.11	0.63
1:B:35:TYR:CD2	1:B:35:TYR:N	2.66	0.63
1:B:169:MET:HA	1:B:177:ARG:HG3	1.79	0.63
1:C:83:VAL:O	1:C:87:VAL:HG23	1.98	0.63
1:C:334:THR:O	1:C:337:GLN:HG2	1.99	0.63
1:A:13:LEU:HD23	1:A:276:ARG:HD3	1.81	0.63
1:A:61:ILE:HG21	1:A:194:MET:HB3	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:ALA:N	1:B:327:ASN:HB3	2.14	0.62
1:C:250:LEU:O	1:C:253:ILE:HG22	1.98	0.62
1:B:250:LEU:O	1:B:253:ILE:HG22	1.99	0.62
1:B:217:MET:SD	1:B:225:VAL:HG22	2.39	0.62
1:B:278:SER:HB2	2:B:901:ASP:O	1.99	0.62
1:A:344:THR:HB	1:A:366:VAL:HG23	1.82	0.62
1:C:13:LEU:HD23	1:C:276:ARG:HD3	1.80	0.62
1:B:129:PRO:CG	1:B:132:HIS:HD2	2.12	0.61
1:C:67:VAL:HG11	1:C:187:ILE:HD12	1.81	0.61
1:A:186:ALA:O	1:A:188:ASN:O	2.19	0.61
1:A:24:ALA:HA	1:A:217:MET:HG3	1.81	0.61
1:B:54:LEU:HD12	1:B:201:VAL:HG11	1.83	0.61
1:B:364:ALA:O	1:B:368:HIS:HB2	2.01	0.60
1:A:250:LEU:O	1:A:253:ILE:HG22	2.01	0.60
1:A:35:TYR:N	1:A:35:TYR:HD2	1.98	0.60
1:C:30:LEU:HD23	1:C:34:GLY:HA3	1.83	0.60
1:C:54:LEU:HD12	1:C:201:VAL:HG11	1.82	0.60
1:C:103:MET:HG3	1:C:238:GLY:HA3	1.83	0.60
1:B:61:ILE:HG22	1:B:194:MET:CB	2.32	0.60
1:C:203:GLN:NE2	1:C:203:GLN:HA	2.17	0.60
1:A:83:VAL:O	1:A:87:VAL:HG23	2.02	0.60
1:B:129:PRO:HG2	1:B:132:HIS:HD2	1.67	0.59
1:C:217:MET:SD	1:C:225:VAL:HG22	2.42	0.59
1:A:143:PHE:CE2	1:C:146:LEU:HD23	2.38	0.59
1:B:24:ALA:HA	1:B:217:MET:HG3	1.85	0.59
1:C:165:ILE:HG21	1:C:184:LEU:HB2	1.84	0.59
1:A:103:MET:HG3	1:A:238:GLY:HA3	1.84	0.59
1:C:165:ILE:HG21	1:C:184:LEU:HD13	1.84	0.59
1:B:37:HIS:HA	1:B:40:HIS:HB3	1.85	0.59
1:C:37:HIS:HA	1:C:40:HIS:HB3	1.83	0.59
1:A:239:LEU:HD22	1:A:400:VAL:HG21	1.84	0.59
1:B:54:LEU:CD1	1:B:201:VAL:HG11	2.33	0.59
1:A:165:ILE:HG21	1:A:184:LEU:HB2	1.84	0.58
1:C:61:ILE:HG21	1:C:194:MET:HB3	1.85	0.58
1:B:155:ILE:HD11	1:B:365:MET:HG3	1.84	0.58
1:B:35:TYR:N	1:B:35:TYR:HD2	2.00	0.58
1:B:129:PRO:HG2	1:B:132:HIS:CD2	2.38	0.58
1:C:24:ALA:HA	1:C:217:MET:HG3	1.86	0.58
1:B:277:SER:N	1:B:398:THR:HG21	2.19	0.58
1:C:54:LEU:CD1	1:C:201:VAL:HG11	2.34	0.58
1:B:146:LEU:HD23	1:C:143:PHE:CE2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:371:GLY:O	1:C:373:PRO:HD3	2.03	0.58
1:B:130:LEU:HA	1:B:133:ILE:HG22	1.86	0.57
1:C:335:VAL:HA	1:C:338:GLN:CB	2.29	0.57
1:B:334:THR:O	1:B:337:GLN:HG2	2.05	0.57
1:C:130:LEU:HA	1:C:133:ILE:CG2	2.34	0.57
1:B:334:THR:HG23	1:B:335:VAL:O	2.05	0.57
1:A:82:GLY:HA2	1:A:85:ILE:HG22	1.86	0.57
1:C:73:ILE:O	1:C:78:LEU:HD22	2.05	0.57
1:A:155:ILE:HD11	1:A:365:MET:HG3	1.87	0.57
1:A:58:VAL:O	1:A:62:VAL:HG23	2.05	0.57
1:B:183:LEU:HD21	1:B:187:ILE:HD11	1.87	0.57
1:B:82:GLY:HA2	1:B:85:ILE:HG22	1.86	0.56
1:C:35:TYR:N	1:C:35:TYR:HD2	2.01	0.56
1:C:271:THR:HG21	1:C:284:VAL:HG21	1.86	0.56
1:C:183:LEU:HD21	1:C:187:ILE:HD11	1.87	0.56
1:B:83:VAL:O	1:B:87:VAL:HG23	2.05	0.56
1:B:341:ILE:HG13	1:B:370:VAL:HG21	1.88	0.56
1:B:183:LEU:HD23	1:B:187:ILE:HG13	1.87	0.56
1:A:37:HIS:HA	1:A:40:HIS:HB3	1.87	0.56
1:C:130:LEU:HA	1:C:133:ILE:HG22	1.88	0.56
1:A:193:ALA:HB2	1:B:168:LEU:HD11	1.87	0.56
1:B:6:LYS:O	1:B:8:ILE:N	2.40	0.55
1:A:64:ALA:HB2	1:A:190:LEU:HD23	1.88	0.55
1:B:227:GLU:O	1:B:231:VAL:HG23	2.06	0.55
1:B:103:MET:HG3	1:B:238:GLY:HA3	1.89	0.55
