Full wwPDB X-ray Structure Validation Report (i)

Feb 18, 2024 – 12:48 AM EST

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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

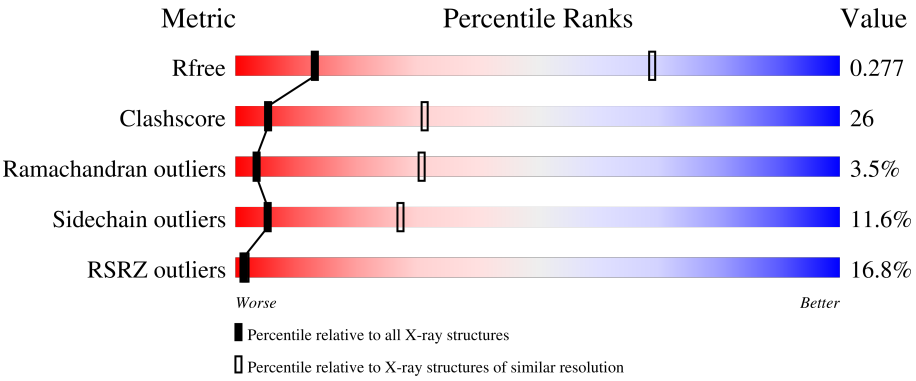
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	24% 48% 43% 6%
1	B	422	15% 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	C	901	-	-	X	-

2 Entry composition (i)

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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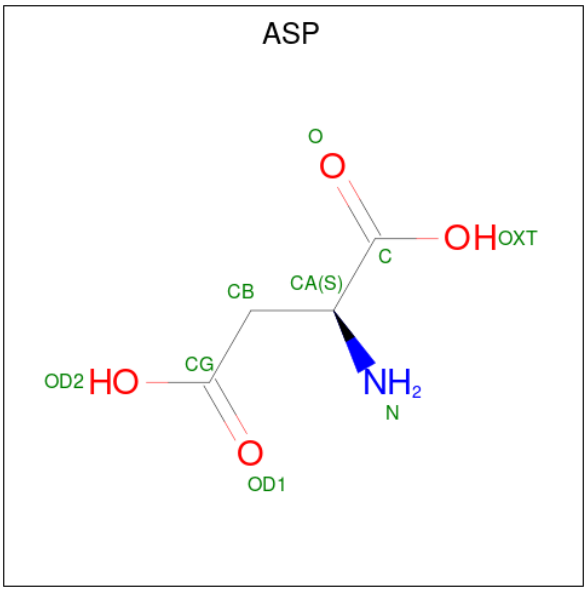
Chain	Residue	Modelled	Actual	Comment	Reference
B	368	HIS	GLU	engineered mutation	UNP O59010
B	385	CYS	MET	engineered mutation	UNP O59010
B	418	THR	-	expression tag	UNP O59010
B	419	LEU	-	expression tag	UNP O59010
B	420	VAL	-	expression tag	UNP O59010
B	421	PRO	-	expression tag	UNP O59010
B	422	ARG	-	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	A	2	Total Na 2 2	0	0
3	B	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).

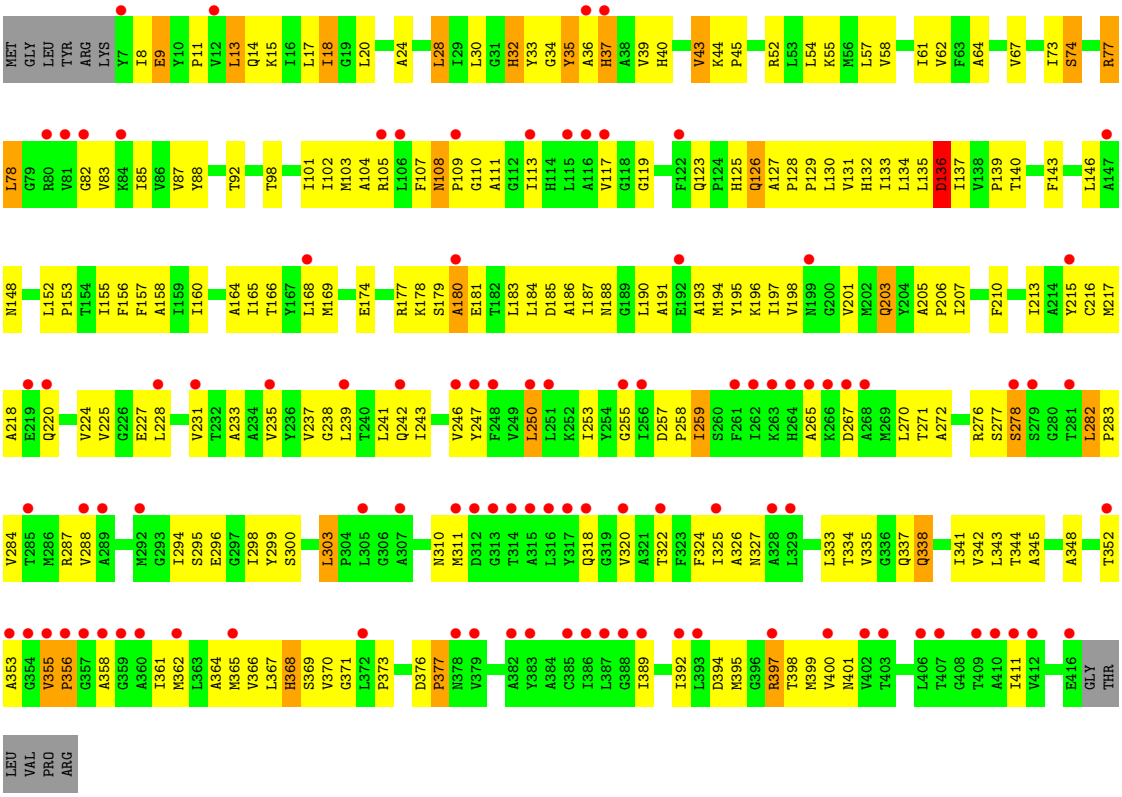
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Hg 1 1	0	0
4	B	1	Total Hg 1 1	0	0
4	C	1	Total Hg 1 1	0	0

