Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:43 PM GMT

PDB ID	:	3RV7
Title	:	Structure of a M. tuberculosis Salicylate Synthase, MbtI, in Complex with an Inhibitor with Isopropyl R-Group
Authors	:	Chi, G.; Bulloch, E.M.M.; Manos-Turvey, A.; Payne, R.J.; Lott, J.S.; TB Structural Genomics Consortium (TBSGC)
Deposited on	:	2011-05-06
Resolution	:	2.50 Å(reported)

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

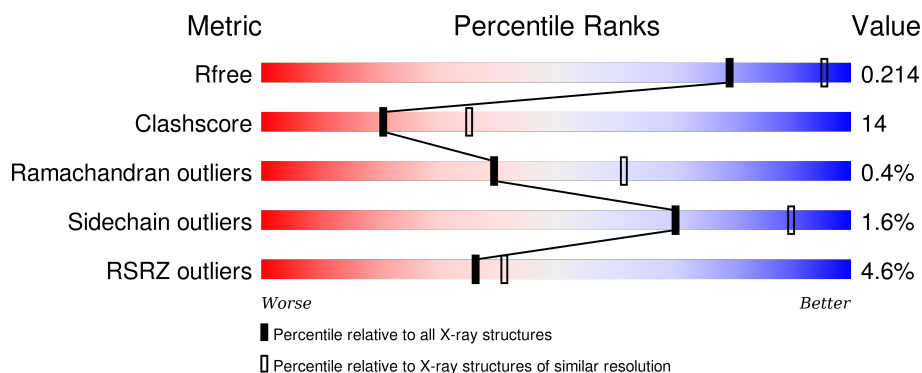|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.214
Clashscore		14
Ramachandran outliers		0.4%
Sidechain outliers		1.6%
RSRZ outliers		4.6%

Worse   *Better*

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

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	450	2% 68% 23% • 8%
1	B	450	4% 71% 22% • 6%
1	C	450	6% 68% 26% • •
1	D	450	6% 74% 19% • 5%

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	RVB	A	451	-	-	X	-
2	RVB	D	451	-	-	-	X

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2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13371 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 Isochorismate synthase/isochorismate-pyruvate lyase mbtI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	2	0
			3151	1981	559	601	10			
1	B	423	Total	C	N	O	S	0	1	0
			3211	2012	580	609	10			
1	C	431	Total	C	N	O	S	0	0	0
			3254	2036	588	620	10			
1	D	428	Total	C	N	O	S	0	0	0
			3222	2021	571	620	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	VAL	-	EXPRESSION TAG	UNP Q7D785
B	1	VAL	-	EXPRESSION TAG	UNP Q7D785
C	1	VAL	-	EXPRESSION TAG	UNP Q7D785
D	1	VAL	-	EXPRESSION TAG	UNP Q7D785

- Molecule 2 is 3-{[(1Z)-1-CARBOXY-3-METHYLBUT-1-EN-1-YL]OXY}-2-HYDROXYBE NZOIC ACID (three-letter code: RVB) (formula: $C_{13}H_{14}O_6$).
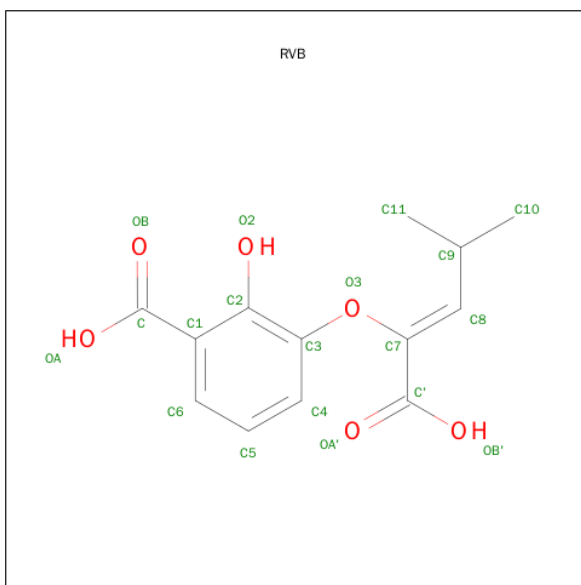
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 19	C 13	O 6	0	0
2	B	1	Total 19	C 13	O 6	0	0
2	C	1	Total 19	C 13	O 6	4	0
2	D	1	Total 19	C 13	O 6	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	121	Total 121	O 121	0	0
3	B	118	Total 118	O 118	0	0
3	C	115	Total 115	O 115	0	0
3	D	103	Total 103	O 103	0	0