1:C:216:CYS:O	1:C:220:GLN:HB2	2.07	0.55
1:B:67:VAL:HG11	1:B:187:ILE:HD12	1.88	0.55
1:A:371:GLY:O	1:A:373:PRO:HD3	2.07	0.55
1:A:44:LYS:N	1:A:45:PRO:HD2	2.21	0.55
1:C:186:ALA:O	1:C:188:ASN:O	2.25	0.55
1:A:54:LEU:CD1	1:A:201:VAL:HG11	2.35	0.55
1:B:61:ILE:HG21	1:B:194:MET:HB3	1.85	0.55
1:A:139:PRO:CB	1:A:153:PRO:HB3	2.36	0.55
1:C:178:LYS:HD3	1:C:178:LYS:O	2.06	0.55
1:A:30:LEU:HD23	1:A:34:GLY:HA3	1.89	0.54
1:B:271:THR:HG21	1:B:284:VAL:HG21	1.89	0.54
1:C:397:ARG:NH1	2:C:901:ASP:OD1	2.40	0.54
1:A:278:SER:HB2	2:A:901:ASP:O	2.08	0.54
1:C:341:ILE:HG13	1:C:370:VAL:HG21	1.90	0.53
1:B:30:LEU:HD23	1:B:34:GLY:HA3	1.89	0.53
1:A:126:GLN:O	1:A:126:GLN:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:LYS:N	1:B:45:PRO:HD2	2.23	0.53
1:A:104:ALA:HB2	1:A:320:VAL:HG13	1.90	0.53
1:C:227:GLU:O	1:C:231:VAL:HG23	2.07	0.53
1:C:237:VAL:O	1:C:241:LEU:HB2	2.09	0.53
1:B:52:ARG:HH12	1:C:136:ASP:HA	1.73	0.53
1:C:44:LYS:N	1:C:45:PRO:HD2	2.22	0.53
1:B:397:ARG:NH1	2:B:901:ASP:OD1	2.42	0.53
1:A:237:VAL:O	1:A:241:LEU:HB2	2.08	0.53
1:B:296:GLU:HA	1:B:299:TYR:CE1	2.44	0.53
1:A:271:THR:HG21	1:A:284:VAL:HG21	1.91	0.53
1:B:130:LEU:HA	1:B:133:ILE:CG2	2.39	0.52
1:A:129:PRO:HG2	1:A:132:HIS:CD2	2.45	0.52
1:C:243:ILE:HA	1:C:247:TYR:CD2	2.45	0.52
1:B:353:ALA:HB3	1:B:358:ALA:HB2	1.92	0.52
1:C:353:ALA:HB3	1:C:358:ALA:HB2	1.90	0.52
1:A:155:ILE:O	1:A:158:ALA:N	2.39	0.52
1:B:193:ALA:CB	1:C:168:LEU:HD11	2.39	0.52
1:B:6:LYS:C	1:B:8:ILE:H	2.13	0.52
1:C:277:SER:N	1:C:398:THR:HG21	2.24	0.52
1:C:343:LEU:C	1:C:343:LEU:HD13	2.30	0.52
1:C:334:THR:HG23	1:C:335:VAL:O	2.09	0.52
1:C:296:GLU:HA	1:C:299:TYR:CE1	2.44	0.52
1:A:130:LEU:HA	1:A:133:ILE:CG2	2.40	0.52
1:A:397:ARG:NH1	2:A:901:ASP:OD1	2.42	0.52
1:C:364:ALA:O	1:C:368:HIS:HB2	2.10	0.52
1:A:129:PRO:HG2	1:A:132:HIS:HD2	1.75	0.52
1:A:130:LEU:HA	1:A:133:ILE:HG22	1.91	0.52
1:B:333:LEU:HD12	1:B:337:GLN:HE21	1.75	0.52
1:C:77:ARG:HG2	1:C:166:THR:HB	1.92	0.51
1:A:183:LEU:HD23	1:A:187:ILE:HG13	1.91	0.51
1:B:277:SER:H	1:B:398:THR:HG21	1.73	0.51
1:A:98:THR:O	1:A:102:ILE:HG13	2.11	0.51
1:C:129:PRO:CG	1:C:132:HIS:HD2	2.24	0.51
1:A:205:ALA:N	1:A:206:PRO:HD2	2.26	0.51
1:B:216:CYS:O	1:B:224:VAL:HG11	2.10	0.51
1:B:24:ALA:O	1:B:28:LEU:HD22	2.11	0.51
1:A:17:LEU:HD22	1:A:392:ILE:HD11	1.92	0.51
1:A:243:ILE:HA	1:A:247:TYR:CD2	2.46	0.51
1:B:74:SER:O	1:B:77:ARG:CB	2.58	0.51
1:A:296:GLU:HA	1:A:299:TYR:CE1	2.46	0.51
1:B:294:ILE:CG2	1:B:299:TYR:HB3	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:ALA:O	1:C:28:LEU:HD22	2.11	0.51
1:A:129:PRO:CG	1:A:132:HIS:HD2	2.23	0.51
1:B:73:ILE:O	1:B:78:LEU:HD22	2.11	0.51
1:C:205:ALA:N	1:C:206:PRO:HD2	2.26	0.51
1:B:243:ILE:HA	1:B:247:TYR:HD2	1.76	0.51
1:A:77:ARG:HG2	1:A:166:THR:HB	1.91	0.50
1:A:216:CYS:O	1:A:224:VAL:HG11	2.11	0.50
1:A:197:ILE:O	1:A:201:VAL:HG23	2.10	0.50
1:A:183:LEU:HD21	1:A:187:ILE:HD11	1.93	0.50
1:A:334:THR:O	1:A:338:GLN:N	2.43	0.50
1:C:243:ILE:HA	1:C:247:TYR:HD2	1.75	0.50
1:B:104:ALA:HB2	1:B:320:VAL:HG13	1.94	0.50
1:A:341:ILE:HG13	1:A:370:VAL:HG21	1.94	0.50
1:A:364:ALA:O	1:A:368:HIS:HB2	2.11	0.50
1:B:239:LEU:HD22	1:B:400:VAL:HG21	1.93	0.50