3 Residue-property plots (i)

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

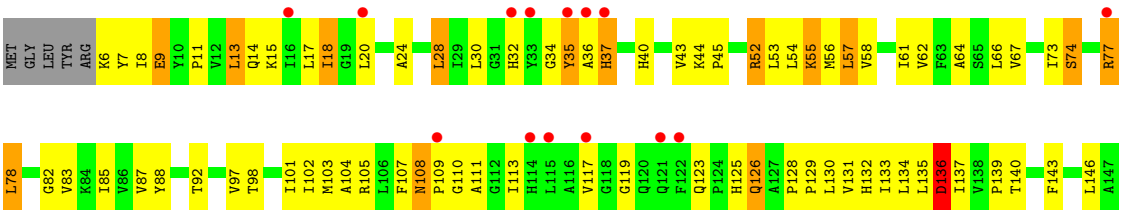
• Molecule 1: sodium-coupled L-aspartate transporter

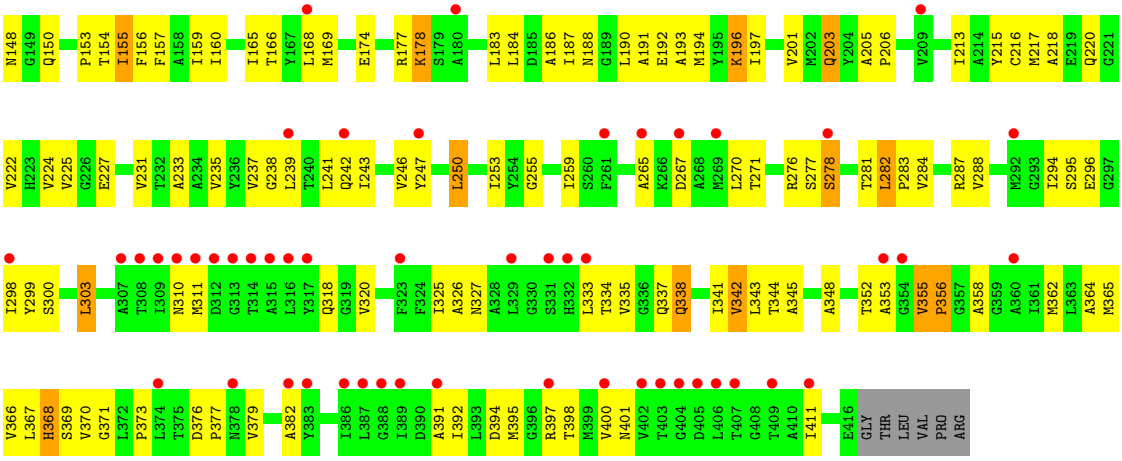
Chain A:



• Molecule 1: sodium-coupled L-aspartate transporter

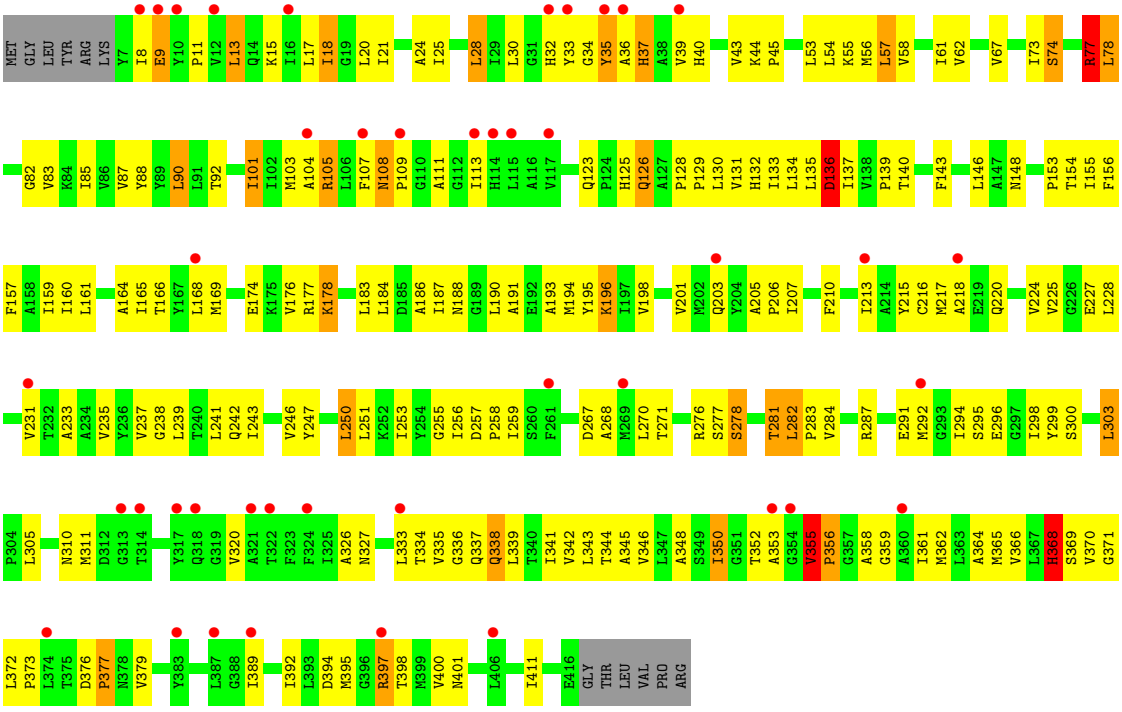
Chain B:





• 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 0.254 , 0.277	Depositor DCC
R_{free} test set	1222 reflections (5.15%)	wwPDB-VP
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 , 238.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 respectively for untwinned datasets, and 0.375, 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:A:55:LYS:O	1:A:58:VAL:HG12	1.84	0.76
1:C:155:ILE:HD11	1:C:365:MET:HG3	1.67	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:A:157:PHE:HA	1:A:160:ILE:HG22	1.67	0.75
1:B:334:THR:HG22	1:B:337:GLN:OE1	1.85	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:HE21	1:B:203:GLN:HA	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:OE1	1:C:123:GLN:HA	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:HA	1:A:203:GLN:HE21	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:HA	1:B:123:GLN:OE1	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:O	1:C:126:GLN:HG2	1.95	0.67
1:A:15:LYS:O	1:A:18:ILE:HG22	1.95	0.67
1:C:169:MET:HA	1:C:177:ARG:HG3	1.76	0.67
1:A:113:ILE:HD11	1:A:224:VAL:HG23	1.77	0.67
1:C:284:VAL:HG13	1:C:287:ARG:HH21	1.60	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:35:TYR:N	1:A:35:TYR:CD2	2.65	0.65
1:A:168:LEU:HD11	1:C:193:ALA:HB2	1.79	0.65
1:A:345:ALA:HA	1:A:348:ALA:HB3	1.80	0.64
1:B:344:THR:HB	1:B:366:VAL:HG23	1.80	0.64
1:B:61:ILE:HG22	1:B:194:MET:HB3	1.79	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:C:61:ILE:HG22	1:C:194:MET:CB	2.27	0.64
1:B:205:ALA:N	1:B:206:PRO:HD2	2.13	0.64
1:A:123:GLN:OE1	1:A:123:GLN:HA	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:A:242:GLN:O	1:A:246:VAL:HB	1.98	0.63
1:B:186:ALA:O	1:B:188:ASN:O	2.17	0.63
1:C:344:THR:HB	1:C:366:VAL:HG23	1.81	0.63
1:B:35:TYR:N	1:B:35:TYR:CD2	2.66	0.63
1:C:111:ALA:N	1:C:327:ASN:HB3	2.11	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:217:MET:SD	1:B:225:VAL:HG22	2.39	0.62
1:B:250:LEU:O	1:B:253:ILE:HG22	1.99	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:A:250:LEU:O	1:A:253:ILE:HG22	2.01	0.60
1:B:364:ALA:O	1:B:368:HIS:HB2	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:HA	1:C:203:GLN:NE2	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:A:143:PHE:CE2	1:C:146:LEU:HD23	2.38	0.59
1:C:217:MET:SD	1:C:225:VAL:HG22	2.42	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:A:239:LEU:HD22	1:A:400:VAL:HG21	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:C:165:ILE:HG21	1:C:184:LEU:HD13	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:B:155:ILE:HD11	1:B:365:MET:HG3	1.84	0.58
1:C:61:ILE:HG21	1:C:194:MET:HB3	1.85	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:B:277:SER:N	1:B:398:THR:HG21	2.19	0.58
1:C:24:ALA:HA	1:C:217:MET:HG3	1.86	0.58
1:B:146:LEU:HD23	1:C:143:PHE:CE2	2.39	0.58
1:C:54:LEU:CD1	1:C:201:VAL:HG11	2.34	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: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:C:335:VAL:HA	1:C:338:GLN:CB	2.29	0.57
1:A:82:GLY:HA2	1:A:85:ILE:HG22	1.86	0.57
1:B:334:THR:HG23	1:B:335:VAL:O	2.05	0.57
1:C:73:ILE:O	1:C:78:LEU:HD22	2.05	0.57
1:A:58:VAL:O	1:A:62:VAL:HG23	2.05	0.57
1:A:155:ILE:HD11	1:A:365:MET:HG3	1.87	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:B:83:VAL:O	1:B:87:VAL:HG23	2.05	0.56
1:C:183:LEU:HD21	1:C:187:ILE:HD11	1.87	0.56
1:C:271:THR:HG21	1:C:284:VAL:HG21	1.86	0.56
1:A:37:HIS:HA	1:A:40:HIS:HB3	1.87	0.56
1:B:183:LEU:HD23	1:B:187:ILE:HG13	1.87	0.56
1:B:341:ILE:HG13	1:B:370:VAL:HG21	1.88	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:A:64:ALA:HB2	1:A:190:LEU:HD23	1.88	0.55
1:B:6:LYS:O	1:B:8:ILE:N	2.40	0.55