3 Residue-property plots ⓘ

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

- Molecule 1: Isochorismate synthase/isochorismate-pyruvate lyase mbtI
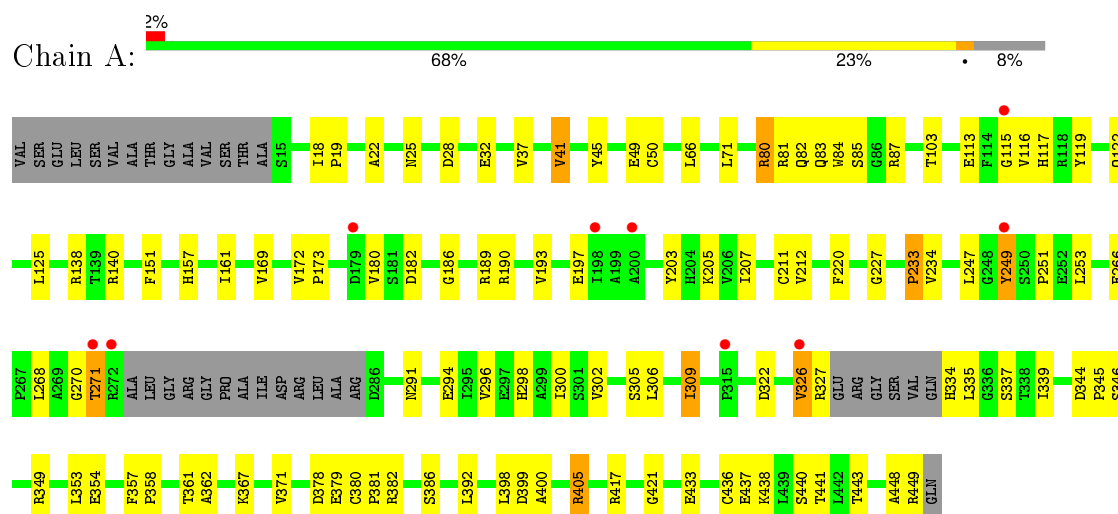
Chain A:
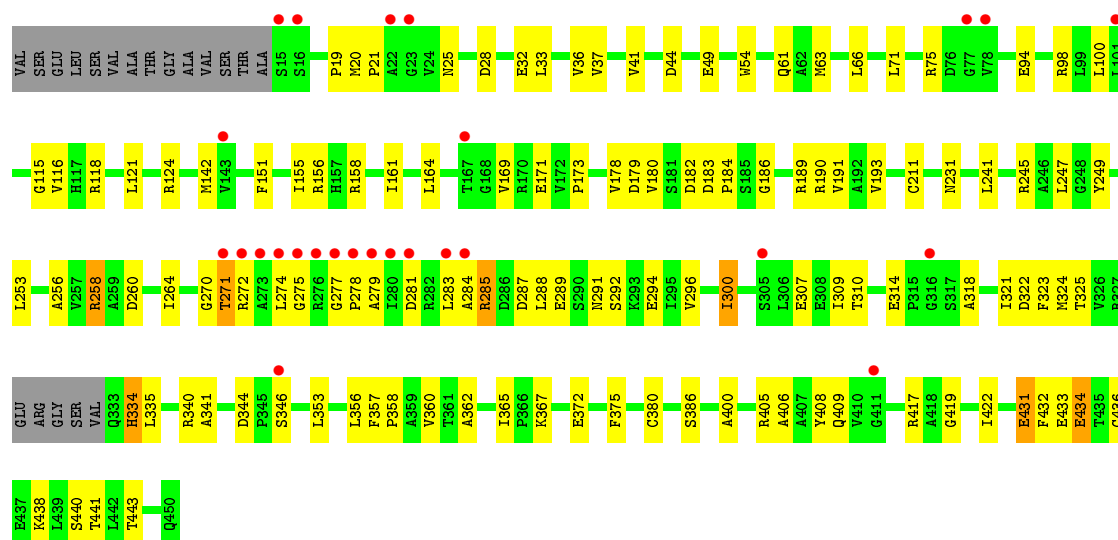
- Molecule 1: Isochorismate synthase/isochorismate-pyruvate lyase mbtI
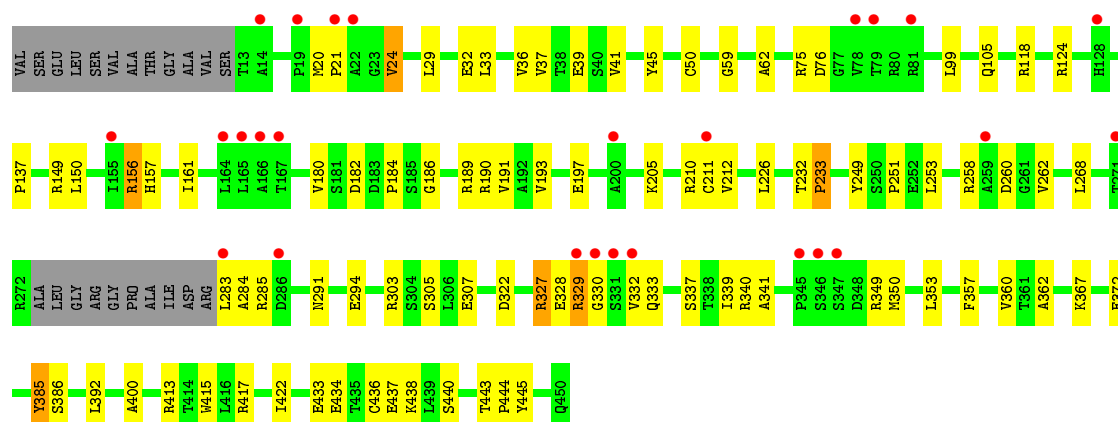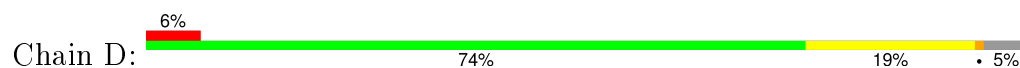
Chain B:

- Molecule 1: Isochorismate synthase/isochorismate-pyruvate lyase mbtI

Chain C:

• Molecule 1: Isochorismate synthase/isochorismate-pyruvate lyase mbtI

Chain D:
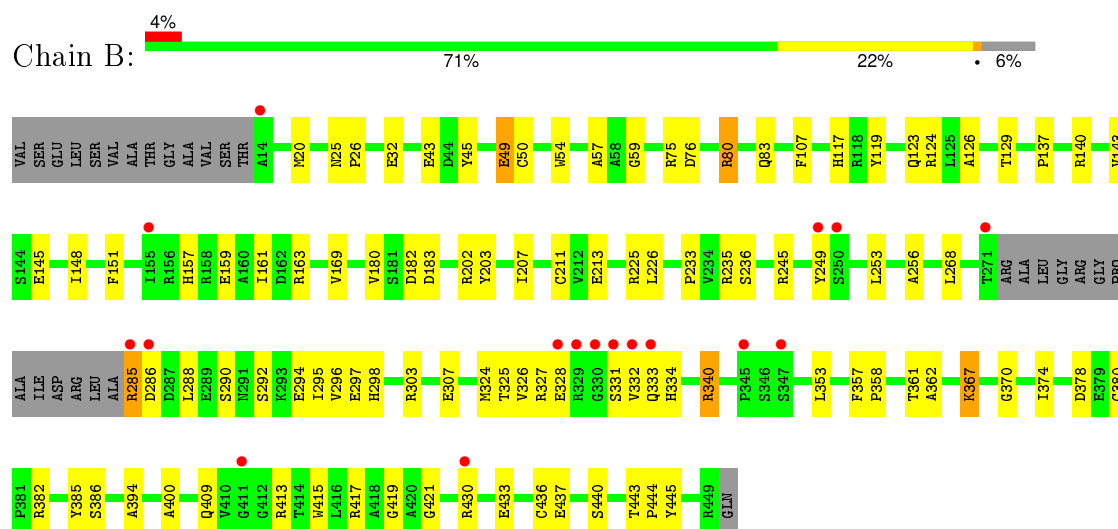
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.67Å 113.94Å 95.23Å 90.00° 91.41° 90.00°	Depositor
Resolution (Å)	19.78 – 2.50 19.78 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.78-2.50) 99.7 (19.78-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 2.50Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.184 , 0.222 0.198 , 0.214	Depositor DCC
R_{free} test set	3224 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	38.0	Xtriage
Anisotropy	0.471	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 67.7	EDS
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Outliers	1 of 63699 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13371	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	1.59	7/3213 (0.2%)	0.80	0/4370
1	B	1.53	6/3270 (0.2%)	0.79	1/4444 (0.0%)
1	C	1.51	6/3311 (0.2%)	0.77	2/4501 (0.0%)
1	D	1.49	4/3278 (0.1%)	0.78	0/4459
All	All	1.53	23/13072 (0.2%)	0.78	3/17774 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	249	TYR	CD1-CE1	-6.39	1.29	1.39
1	B	119	TYR	CD1-CE1	-5.96	1.30	1.39
1	C	380	CYS	CB-SG	-5.91	1.72	1.81
1	B	50	CYS	CB-SG	-5.91	1.72	1.81
1	B	45	TYR	CD1-CE1	-5.78	1.30	1.39
1	A	234	VAL	CB-CG2	-5.76	1.40	1.52
1	A	50	CYS	CB-SG	-5.73	1.72	1.81
1	A	49	GLU	CD-OE1	-5.72	1.19	1.25
1	D	50	CYS	CB-SG	-5.70	1.72	1.81
1	D	45	TYR	CD2-CE2	-5.55	1.31	1.39
1	C	249	TYR	CD2-CE2	-5.46	1.31	1.39
1	A	41	VAL	CB-CG1	-5.43	1.41	1.52
1	D	249	TYR	CD2-CE2	-5.39	1.31	1.39
1	A	203	TYR	CD2-CE2	-5.37	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	45	TYR	CD1-CE1	-5.33	1.31	1.39
1	B	45	TYR	CD2-CE2	-5.25	1.31	1.39
1	B	49	GLU	CD-OE1	-5.22	1.20	1.25
1	C	193	VAL	CB-CG2	-5.21	1.42	1.52
1	D	385	TYR	CD2-CE2	-5.15	1.31	1.39
1	C	249	TYR	CE1-CZ	-5.05	1.31	1.38
1	B	380	CYS	CB-SG	-5.05	1.73	1.81
1	A	45	TYR	CD2-CE2	-5.04	1.31	1.39
1	C	408	TYR	CD1-CE1	-5.00	1.31	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	124	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	C	20	MET	C-N-CD	-5.21	109.15	120.60
1	C	44	ASP	CB-CG-OD1	5.04	122.84	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	182[A]	ASP	Mainchain
1	A	182[B]	ASP	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3151	0	3107	90	0
1	B	3211	0	3191	89	0
1	C	3254	0	3209	110	0
1	D	3222	0	3164	82	0
2	A	19	0	11	11	0
2	B	19	0	11	4	0
2	C	19	0	11	2	0
2	D	19	0	11	6	0
3	A	121	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	118	0	0	5	0
3	C	115	0	0	0	0
3	D	103	0	0	0	0
All	All	13371	0	12715	371	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 14.