1:A:179:SER:O	1:A:181:GLU:N	2.45	0.50
1:C:294:ILE:CG2	1:C:299:TYR:HB3	2.41	0.50
1:B:243:ILE:HA	1:B:247:TYR:CD2	2.46	0.50
1:A:265:ALA:HA	1:A:288:VAL:HG11	1.94	0.50
1:C:73:ILE:O	1:C:74:SER:C	2.51	0.49
1:C:334:THR:O	1:C:338:GLN:N	2.45	0.49
1:C:287:ARG:HG2	1:C:291:GLU:OE2	2.11	0.49
1:C:54:LEU:N	1:C:54:LEU:HD12	2.27	0.49
1:C:394:ASP:O	1:C:398:THR:OG1	2.26	0.49
1:B:343:LEU:C	1:B:343:LEU:HD13	2.32	0.49
1:B:216:CYS:O	1:B:220:GLN:HB2	2.13	0.49
1:B:8:ILE:HG12	1:B:15:LYS:HE3	1.93	0.49
1:C:77:ARG:HD3	1:C:77:ARG:O	2.12	0.49
1:B:77:ARG:HG2	1:B:166:THR:HB	1.94	0.49
1:B:139:PRO:CB	1:B:153:PRO:HB3	2.39	0.49
1:A:243:ILE:HA	1:A:247:TYR:HD2	1.76	0.49
1:A:227:GLU:O	1:A:231:VAL:HG23	2.11	0.49
1:A:157:PHE:HA	1:A:160:ILE:CG2	2.38	0.49
1:A:355:VAL:HG13	1:A:356:PRO:N	2.28	0.49
1:A:294:ILE:CG2	1:A:299:TYR:HB3	2.43	0.49
1:C:228:LEU:HD22	1:C:389:ILE:CG2	2.42	0.49
1:A:52:ARG:NH1	1:B:136:ASP:HA	2.28	0.49
1:B:203:GLN:HA	1:B:203:GLN:NE2	2.24	0.49
1:C:166:THR:HA	1:C:169:MET:CE	2.43	0.49
1:A:185:ASP:O	1:A:188:ASN:O	2.31	0.49
1:C:278:SER:HB2	2:C:901:ASP:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:ASP:O	1:C:379:VAL:N	2.46	0.49
1:A:74:SER:O	1:A:77:ARG:CB	2.60	0.49
1:A:73:ILE:O	1:A:78:LEU:HD22	2.13	0.49
1:C:183:LEU:HD23	1:C:187:ILE:HG13	1.94	0.49
1:A:203:GLN:NE2	1:A:203:GLN:HA	2.24	0.48
1:B:155:ILE:O	1:B:159:ILE:HD12	2.13	0.48
1:C:82:GLY:HA2	1:C:85:ILE:HG22	1.94	0.48
1:C:74:SER:OG	1:C:166:THR:HG21	2.13	0.48
1:C:239:LEU:HD22	1:C:400:VAL:CG2	2.39	0.48
1:A:134:LEU:O	1:A:137:ILE:HG12	2.12	0.48
1:C:277:SER:H	1:C:398:THR:HG21	1.79	0.48
1:B:20:LEU:HA	1:B:213:ILE:HD11	1.95	0.48
1:A:146:LEU:HD12	1:A:146:LEU:H	1.79	0.48
1:A:334:THR:HG23	1:A:335:VAL:O	2.14	0.48
1:B:237:VAL:O	1:B:241:LEU:HB2	2.13	0.48
1:C:187:ILE:O	1:C:190:LEU:HB3	2.13	0.48
1:B:325:ILE:HG13	1:B:367:LEU:HD21	1.95	0.48
1:A:343:LEU:C	1:A:343:LEU:HD13	2.34	0.48
1:C:216:CYS:O	1:C:224:VAL:HG11	2.14	0.48
1:C:103:MET:CE	1:C:237:VAL:HG23	2.44	0.47
1:A:216:CYS:O	1:A:220:GLN:HB2	2.14	0.47
1:C:341:ILE:CG1	1:C:370:VAL:HG21	2.44	0.47
1:B:52:ARG:NH1	1:C:136:ASP:HA	2.30	0.47
1:C:129:PRO:HG2	1:C:132:HIS:HD2	1.79	0.47
1:B:131:VAL:O	1:B:135:LEU:HB2	2.14	0.47
1:B:146:LEU:N	1:B:146:LEU:HD12	2.29	0.47
1:B:98:THR:O	1:B:102:ILE:HG13	2.15	0.47
1:C:343:LEU:O	1:C:343:LEU:HD13	2.14	0.47
1:A:139:PRO:HB3	1:A:153:PRO:CB	2.39	0.47
1:C:74:SER:O	1:C:77:ARG:CB	2.63	0.47
1:B:344:THR:HG21	1:B:369:SER:OG	2.15	0.47
1:A:165:ILE:HG21	1:A:184:LEU:HD13	1.96	0.47
1:B:334:THR:O	1:B:338:GLN:N	2.48	0.47
1:C:196:LYS:HA	1:C:196:LYS:HD3	1.67	0.47
1:B:311:MET:HB3	1:B:401:ASN:CG	2.35	0.47
1:A:353:ALA:HB3	1:A:358:ALA:HB2	1.96	0.47
1:A:322:THR:HG21	1:A:341:ILE:HG12	1.95	0.47
1:C:157:PHE:HA	1:C:160:ILE:CG2	2.43	0.47
1:A:8:ILE:HG12	1:A:15:LYS:HE3	1.97	0.47
1:C:276:ARG:HG2	1:C:395:MET:HG2	1.96	0.47
1:A:352:THR:HA	1:A:362:MET:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:MET:HB3	1:C:401:ASN:CG	2.35	0.47
1:A:187:ILE:O	1:A:190:LEU:HB3	2.15	0.47
1:B:97:VAL:HG13	1:B:342:VAL:HG22	1.96	0.47
1:B:165:ILE:CG2	1:B:184:LEU:HB2	2.41	0.46
1:A:277:SER:N	1:A:398:THR:HG21	2.30	0.46
1:B:146:LEU:H	1:B:146:LEU:HD12	1.80	0.46