1:B:103:MET:HG3	1:B:238:GLY:HA3	1.89	0.55
1:B:227:GLU:O	1:B:231:VAL:HG23	2.06	0.55
1:B:67:VAL:HG11	1:B:187:ILE:HD12	1.88	0.55
1:C:216:CYS:O	1:C:220:GLN:HB2	2.07	0.55
1:A:44:LYS:N	1:A:45:PRO:HD2	2.21	0.55
1:A:371:GLY:O	1:A:373:PRO:HD3	2.07	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:A:139:PRO:CB	1:A:153:PRO:HB3	2.36	0.55
1:B:61:ILE:HG21	1:B:194:MET:HB3	1.85	0.55
1:C:178:LYS:O	1:C:178:LYS:HD3	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:A:126:GLN:O	1:A:126:GLN:HG2	2.08	0.53
1:B:30:LEU:HD23	1:B:34:GLY:HA3	1.89	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: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: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: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:B:353:ALA:HB3	1:B:358:ALA:HB2	1.92	0.52
1:C:243:ILE:HA	1:C:247:TYR:CD2	2.45	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:6:LYS:C	1:B:8:ILE:H	2.13	0.52
1:B:193:ALA:CB	1:C:168:LEU:HD11	2.39	0.52
1:C:277:SER:N	1:C:398:THR:HG21	2.24	0.52
1:C:343:LEU:HD13	1:C:343:LEU:C	2.30	0.52
1:A:130:LEU:HA	1:A:133:ILE:CG2	2.40	0.52
1:C:296:GLU:HA	1:C:299:TYR:CE1	2.44	0.52
1:C:334:THR:HG23	1:C:335:VAL:O	2.09	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:A:183:LEU:HD23	1:A:187:ILE:HG13	1.91	0.51
1:C:77:ARG:HG2	1:C:166:THR:HB	1.92	0.51
1:A:98:THR:O	1:A:102:ILE:HG13	2.11	0.51
1:B:277:SER:H	1:B:398:THR:HG21	1.73	0.51
1:A:205:ALA:N	1:A:206:PRO:HD2	2.26	0.51
1:C:129:PRO:CG	1:C:132:HIS:HD2	2.24	0.51
1:A:17:LEU:HD22	1:A:392:ILE:HD11	1.92	0.51
1:B:24:ALA:O	1:B:28:LEU:HD22	2.11	0.51
1:B:216:CYS:O	1:B:224:VAL:HG11	2.10	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:B:243:ILE:HA	1:B:247:TYR:HD2	1.76	0.51
1:C:205:ALA:N	1:C:206:PRO:HD2	2.26	0.51
1:A:77:ARG:HG2	1:A:166:THR:HB	1.91	0.50
1:A:183:LEU:HD21	1:A:187:ILE:HD11	1.93	0.50
1:A:197:ILE:O	1:A:201:VAL:HG23	2.10	0.50
1:A:216:CYS:O	1:A:224:VAL:HG11	2.11	0.50
1:A:334:THR:O	1:A:338:GLN:N	2.43	0.50
1:B:104:ALA:HB2	1:B:320:VAL:HG13	1.94	0.50
1:C:243:ILE:HA	1:C:247:TYR:HD2	1.75	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:A:179:SER:O	1:A:181:GLU:N	2.45	0.50
1:B:239:LEU:HD22	1:B:400:VAL:HG21	1.93	0.50
1:A:265:ALA:HA	1:A:288:VAL:HG11	1.94	0.50
1:B:243:ILE:HA	1:B:247:TYR:CD2	2.46	0.50
1:C:294:ILE:CG2	1:C:299:TYR:HB3	2.41	0.50
1:C:73:ILE:O	1:C:74:SER:C	2.51	0.49
1:B:343:LEU:HD13	1:B:343:LEU:C	2.32	0.49
1:C:54:LEU:HD12	1:C:54:LEU:N	2.27	0.49
1:C:287:ARG:HG2	1:C:291:GLU:OE2	2.11	0.49
1:C:334:THR:O	1:C:338:GLN:N	2.45	0.49
1:C:394:ASP:O	1:C:398:THR:OG1	2.26	0.49
1:B:8:ILE:HG12	1:B:15:LYS:HE3	1.93	0.49
1:B:77:ARG:HG2	1:B:166:THR:HB	1.94	0.49
1:B:216:CYS:O	1:B:220:GLN:HB2	2.13	0.49
1:C:77:ARG:O	1:C:77:ARG:HD3	2.12	0.49
1:A:243:ILE:HA	1:A:247:TYR:HD2	1.76	0.49
1:B:139:PRO:CB	1:B:153:PRO:HB3	2.39	0.49
1:A:157:PHE:HA	1:A:160:ILE:CG2	2.38	0.49
1:A:227:GLU:O	1:A:231:VAL:HG23	2.11	0.49
1:A:294:ILE:CG2	1:A:299:TYR:HB3	2.43	0.49
1:A:355:VAL:HG13	1:A:356:PRO:N	2.28	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:A:185:ASP:O	1:A:188:ASN:O	2.31	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: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:HA	1:A:203:GLN:NE2	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:A:134:LEU:O	1:A:137:ILE:HG12	2.12	0.48
1:C:239:LEU:HD22	1:C:400:VAL:CG2	2.39	0.48
1:A:146:LEU:HD12	1:A:146:LEU:H	1.79	0.48
1:B:20:LEU:HA	1:B:213:ILE:HD11	1.95	0.48
1:C:277:SER:H	1:C:398:THR:HG21	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:A:343:LEU:C	1:A:343:LEU:HD13	2.34	0.48
1:B:325:ILE:HG13	1:B:367:LEU:HD21	1.95	0.48
1:C:216:CYS:O	1:C:224:VAL:HG11	2.14	0.48