All (371) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:THR:HG21	2:A:451:RVB:C10	1.62	1.27
1:A:361:THR:CG2	2:A:451:RVB:H10	1.69	1.21
1:C:291:ASN:HD22	1:C:294:GLU:HG2	1.05	1.17
1:C:272:ARG:HG3	1:C:284:ALA:HB1	1.24	1.16
1:C:271:THR:H	1:C:334:HIS:HB3	1.13	1.13
1:A:291:ASN:HD22	1:A:294:GLU:HG2	1.12	1.13
1:B:20:MET:HE2	1:B:148:ILE:HD11	1.27	1.11
1:C:274:LEU:HD23	1:C:275:GLY:N	1.68	1.07
1:B:331:SER:HA	1:B:332:VAL:HG22	1.32	1.06
1:C:431:GLU:OE1	1:C:431:GLU:HA	1.54	1.02
1:A:361:THR:HG21	2:A:451:RVB:H10	1.03	1.02
1:C:274:LEU:HD23	1:C:275:GLY:H	1.19	1.01
1:A:233:PRO:HG3	1:A:249:TYR:HB3	1.39	1.00
2:D:451:RVB:H10	2:D:451:RVB:O3	1.63	0.98
1:B:20:MET:HE3	1:B:148:ILE:HG13	1.43	0.98
1:C:36:VAL:HG12	1:C:37:VAL:N	1.78	0.95
1:C:271:THR:HG23	1:C:271:THR:O	1.64	0.95
1:C:291:ASN:ND2	1:C:294:GLU:HG2	1.83	0.93
1:A:358:PRO:O	1:A:367:LYS:HE3	1.69	0.93
1:A:448:ALA:O	1:A:449:ARG:HB2	1.68	0.92
1:A:205:LYS:HE2	3:A:564:HOH:O	1.68	0.91
1:B:20:MET:CE	1:B:148:ILE:CG1	2.50	0.90
1:D:283:LEU:O	1:D:284:ALA:HB3	1.71	0.90
1:B:340:ARG:HH11	1:B:340:ARG:HG3	1.36	0.89
1:A:291:ASN:ND2	1:A:294:GLU:HG2	1.89	0.87
1:B:20:MET:HE2	1:B:148:ILE:CD1	2.03	0.87
1:B:303:ARG:O	1:B:307:GLU:HG3	1.74	0.87
1:A:271:THR:HB	1:A:334:HIS:CD2	2.10	0.86
1:C:270:GLY:O	1:C:271:THR:HG22	1.74	0.86
1:B:331:SER:HA	1:B:332:VAL:CG2	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:THR:HG21	2:B:451:RVB:H10	1.58	0.85
1:D:291:ASN:HD22	1:D:294:GLU:HG2	1.40	0.84
1:A:358:PRO:O	1:A:367:LYS:CE	2.24	0.84
1:A:380:CYS:HB3	1:A:381:PRO:HA	1.60	0.84
1:C:271:THR:N	1:C:334:HIS:HB3	1.93	0.84
1:B:20:MET:HE3	1:B:148:ILE:CG1	2.07	0.83
1:D:75:ARG:HG2	1:D:76:ASP:OD2	1.77	0.83
1:C:272:ARG:HG3	1:C:284:ALA:CB	2.08	0.83
1:C:272:ARG:CG	1:C:284:ALA:HB1	2.09	0.81
1:B:285:ARG:HB2	1:B:333:GLN:OE1	1.80	0.81
1:C:270:GLY:HA3	1:C:335:LEU:H	1.47	0.80
1:C:284:ALA:O	1:C:288:LEU:HB3	1.80	0.80
1:C:271:THR:O	1:C:271:THR:CG2	2.28	0.79
1:B:340:ARG:NH1	1:B:340:ARG:HG3	1.89	0.79