1:A:20:LEU:HA	1:A:213:ILE:HD11	1.98	0.46
1:A:207:ILE:O	1:A:210:PHE:HB3	2.16	0.46
1:C:129:PRO:HG2	1:C:132:HIS:CD2	2.50	0.46
1:A:190:LEU:O	1:A:191:ALA:C	2.53	0.46
1:A:196:LYS:HD3	1:A:196:LYS:HA	1.70	0.46
1:C:132:HIS:O	1:C:136:ASP:HB2	2.16	0.46
1:C:58:VAL:O	1:C:62:VAL:HG23	2.15	0.46
1:C:271:THR:HB	1:C:281:THR:HG23	1.96	0.46
1:C:57:LEU:HD12	1:C:361:ILE:CD1	2.45	0.46
1:B:64:ALA:HB2	1:B:190:LEU:HD23	1.96	0.46
1:A:146:LEU:HD23	1:B:143:PHE:CE2	2.50	0.46
1:C:335:VAL:CA	1:C:338:GLN:HB2	2.31	0.46
1:B:355:VAL:HG13	1:B:356:PRO:N	2.29	0.46
1:C:104:ALA:HB2	1:C:320:VAL:HG13	1.97	0.46
1:B:128:PRO:HB2	1:B:129:PRO:CD	2.36	0.46
1:C:251:LEU:HD22	1:C:256:ILE:CG2	2.46	0.46
1:C:139:PRO:CB	1:C:153:PRO:HB3	2.39	0.46
1:B:77:ARG:O	1:B:77:ARG:HD3	2.15	0.46
1:B:178:LYS:O	1:B:178:LYS:HD3	2.16	0.46
1:C:352:THR:HA	1:C:362:MET:HG3	1.98	0.46
1:C:295:SER:HB3	1:C:298:ILE:HD13	1.98	0.46
1:B:113:ILE:O	1:B:113:ILE:HG23	2.16	0.45
1:A:24:ALA:O	1:A:28:LEU:HD22	2.17	0.45
1:B:17:LEU:HD22	1:B:392:ILE:HD11	1.98	0.45
1:C:8:ILE:HG12	1:C:15:LYS:HE3	1.97	0.45
1:B:117:VAL:C	1:B:119:GLY:H	2.20	0.45
1:C:282:LEU:H	1:C:283:PRO:CD	2.30	0.45
1:A:341:ILE:CG1	1:A:370:VAL:HG21	2.46	0.45
1:B:376:ASP:O	1:B:379:VAL:N	2.50	0.45
1:C:207:ILE:O	1:C:210:PHE:HB3	2.17	0.45
1:B:341:ILE:CG1	1:B:370:VAL:HG21	2.47	0.45
1:A:74:SER:OG	1:A:166:THR:HG21	2.17	0.45
1:B:215:TYR:HA	1:B:218:ALA:HB3	1.97	0.45
1:A:344:THR:HG21	1:A:369:SER:OG	2.17	0.45
1:A:295:SER:HB3	1:A:298:ILE:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:LEU:O	1:C:137:ILE:HG12	2.17	0.45
1:C:113:ILE:HG23	1:C:113:ILE:O	2.15	0.45
1:C:183:LEU:CD2	1:C:187:ILE:HD11	2.46	0.45
1:A:333:LEU:HD11	1:A:370:VAL:HG11	1.99	0.45
1:A:132:HIS:O	1:A:136:ASP:HB2	2.17	0.45
1:B:265:ALA:HA	1:B:288:VAL:HG11	1.97	0.45
1:C:161:LEU:O	1:C:165:ILE:HG12	2.17	0.44
1:B:352:THR:HA	1:B:362:MET:HG3	1.98	0.44
1:A:213:ILE:C	1:A:215:TYR:H	2.21	0.44
1:C:195:TYR:O	1:C:198:VAL:HB	2.17	0.44
1:A:57:LEU:HD12	1:A:361:ILE:CD1	2.47	0.44
1:C:376:ASP:HA	1:C:377:PRO:HD2	1.75	0.44
1:A:146:LEU:HD12	1:A:146:LEU:N	2.32	0.44
1:A:259:ILE:H	1:A:259:ILE:HG13	1.58	0.44
1:B:318:GLN:HB3	1:B:366:VAL:HG11	1.99	0.44
1:B:190:LEU:O	1:B:191:ALA:C	2.55	0.44
1:B:196:LYS:HD3	1:B:196:LYS:HA	1.61	0.44
1:B:157:PHE:HA	1:B:160:ILE:CG2	2.42	0.44
1:B:135:LEU:C	1:B:137:ILE:H	2.21	0.44
1:A:156:PHE:O	1:A:160:ILE:HG22	2.17	0.44
1:B:282:LEU:HB3	1:B:283:PRO:HD3	1.99	0.44
1:A:127:ALA:HA	1:A:128:PRO:HD3	1.89	0.44
1:A:52:ARG:HH12	1:B:136:ASP:HA	1.82	0.44
1:A:117:VAL:C	1:A:119:GLY:H	2.22	0.43
1:B:295:SER:HB3	1:B:298:ILE:HD13	1.99	0.43
1:C:155:ILE:O	1:C:156:PHE:C	2.57	0.43
1:A:109:PRO:O	1:A:324:PHE:HA	2.18	0.43
1:B:342:VAL:HG12	1:B:343:LEU:N	2.33	0.43
1:B:282:LEU:H	1:B:283:PRO:CD	2.31	0.43
1:A:272:ALA:HB1	1:A:399:MET:HA	1.99	0.43
1:A:246:VAL:O	1:A:250:LEU:HG	2.18	0.43
1:B:74:SER:OG	1:B:166:THR:HG21	2.18	0.43
1:A:166:THR:HA	1:A:169:MET:CE	2.48	0.43
1:C:213:ILE:C	1:C:215:TYR:H	2.21	0.43
1:C:190:LEU:O	1:C:191:ALA:C	2.56	0.43
1:A:333:LEU:HD21	1:A:341:ILE:HD11	1.99	0.43
1:C:20:LEU:HA	1:C:213:ILE:HD11	2.00	0.43
1:B:8:ILE:C	1:B:9:GLU:HG3	2.39	0.43
1:B:17:LEU:CD2	1:B:392:ILE:HD11	2.49	0.43