1:A:216:CYS:O	1:A:220:GLN:HB2	2.14	0.47
1:C:103:MET:CE	1:C:237:VAL:HG23	2.44	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:B:98:THR:O	1:B:102:ILE:HG13	2.15	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:C:129:PRO:HG2	1:C:132:HIS:HD2	1.79	0.47
1:C:343:LEU:HD13	1:C:343:LEU:O	2.14	0.47
1:A:139:PRO:HB3	1:A:153:PRO:CB	2.39	0.47
1:A:165:ILE:HG21	1:A:184:LEU:HD13	1.96	0.47
1:B:344:THR:HG21	1:B:369:SER:OG	2.15	0.47
1:C:74:SER:O	1:C:77:ARG:CB	2.63	0.47
1:A:353:ALA:HB3	1:A:358:ALA:HB2	1.96	0.47
1:B:311:MET:HB3	1:B:401:ASN:CG	2.35	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:A:8:ILE:HG12	1:A:15:LYS:HE3	1.97	0.47
1:A:322:THR:HG21	1:A:341:ILE:HG12	1.95	0.47
1:A:352:THR:HA	1:A:362:MET:HG3	1.97	0.47
1:C:157:PHE:HA	1:C:160:ILE:CG2	2.43	0.47
1:C:276:ARG:HG2	1:C:395:MET:HG2	1.96	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:A:277:SER:N	1:A:398:THR:HG21	2.30	0.46
1:B:165:ILE:CG2	1:B:184:LEU:HB2	2.41	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:B:146:LEU:HD12	1:B:146:LEU:H	1.80	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:129:PRO:HG2	1:C:132:HIS:CD2	2.50	0.46
1:C:57:LEU:HD12	1:C:361:ILE:CD1	2.45	0.46
1:C:58:VAL:O	1:C:62:VAL:HG23	2.15	0.46
1:C:132:HIS:O	1:C:136:ASP:HB2	2.16	0.46
1:C:271:THR:HB	1:C:281:THR:HG23	1.96	0.46
1:A:146:LEU:HD23	1:B:143:PHE:CE2	2.50	0.46
1:B:64:ALA:HB2	1:B:190:LEU:HD23	1.96	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:C:335:VAL:CA	1:C:338:GLN:HB2	2.31	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: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:139:PRO:CB	1:C:153:PRO:HB3	2.39	0.46
1:C:295:SER:HB3	1:C:298:ILE:HD13	1.98	0.46
1:C:352:THR:HA	1:C:362:MET:HG3	1.98	0.46
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:B:113:ILE:O	1:B:113:ILE:HG23	2.16	0.45
1:B:117:VAL:C	1:B:119:GLY:H	2.20	0.45
1:C:8:ILE:HG12	1:C:15:LYS:HE3	1.97	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: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:B:341:ILE:CG1	1:B:370:VAL:HG21	2.47	0.45
1:A:295:SER:HB3	1:A:298:ILE:HD13	1.98	0.45
1:A:344:THR:HG21	1:A:369:SER:OG	2.17	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:132:HIS:O	1:A:136:ASP:HB2	2.17	0.45
1:A:333:LEU:HD11	1:A:370:VAL:HG11	1.99	0.45
1:B:265:ALA:HA	1:B:288:VAL:HG11	1.97	0.45
1:A:57:LEU:HD12	1:A:361:ILE:CD1	2.47	0.44
1:A:213:ILE:C	1:A:215:TYR:H	2.21	0.44
1:B:352:THR:HA	1:B:362:MET:HG3	1.98	0.44
1:C:161:LEU:O	1:C:165:ILE:HG12	2.17	0.44
1:C:195:TYR:O	1:C:198:VAL:HB	2.17	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:C:376:ASP:HA	1:C:377:PRO:HD2	1.75	0.44
1:B:190:LEU:O	1:B:191:ALA:C	2.55	0.44
1:B:196:LYS:HA	1:B:196:LYS:HD3	1.61	0.44
1:B:318:GLN:HB3	1:B:366:VAL:HG11	1.99	0.44
1:B:135:LEU:C	1:B:137:ILE:H	2.21	0.44
1:B:157:PHE:HA	1:B:160:ILE:CG2	2.42	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:52:ARG:HH12	1:B:136:ASP:HA	1.82	0.44
1:A:127:ALA:HA	1:A:128:PRO:HD3	1.89	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:A:272:ALA:HB1	1:A:399:MET:HA	1.99	0.43
1:B:282:LEU:H	1:B:283:PRO:CD	2.31	0.43
1:B:342:VAL:HG12	1:B:343:LEU:N	2.33	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:190:LEU:O	1:C:191:ALA:C	2.56	0.43
1:C:213:ILE:C	1:C:215:TYR:H	2.21	0.43
1:A:195:TYR:O	1:A:198:VAL:HB	2.19	0.43
1:A:333:LEU:HD21	1:A:341:ILE:HD11	1.99	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:C:20:LEU:HA	1:C:213:ILE:HD11	2.00	0.43
1:A:168:LEU:HD11	1:C:193:ALA:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:ILE:HG21	1:B:184:LEU:HD13	1.99	0.43
1:C:17:LEU:HD22	1:C:392:ILE:HD11	2.00	0.43