1:A:195:TYR:O	1:A:198:VAL:HB	2.19	0.43
1:B:165:ILE:HG21	1:B:184:LEU:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:ALA:O	1:C:281:THR:HG21	2.19	0.43
1:A:168:LEU:HD11	1:C:193:ALA:CB	2.48	0.43
1:C:17:LEU:HD22	1:C:392:ILE:HD11	2.00	0.43
1:A:333:LEU:HD12	1:A:337:GLN:HE21	1.84	0.43
1:A:8:ILE:C	1:A:9:GLU:HG3	2.38	0.43
1:B:197:ILE:O	1:B:201:VAL:HG23	2.19	0.43
1:A:107:PHE:C	1:A:109:PRO:HD3	2.38	0.43
1:C:9:GLU:HA	1:C:15:LYS:HZ1	1.84	0.43
1:C:164:ALA:O	1:C:165:ILE:C	2.55	0.43
1:B:187:ILE:O	1:B:190:LEU:HB3	2.19	0.43
1:B:44:LYS:HD2	1:B:215:TYR:CZ	2.53	0.43
1:B:311:MET:HB3	1:B:401:ASN:OD1	2.19	0.43
1:A:325:ILE:HG13	1:A:367:LEU:HD21	2.00	0.43
1:B:294:ILE:HG22	1:B:299:TYR:HB3	2.01	0.42
1:B:246:VAL:O	1:B:250:LEU:HG	2.19	0.42
1:A:276:ARG:HG2	1:A:395:MET:HG2	2.01	0.42
1:B:155:ILE:O	1:B:156:PHE:C	2.58	0.42
1:C:131:VAL:O	1:C:135:LEU:HB2	2.19	0.42
1:B:54:LEU:HD12	1:B:54:LEU:N	2.33	0.42
1:C:101:ILE:O	1:C:105:ARG:HG2	2.19	0.42
1:C:294:ILE:HG22	1:C:299:TYR:HB3	2.00	0.42
1:A:376:ASP:HA	1:A:377:PRO:HD2	1.72	0.42
1:B:57:LEU:O	1:B:61:ILE:HG12	2.19	0.42
1:B:294:ILE:HG21	1:B:299:TYR:HB3	2.00	0.42
1:B:271:THR:HB	1:B:281:THR:HG23	2.01	0.42
1:B:13:LEU:HB2	1:B:276:ARG:HE	1.85	0.42
1:A:165:ILE:CG2	1:A:184:LEU:HB2	2.50	0.42
1:A:103:MET:HG3	1:A:238:GLY:CA	2.48	0.42
1:B:123:GLN:OE1	1:B:123:GLN:CA	2.66	0.42
1:C:401:ASN:ND2	2:C:901:ASP:HA	2.34	0.42
1:C:90:LEU:HD11	1:C:350:ILE:HD11	2.02	0.42
1:B:53:LEU:HA	1:B:53:LEU:HD23	1.90	0.42
1:B:333:LEU:HD21	1:B:341:ILE:HD11	2.02	0.42
1:C:107:PHE:C	1:C:109:PRO:HD3	2.37	0.42
1:C:166:THR:HA	1:C:169:MET:HE2	2.01	0.42
1:C:39:VAL:HG13	1:C:43:VAL:HG12	2.01	0.42
1:B:66:LEU:HA	1:B:66:LEU:HD23	1.66	0.42
1:A:294:ILE:HG22	1:A:299:TYR:HB3	2.01	0.42
1:B:13:LEU:CD2	1:B:276:ARG:HD3	2.47	0.42
1:C:336:GLY:O	1:C:339:LEU:N	2.52	0.42
1:A:20:LEU:HD12	1:A:213:ILE:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:PRO:CB	1:B:129:PRO:CD	2.93	0.41
1:A:152:LEU:O	1:A:153:PRO:C	2.58	0.41
1:C:352:THR:HG23	1:C:358:ALA:HB1	2.02	0.41
1:B:58:VAL:O	1:B:62:VAL:HG23	2.20	0.41
1:C:228:LEU:HD22	1:C:389:ILE:HG21	2.01	0.41
1:A:32:HIS:HB3	1:A:33:TYR:H	1.65	0.41
1:B:343:LEU:O	1:B:343:LEU:HD13	2.20	0.41
1:C:103:MET:HG3	1:C:238:GLY:CA	2.51	0.41
1:B:58:VAL:HG21	1:B:364:ALA:HB3	2.03	0.41
1:A:257:ASP:HA	1:A:258:PRO:HD3	1.83	0.41
1:B:103:MET:CE	1:B:237:VAL:HG23	2.50	0.41
1:B:107:PHE:C	1:B:109:PRO:HD3	2.39	0.41
1:B:110:GLY:O	1:B:111:ALA:C	2.58	0.41
1:B:342:VAL:CG1	1:B:343:LEU:N	2.83	0.41
1:A:343:LEU:HD13	1:A:343:LEU:O	2.20	0.41
1:A:311:MET:HB3	1:A:401:ASN:CG	2.41	0.41
1:A:152:LEU:O	1:A:155:ILE:HB	2.21	0.41
1:C:213:ILE:HG22	1:C:216:CYS:HB2	2.03	0.41
1:A:164:ALA:O	1:A:165:ILE:C	2.57	0.41
1:A:282:LEU:HB3	1:A:283:PRO:HD3	2.02	0.41
1:C:305:LEU:HG	1:C:305:LEU:O	2.20	0.41
1:A:77:ARG:O	1:A:77:ARG:HD3	2.19	0.41
1:C:294:ILE:HG21	1:C:299:TYR:HB3	2.02	0.41
1:C:130:LEU:HD12	1:C:133:ILE:HG23	2.02	0.41
1:A:228:LEU:HD22	1:A:389:ILE:CG2	2.51	0.41
1:C:21:ILE:O	1:C:25:ILE:HD13	2.21	0.41
1:A:73:ILE:O	1:A:74:SER:C	2.58	0.41
1:B:192:GLU:HG2	1:C:176:VAL:HG13	2.02	0.41
1:A:157:PHE:CA	1:A:160:ILE:HG22	2.44	0.41
1:A:103:MET:CE	1:A:237:VAL:HG23	2.51	0.41
1:A:318:GLN:HB3	1:A:366:VAL:HG11	2.02	0.41
1:A:277:SER:H	1:A:398:THR:HG21	1.86	0.41
1:B:391:ALA:O	1:B:395:MET:HG3	2.21	0.41
1:B:183:LEU:HD23	1:B:183:LEU:C	2.42	0.41
1:C:128:PRO:HB2	1:C:129:PRO:CD	2.39	0.40
1:C:344:THR:HG21	1:C:369:SER:OG	2.21	0.40
1:B:362:MET:O	1:B:365:MET:HB3	2.21	0.40
1:B:190:LEU:HA	1:B:190:LEU:HD12	1.89	0.40
1:C:359:GLY:H	2:C:901:ASP:CG	2.25	0.40
1:A:17:LEU:CD2	1:A:392:ILE:HD11	2.50	0.40
1:A:303:LEU:HD13	1:A:303:LEU:HA	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:TYR:HA	1:C:218:ALA:HB3	2.03	0.40
1:B:177:ARG:HH11	1:B:177:ARG:HD2	1.77	0.40
1:B:73:ILE:O	1:B:74:SER:C	2.59	0.40
1:B:325:ILE:HG23	1:B:382:ALA:HB3	2.03	0.40
1:A:39:VAL:HG13	1:A:43:VAL:HG12	2.04	0.40
1:B:222:VAL:O	1:B:225:VAL:HG23	2.21	0.40
1:A:131:VAL:O	1:A:135:LEU:HB2	2.22	0.40
1:C:333:LEU:HD12	1:C:337:GLN:HE21	1.86	0.40
1:A:137:ILE:HA	1:A:153:PRO:HG3	2.04	0.40
1:C:355:VAL:HG13	1:C:356:PRO:N	2.36	0.40
1:B:155:ILE:HG23	1:B:159:ILE:CD1	2.52	0.40
1:A:179:SER:O	1:A:180:ALA:C	2.60	0.40
1:A:110:GLY:O	1:A:111:ALA:C	2.59	0.40
1:C:155:ILE:O	1:C:159:ILE:HD12	2.22	0.40
1:C:24:ALA:O	1:C:28:LEU:CD2	2.69	0.40
1:A:215:TYR:HA	1:A:218:ALA:HB3	2.02	0.40
1:C:90:LEU:CD1	1:C:350:ILE:HD11	2.51	0.40
1:C:257:ASP:HA	1:C:258:PRO:HD3	1.82	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	408/422 (97%)	329 (81%)	66 (16%)	13 (3%)	5 44
1	B	409/422 (97%)	328 (80%)	67 (16%)	14 (3%)	5 43
1	C	408/422 (97%)	322 (79%)	70 (17%)	16 (4%)	4 38
All	All	1225/1266 (97%)	979 (80%)	203 (17%)	43 (4%)	4 42

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	356	PRO
1	B	356	PRO
1	C	356	PRO
1	B	7	TYR
1	B	310	ASN
1	B	377	PRO
1	C	310	ASN
1	A	136	ASP
1	A	180	ALA
1	A	282	LEU
1	A	310	ASN
1	A	377	PRO
1	B	282	LEU
1	B	394	ASP
1	C	108	ASN
1	C	154	THR
1	C	282	LEU
1	C	377	PRO
1	C	397	ARG
1	A	36	ALA
1	A	394	ASP
1	B	36	ALA
1	B	55	LYS
1	B	74	SER
1	C	36	ALA
1	C	292	MET
1	C	368	HIS
1	A	74	SER
1	A	108	ASN
1	B	136	ASP
1	B	154	THR
1	C	11	PRO
1	C	33	TYR
1	C	74	SER
1	C	136	ASP
1	A	11	PRO
1	A	397	ARG
1	B	11	PRO
1	B	108	ASN
1	A	255	GLY
1	B	255	GLY
1	C	255	GLY
1	C	355	VAL

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	319/329 (97%)	285 (89%)	34 (11%)	8 41
1	B	319/329 (97%)	280 (88%)	39 (12%)	6 34
1	C	319/329 (97%)	281 (88%)	38 (12%)	6 35
All	All	957/987 (97%)	846 (88%)	111 (12%)	7 36

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLU
1	A	13	LEU
1	A	14	GLN
1	A	18	ILE
1	A	28	LEU
1	A	32	HIS
1	A	35	TYR
1	A	37	HIS
1	A	43	VAL
1	A	77	ARG
1	A	78	LEU
1	A	101	ILE
1	A	105	ARG
1	A	108	ASN
1	A	125	HIS
1	A	126	GLN
1	A	136	ASP
1	A	140	THR
1	A	148	ASN
1	A	174	GLU
1	A	178	LYS
1	A	203	GLN
1	A	250	LEU
1	A	259	ILE
1	A	267	ASP
1	A	270	LEU

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Mol	Chain	Res	Type
1	A	278	SER
1	A	300	SER
1	A	303	LEU
1	A	338	GLN
1	A	342	VAL
1	A	355	VAL
1	A	368	HIS
1	A	411	ILE
1	B	9	GLU
1	B	13	LEU
1	B	14	GLN
1	B	18	ILE
1	B	28	LEU
1	B	32	HIS
1	B	35	TYR
1	B	37	HIS
1	B	43	VAL
1	B	52	ARG
1	B	57	LEU
1	B	77	ARG
1	B	78	LEU
1	B	101	ILE
1	B	105	ARG
1	B	108	ASN
1	B	125	HIS
1	B	126	GLN
1	B	136	ASP
1	B	140	THR
1	B	148	ASN