1:C:268:ALA:O	1:C:281:THR:HG21	2.19	0.43
1:A:8:ILE:C	1:A:9:GLU:HG3	2.38	0.43
1:A:333:LEU:HD12	1:A:337:GLN:HE21	1.84	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:A:325:ILE:HG13	1:A:367:LEU:HD21	2.00	0.43
1:B:44:LYS:HD2	1:B:215:TYR:CZ	2.53	0.43
1:B:187:ILE:O	1:B:190:LEU:HB3	2.19	0.43
1:B:311:MET:HB3	1:B:401:ASN:OD1	2.19	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: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:B:246:VAL:O	1:B:250:LEU:HG	2.19	0.42
1:B:294:ILE:HG22	1:B:299:TYR:HB3	2.01	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:A:376:ASP:HA	1:A:377:PRO:HD2	1.72	0.42
1:C:294:ILE:HG22	1:C:299:TYR:HB3	2.00	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:A:165:ILE:CG2	1:A:184:LEU:HB2	2.50	0.42
1:B:13:LEU:HB2	1:B:276:ARG:HE	1.85	0.42
1:B:271:THR:HB	1:B:281:THR:HG23	2.01	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:B:53:LEU:HD23	1:B:53:LEU:HA	1.90	0.42
1:C:90:LEU:HD11	1:C:350:ILE:HD11	2.02	0.42
1:C:401:ASN:ND2	2:C:901:ASP:HA	2.34	0.42
1:B:66:LEU:HD23	1:B:66:LEU:HA	1.66	0.42
1:B:333:LEU:HD21	1:B:341:ILE:HD11	2.02	0.42
1:C:39:VAL:HG13	1:C:43:VAL:HG12	2.01	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: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:A:152:LEU:O	1:A:153:PRO:C	2.58	0.41
1:B:128:PRO:CB	1:B:129:PRO:CD	2.93	0.41
1:C:352:THR:HG23	1:C:358:ALA:HB1	2.02	0.41
1:A:32:HIS:HB3	1:A:33:TYR:H	1.65	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:B:343:LEU:HD13	1:B:343:LEU:O	2.20	0.41
1:A:257:ASP:HA	1:A:258:PRO:HD3	1.83	0.41
1:B:58:VAL:HG21	1:B:364:ALA:HB3	2.03	0.41
1:C:103:MET:HG3	1:C:238:GLY:CA	2.51	0.41
1:A:311:MET:HB3	1:A:401:ASN:CG	2.41	0.41
1:A:343:LEU:HD13	1:A:343:LEU:O	2.20	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:152:LEU:O	1:A:155:ILE:HB	2.21	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:213:ILE:HG22	1:C:216:CYS:HB2	2.03	0.41
1:C:305:LEU:O	1:C:305:LEU:HG	2.20	0.41
1:A:77:ARG:O	1:A:77:ARG:HD3	2.19	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:C:130:LEU:HD12	1:C:133:ILE:HG23	2.02	0.41
1:C:294:ILE:HG21	1:C:299:TYR:HB3	2.02	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:103:MET:CE	1:A:237:VAL:HG23	2.51	0.41
1:A:157:PHE:CA	1:A:160:ILE:HG22	2.44	0.41
1:A:277:SER:H	1:A:398:THR:HG21	1.86	0.41
1:A:318:GLN:HB3	1:A:366:VAL:HG11	2.02	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:A:17:LEU:CD2	1:A:392:ILE:HD11	2.50	0.40
1:B:190:LEU:HA	1:B:190:LEU:HD12	1.89	0.40
1:B:362:MET:O	1:B:365:MET:HB3	2.21	0.40
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:C:359:GLY:H	2:C:901:ASP:CG	2.25	0.40
1:A:39:VAL:HG13	1:A:43:VAL:HG12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:LEU:HD13	1:A:303:LEU:HA	1.94	0.40
1:B:73:ILE:O	1:B:74:SER:C	2.59	0.40
1:B:177:ARG:HH11	1:B:177:ARG:HD2	1.77	0.40
1:B:325:ILE:HG23	1:B:382:ALA:HB3	2.03	0.40
1:C:215:TYR:HA	1:C:218:ALA:HB3	2.03	0.40
1:A:131:VAL:O	1:A:135:LEU:HB2	2.22	0.40
1:B:222:VAL:O	1:B:225:VAL:HG23	2.21	0.40
1:A:137:ILE:HA	1:A:153:PRO:HG3	2.04	0.40
1:A:179:SER:O	1:A:180:ALA:C	2.60	0.40
1:B:155:ILE:HG23	1:B:159:ILE:CD1	2.52	0.40
1:C:333:LEU:HD12	1:C:337:GLN:HE21	1.86	0.40
1:C:355:VAL:HG13	1:C:356:PRO:N	2.36	0.40
1:A:110:GLY:O	1:A:111:ALA:C	2.59	0.40
1:A:215:TYR:HA	1:A:218:ALA:HB3	2.02	0.40
1:C:24:ALA:O	1:C:28:LEU:CD2	2.69	0.40
1:C:90:LEU:CD1	1:C:350:ILE:HD11	2.51	0.40
1:C:155:ILE:O	1:C:159:ILE:HD12	2.22	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%)	4	32
1	B	409/422 (97%)	328 (80%)	67 (16%)	14 (3%)	3	31
1	C	408/422 (97%)	322 (79%)	70 (17%)	16 (4%)	3	28
All	All	1225/1266 (97%)	979 (80%)	203 (17%)	43 (4%)	3	31

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%)	6 30
1	B	319/329 (97%)	280 (88%)	39 (12%)	5 25
1	C	319/329 (97%)	281 (88%)	38 (12%)	5 26
All	All	957/987 (97%)	846 (88%)	111 (12%)	5 27

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

Sometimes 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 monosaccharides 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	-	6,8,8	1.25	1 (16%)	8,10,10	1.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	ASP	C	901	-	6,8,8	1.23	1 (16%)	8,10,10	1.34	2 (25%)
2	ASP	B	901	-	6,8,8	1.35	1 (16%)	8,10,10	1.38	1 (12%)

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	-	-	4/8/8/8	-
2	ASP	C	901	-	-	5/8/8/8	-
2	ASP	B	901	-	-	5/8/8/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	ASP	OXT-C	-2.46	1.22	1.30
2	A	901	ASP	OXT-C	-2.21	1.23	1.30
2	C	901	ASP	OXT-C	-2.21	1.23	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	901	ASP	OXT-C-O	-2.82	117.70	124.09
2	C	901	ASP	OXT-C-CA	2.26	121.10	113.38
2	C	901	ASP	OXT-C-O	-2.12	119.28	124.09

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	ASP	O-C-CA-N
2	B	901	ASP	O-C-CA-N
2	C	901	ASP	O-C-CA-N
2	B	901	ASP	OXT-C-CA-N
2	A	901	ASP	OXT-C-CA-N
2	C	901	ASP	OXT-C-CA-N
2	A	901	ASP	CA-CB-CG-OD1
2	A	901	ASP	CA-CB-CG-OD2
2	B	901	ASP	CA-CB-CG-OD1

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Mol	Chain	Res	Type	Atoms
2	B	901	ASP	CA-CB-CG-OD2
2	C	901	ASP	CA-CB-CG-OD1
2	C	901	ASP	CA-CB-CG-OD2
2	B	901	ASP	N-CA-CB-CG
2	C	901	ASP	N-CA-CB-CG

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	C	901	ASP	4	0
2	B	901	ASP	2	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

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%)	1.15	100 (24%) 0 0	164, 286, 403, 467	0
1	B	411/422 (97%)	0.78	65 (15%) 2 2	135, 215, 334, 372	0
1	C	410/422 (97%)	0.64	42 (10%) 6 6	132, 219, 316, 424	0
All	All	1231/1266 (97%)	0.85	207 (16%) 1 2	132, 237, 359, 467	0