1	B	150	GLN
1	B	155	ILE
1	B	174	GLU
1	B	178	LYS
1	B	196	LYS
1	B	203	GLN
1	B	250	LEU
1	B	259	ILE
1	B	267	ASP
1	B	270	LEU
1	B	278	SER
1	B	300	SER
1	B	303	LEU

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Mol	Chain	Res	Type
1	B	338	GLN
1	B	342	VAL
1	B	355	VAL
1	B	368	HIS
1	B	411	ILE
1	C	9	GLU
1	C	13	LEU
1	C	18	ILE
1	C	28	LEU
1	C	32	HIS
1	C	35	TYR
1	C	37	HIS
1	C	57	LEU
1	C	77	ARG
1	C	78	LEU
1	C	90	LEU
1	C	101	ILE
1	C	105	ARG
1	C	108	ASN
1	C	125	HIS
1	C	126	GLN
1	C	136	ASP
1	C	140	THR
1	C	148	ASN
1	C	174	GLU
1	C	178	LYS
1	C	196	LYS
1	C	250	LEU
1	C	259	ILE
1	C	267	ASP
1	C	270	LEU
1	C	278	SER
1	C	281	THR
1	C	300	SER
1	C	303	LEU
1	C	338	GLN
1	C	342	VAL
1	C	346	VAL
1	C	350	ILE
1	C	355	VAL
1	C	368	HIS
1	C	372	LEU

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Mol	Chain	Res	Type
1	C	411	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	HIS
1	A	108	ASN
1	A	132	HIS
1	B	108	ASN
1	B	132	HIS
1	C	108	ASN
1	C	132	HIS

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

Of 12 ligands modelled in this entry, 9 are monoatomic - leaving 3 for Mogul analysis.

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	ASP	A	901	-	2,8,8	0.40	0	0,10,10	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	ASP	B	901	-	2,8,8	0.40	0	0,10,10	0.00	-
2	ASP	C	901	-	2,8,8	0.28	0	0,10,10	0.00	-

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	ASP	A	901	-	-	0/2/8/8	0/0/0/0
2	ASP	B	901	-	-	0/2/8/8	0/0/0/0
2	ASP	C	901	-	-	0/2/8/8	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	ASP	2	0
2	B	901	ASP	2	0
2	C	901	ASP	4	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	410/422 (97%)	1.16	98 (23%)	1 1	164, 286, 403, 467	0
1	B	411/422 (97%)	0.80	66 (16%)	3 2	135, 215, 334, 372	0
1	C	410/422 (97%)	0.66	41 (10%)	9 6	132, 219, 316, 424	0
All	All	1231/1266 (97%)	0.87	205 (16%)	2 2	132, 237, 359, 467	0

All (205) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	33	TYR	9.5
1	A	115	LEU	8.2
1	A	261	PHE	7.2
1	A	313	GLY	7.1
1	A	247	TYR	6.6
1	A	354	GLY	6.5
1	A	314	THR	6.3
1	A	329	LEU	6.3
1	A	412	VAL	6.2
1	B	312	ASP	6.1
1	A	353	ALA	6.1
1	A	407	THR	6.0
1	A	113	ILE	5.9
1	A	264	HIS	5.9
1	B	35	TYR	5.8
1	A	268	ALA	5.8
1	A	265	ALA	5.7
1	A	358	ALA	5.5
1	A	84	LYS	5.5
1	A	281	THR	5.4
1	B	314	THR	5.3
1	A	403	THR	5.2
1	A	278	SER	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	278	SER	5.2
1	C	322	THR	5.0
1	C	10	TYR	4.8
1	A	292	MET	4.7
1	B	36	ALA	4.7
1	A	250	LEU	4.6
1	B	404	GLY	4.5
1	A	411	ILE	4.5
1	A	389	ILE	4.4
1	B	387	LEU	4.4
1	A	386	ILE	4.3
1	A	307	ALA	4.2
1	A	315	ALA	4.2
1	B	247	TYR	4.2
1	A	117	VAL	4.2
1	A	239	LEU	4.2
1	B	382	ALA	4.2
1	B	402	VAL	4.2
1	B	310	ASN	4.2
1	C	115	LEU	4.1
1	A	262	ILE	4.1
1	C	353	ALA	4.0
1	B	115	LEU	3.9
1	A	378	ASN	3.9
1	A	382	ALA	3.9
1	A	365	MET	3.9
1	A	116	ALA	3.9
1	B	353	ALA	3.9
1	C	113	ILE	3.9
1	B	329	LEU	3.9
1	B	409	THR	3.8
1	B	311	MET	3.8
1	C	318	GLN	3.7
1	A	279	SER	3.7
1	A	355	VAL	3.7
1	A	316	LEU	3.7
1	A	356	PRO	3.7
1	B	333	LEU	3.6
1	A	318	GLN	3.6
1	A	416	GLU	3.6
1	A	359	GLY	3.5
1	B	33	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	312	ASP	3.4
1	B	313	GLY	3.4