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	33	TYR	9.5
1	A	115	LEU	8.2
1	A	313	GLY	7.2
1	A	261	PHE	7.2
1	A	247	TYR	6.6
1	A	354	GLY	6.6
1	A	329	LEU	6.3
1	A	314	THR	6.3
1	A	412	VAL	6.2
1	A	264	HIS	6.1
1	A	353	ALA	6.0
1	A	407	THR	6.0
1	B	312	ASP	6.0
1	A	113	ILE	6.0
1	B	35	TYR	5.8
1	A	268	ALA	5.8
1	A	265	ALA	5.7
1	A	84	LYS	5.6
1	A	358	ALA	5.5
1	A	281	THR	5.4
1	B	314	THR	5.3
1	A	403	THR	5.2
1	A	278	SER	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	278	SER	5.1
1	C	322	THR	5.0
1	A	292	MET	4.8
1	C	10	TYR	4.7
1	B	36	ALA	4.7
1	A	250	LEU	4.6
1	B	404	GLY	4.6
1	A	411	ILE	4.5
1	A	389	ILE	4.5
1	B	387	LEU	4.4
1	A	386	ILE	4.3
1	A	117	VAL	4.2
1	B	247	TYR	4.2
1	A	239	LEU	4.2
1	A	307	ALA	4.2
1	A	315	ALA	4.2
1	B	402	VAL	4.2
1	C	115	LEU	4.2
1	B	382	ALA	4.2
1	A	262	ILE	4.1
1	B	310	ASN	4.1
1	C	353	ALA	4.0
1	B	115	LEU	4.0
1	A	365	MET	3.9
1	C	113	ILE	3.9
1	A	382	ALA	3.9
1	A	378	ASN	3.9
1	B	329	LEU	3.9
1	A	116	ALA	3.9
1	B	353	ALA	3.9
1	B	409	THR	3.8
1	B	311	MET	3.8
1	A	316	LEU	3.8
1	A	355	VAL	3.8
1	C	318	GLN	3.7
1	A	356	PRO	3.7
1	A	279	SER	3.7
1	B	333	LEU	3.7
1	A	318	GLN	3.6
1	A	359	GLY	3.5
1	A	416	GLU	3.5
1	B	313	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	33	TYR	3.4
1	B	269	MET	3.4
1	B	122	PHE	3.4
1	A	168	LEU	3.4
1	A	122	PHE	3.4
1	A	387	LEU	3.4
1	A	312	ASP	3.4
1	C	314	THR	3.4
1	A	228	LEU	3.3
1	B	411	ILE	3.3
1	A	317	TYR	3.3
1	C	203	GLN	3.2
1	A	180	ALA	3.2
1	A	406	LEU	3.2
1	C	104	ALA	3.1
1	A	82	GLY	3.1
1	A	288	VAL	3.1
1	A	362	MET	3.1
1	A	263	LYS	3.1
1	B	239	LEU	3.1
1	A	357	GLY	3.1
1	B	117	VAL	3.0
1	C	12	VAL	3.0
1	C	168	LEU	3.0
1	A	251	LEU	3.0
1	C	8	ILE	3.0
1	A	393	LEU	3.0
1	A	360	ALA	3.0
1	B	389	ILE	2.9
1	A	311	MET	2.9
1	A	242	GLN	2.9
1	C	383	TYR	2.9
1	A	256	ILE	2.9
1	B	261	PHE	2.9
1	A	352	THR	2.8
1	B	407	THR	2.8
1	A	388	GLY	2.8
1	A	266	LYS	2.8
1	B	323	PHE	2.8
1	A	383	TYR	2.7
1	A	410	ALA	2.7
1	C	261	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	292	MET	2.7
1	B	309	ILE	2.7
1	A	220	GLN	2.7
1	C	35	TYR	2.7
1	A	7	TYR	2.6
1	A	285	THR	2.6
1	A	385	CYS	2.6
1	B	265	ALA	2.6
1	B	109	PRO	2.6
1	C	114	HIS	2.6
1	C	218	ALA	2.6
1	A	328	ALA	2.6
1	C	313	GLY	2.6
1	C	354	GLY	2.6
1	B	397	ARG	2.6
1	B	317	TYR	2.6
1	A	320	VAL	2.6
1	C	109	PRO	2.5
1	B	121	GLN	2.5
1	B	180	ALA	2.5
1	B	388	GLY	2.5
1	A	402	VAL	2.5
1	B	315	ALA	2.5
1	B	400	VAL	2.5
1	A	255	GLY	2.5
1	A	81	VAL	2.5
1	B	406	LEU	2.5
1	A	199	ASN	2.4
1	A	400	VAL	2.4
1	B	383	TYR	2.4
1	C	387	LEU	2.4
1	A	379	VAL	2.4
1	C	374	LEU	2.4
1	B	16	ILE	2.4
1	A	109	PRO	2.4
1	A	231	VAL	2.3
1	A	372	LEU	2.3
1	C	9	GLU	2.3
1	B	378	ASN	2.3
1	B	114	HIS	2.3
1	C	269	MET	2.3
1	B	308	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	80	ARG	2.3
1	B	77	ARG	2.3
1	B	360	ALA	2.3
1	B	242	GLN	2.3
1	A	325	ILE	2.3
1	A	235	VAL	2.3
1	C	397	ARG	2.3
1	A	246	VAL	2.3
1	B	20	LEU	2.3
1	C	389	ILE	2.3
1	B	354	GLY	2.2
1	A	36	ALA	2.2
1	C	360	ALA	2.2
1	A	248	PHE	2.2
1	B	298	ILE	2.2
1	C	117	VAL	2.2
1	A	12	VAL	2.2
1	B	209	VAL	2.2
1	B	391	ALA	2.2
1	B	32	HIS	2.2
1	B	386	ILE	2.2
1	C	16	ILE	2.2
1	B	37	HIS	2.2
1	B	374	LEU	2.2
1	C	406	LEU	2.2
1	A	192	GLU	2.2
1	C	321	ALA	2.1
1	B	331	SER	2.1
1	C	324	PHE	2.1
1	C	333	LEU	2.1
1	A	267	ASP	2.1
1	C	39	VAL	2.1
1	A	289	ALA	2.1
1	A	305	LEU	2.1
1	B	292	MET	2.1
1	C	317	TYR	2.1
1	B	168	LEU	2.1
1	A	322	THR	2.1
1	B	403	THR	2.1
1	A	219	GLU	2.1
1	C	107	PHE	2.1
1	A	215	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	332	HIS	2.1
1	A	105	ARG	2.1
1	C	36	ALA	2.1
1	C	213	ILE	2.1
1	B	316	LEU	2.1
1	B	267	ASP	2.1
1	A	409	THR	2.0
1	B	307	ALA	2.0
1	A	37	HIS	2.0
1	A	392	ILE	2.0
1	A	397	ARG	2.0
1	C	32	HIS	2.0
1	B	405	ASP	2.0
1	A	106	LEU	2.0
1	A	147	ALA	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{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	B-factors(Å^2)	Q<0.9
2	ASP	A	901	9/9	0.89	0.89	253,255,264,269	0
4	HG	A	904	1/1	0.89	0.29	312,312,312,312	1
2	ASP	C	901	9/9	0.91	0.52	178,184,191,191	0
3	NA	B	903	1/1	0.92	0.29	184,184,184,184	0
3	NA	C	903	1/1	0.93	0.17	178,178,178,178	0
2	ASP	B	901	9/9	0.93	0.68	173,178,187,190	0
3	NA	A	903	1/1	0.95	0.27	258,258,258,258	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	HG	B	904	1/1	0.96	0.09	248,248,248,248	1
3	NA	C	902	1/1	0.97	0.41	183,183,183,183	0
4	HG	C	904	1/1	0.97	0.14	284,284,284,284	1
3	NA	A	902	1/1	0.99	0.61	275,275,275,275	0
3	NA	B	902	1/1	0.99	1.19	194,194,194,194	0

6.5 Other polymers (i)

There are no such residues in this entry.