1	B	269	MET	3.4
1	B	122	PHE	3.4
1	A	122	PHE	3.4
1	C	314	THR	3.4
1	A	168	LEU	3.4
1	A	387	LEU	3.4
1	A	228	LEU	3.3
1	A	317	TYR	3.3
1	B	411	ILE	3.2
1	C	203	GLN	3.2
1	A	180	ALA	3.2
1	C	104	ALA	3.2
1	A	406	LEU	3.2
1	A	82	GLY	3.1
1	A	288	VAL	3.1
1	A	362	MET	3.1
1	B	239	LEU	3.1
1	A	357	GLY	3.0
1	A	263	LYS	3.0
1	B	117	VAL	3.0
1	C	12	VAL	3.0
1	A	360	ALA	3.0
1	A	251	LEU	3.0
1	C	168	LEU	3.0
1	A	242	GLN	2.9
1	A	393	LEU	2.9
1	A	311	MET	2.9
1	C	8	ILE	2.9
1	C	383	TYR	2.9
1	B	389	ILE	2.9
1	B	261	PHE	2.9
1	A	256	ILE	2.9
1	A	352	THR	2.8
1	B	407	THR	2.8
1	A	385	CYS	2.8
1	A	410	ALA	2.8
1	A	383	TYR	2.8
1	B	323	PHE	2.8
1	C	261	PHE	2.8
1	A	388	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	266	LYS	2.7
1	C	292	MET	2.7
1	A	220	GLN	2.7
1	C	35	TYR	2.7
1	B	309	ILE	2.7
1	A	7	TYR	2.7
1	B	265	ALA	2.7
1	A	285	THR	2.7
1	C	218	ALA	2.6
1	A	328	ALA	2.6
1	B	109	PRO	2.6
1	B	317	TYR	2.6
1	C	313	GLY	2.6
1	C	354	GLY	2.6
1	B	121	GLN	2.6
1	C	114	HIS	2.6
1	A	320	VAL	2.5
1	B	180	ALA	2.6
1	C	109	PRO	2.5
1	B	397	ARG	2.5
1	B	315	ALA	2.5
1	A	402	VAL	2.5
1	A	199	ASN	2.5
1	B	400	VAL	2.5
1	B	388	GLY	2.5
1	A	81	VAL	2.5
1	A	255	GLY	2.5
1	B	383	TYR	2.4
1	B	406	LEU	2.4
1	A	400	VAL	2.4
1	C	387	LEU	2.4
1	C	9	GLU	2.4
1	A	379	VAL	2.4
1	B	378	ASN	2.4
1	C	374	LEU	2.4
1	A	109	PRO	2.3
1	A	231	VAL	2.3
1	B	16	ILE	2.3
1	A	372	LEU	2.3
1	B	308	THR	2.3
1	B	360	ALA	2.3
1	C	269	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	242	GLN	2.3
1	A	36	ALA	2.3
1	A	235	VAL	2.3
1	C	360	ALA	2.3
1	A	246	VAL	2.3
1	B	20	LEU	2.2
1	A	80	ARG	2.2
1	A	325	ILE	2.2
1	B	114	HIS	2.2
1	A	248	PHE	2.2
1	B	77	ARG	2.2
1	C	389	ILE	2.2
1	B	354	GLY	2.2
1	A	192	GLU	2.2
1	C	117	VAL	2.2
1	C	397	ARG	2.2
1	B	331	SER	2.2
1	A	12	VAL	2.2
1	A	267	ASP	2.2
1	B	391	ALA	2.2
1	B	298	ILE	2.2
1	B	209	VAL	2.2
1	C	321	ALA	2.2
1	C	324	PHE	2.2
1	A	219	GLU	2.2
1	B	374	LEU	2.1
1	A	289	ALA	2.1
1	C	406	LEU	2.1
1	B	386	ILE	2.1
1	C	16	ILE	2.1
1	C	333	LEU	2.1
1	C	39	VAL	2.1
1	C	317	TYR	2.1
1	B	292	MET	2.1
1	A	305	LEU	2.1
1	A	322	THR	2.1
1	B	403	THR	2.1
1	B	267	ASP	2.1
1	A	215	TYR	2.1
1	B	32	HIS	2.1
1	C	36	ALA	2.1
1	C	107	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	37	HIS	2.1
1	B	168	LEU	2.1
1	B	405	ASP	2.1
1	B	307	ALA	2.1
1	A	409	THR	2.1
1	B	316	LEU	2.1
1	C	213	ILE	2.0
1	A	105	ARG	2.0
1	A	147	ALA	2.0
1	B	332	HIS	2.0
1	A	392	ILE	2.0
1	B	390	ASP	2.0
1	A	106	LEU	2.0
1	C	231	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NA	B	902	1/1	0.99	1.19	2.74	194,194,194,194	0
2	ASP	A	901	9/9	0.89	0.89	0.83	253,255,264,269	0
2	ASP	B	901	9/9	0.93	0.68	0.82	173,178,187,190	0
2	ASP	C	901	9/9	0.91	0.52	0.73	178,184,191,191	0
3	NA	C	902	1/1	0.97	0.41	0.33	183,183,183,183	0
3	NA	A	902	1/1	0.99	0.61	0.16	275,275,275,275	0
3	NA	C	903	1/1	0.93	0.17	-1.43	178,178,178,178	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NA	A	903	1/1	0.95	0.27	-1.44	258,258,258,258	0
3	NA	B	903	1/1	0.92	0.29	-1.45	184,184,184,184	0
4	HG	C	904	1/1	0.97	0.14	-	284,284,284,284	1
4	HG	A	904	1/1	0.89	0.29	-	312,312,312,312	1
4	HG	B	904	1/1	0.96	0.09	-	248,248,248,248	1

6.5 Other polymers

There are no such residues in this entry.