1:C:434:GLU:O	1:C:434:GLU:OE1	2.01	0.78
1:D:118:ARG:HH21	1:D:118:ARG:HG3	1.48	0.78
1:C:36:VAL:CG1	1:C:37:VAL:N	2.46	0.78
1:D:20:MET:CE	1:D:24:VAL:HG22	2.12	0.78
1:A:448:ALA:O	1:A:449:ARG:CB	2.32	0.76
1:B:419:GLY:N	2:B:451:RVB:OA	2.18	0.76
2:D:451:RVB:C10	2:D:451:RVB:O3	2.29	0.76
1:A:270:GLY:HA3	1:A:335:LEU:H	1.50	0.76
1:C:360:VAL:HG23	1:C:367:LYS:HE3	1.66	0.76
1:D:205:LYS:HG3	1:D:422:ILE:O	1.85	0.75
1:A:270:GLY:O	1:A:271:THR:HG22	1.86	0.75
1:D:303:ARG:O	1:D:307:GLU:HG3	1.87	0.74
1:D:327:ARG:HH21	1:D:327:ARG:HG3	1.51	0.74
1:D:156:ARG:HG2	1:D:157:HIS:N	2.02	0.73
1:C:291:ASN:HD22	1:C:294:GLU:CG	1.94	0.72
1:C:431:GLU:OE1	1:C:431:GLU:CA	2.34	0.71
1:B:328:GLU:O	1:B:328:GLU:CD	2.29	0.71
1:B:362:ALA:HB1	1:B:386:SER:HB2	1.72	0.71
1:C:274:LEU:CD2	1:C:275:GLY:N	2.52	0.71
1:A:233:PRO:CG	1:A:249:TYR:HB3	2.20	0.71
1:B:294:GLU:HA	1:B:294:GLU:OE2	1.91	0.70
1:D:32:GLU:O	1:D:36:VAL:HG12	1.90	0.70
1:D:413:ARG:HG2	1:D:415:TRP:HE3	1.57	0.70
1:D:413:ARG:HG2	1:D:415:TRP:CE3	2.26	0.69
1:B:233:PRO:HG3	1:B:249:TYR:HB3	1.74	0.69
1:A:271:THR:HB	1:A:334:HIS:NE2	2.06	0.69
1:D:253:LEU:HD12	1:D:400:ALA:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:ARG:HG2	1:B:415:TRP:CE3	2.27	0.68
1:B:378:ASP:OD2	1:B:382:ARG:NH2	2.27	0.68
1:A:227:GLY:HA3	1:A:249:TYR:OH	1.94	0.67
1:B:340:ARG:HH11	1:B:340:ARG:CG	2.06	0.67
1:D:20:MET:HE3	1:D:24:VAL:HG22	1.76	0.66
1:A:180:VAL:HG12	1:A:212:VAL:HG11	1.76	0.66
1:D:211:CYS:SG	1:D:417:ARG:HG3	2.35	0.66
1:B:20:MET:CE	1:B:148:ILE:HG13	2.15	0.66
1:D:283:LEU:C	1:D:285:ARG:H	1.97	0.66
1:A:298:HIS:O	1:A:302:VAL:HG23	1.97	0.64
1:A:113:GLU:O	1:A:116:VAL:HG22	1.98	0.64
1:A:362:ALA:HB1	1:A:386:SER:HB2	1.77	0.64
1:C:253:LEU:HD12	1:C:400:ALA:O	1.98	0.64
1:C:284:ALA:O	1:C:288:LEU:CB	2.45	0.64
1:A:361:THR:CG2	2:A:451:RVB:C10	2.48	0.63
1:A:398:LEU:HD12	1:A:399:ASP:N	2.12	0.63
1:B:353:LEU:O	1:B:357:PHE:HB2	1.99	0.63
1:B:20:MET:CE	1:B:148:ILE:HD11	2.17	0.63
1:B:80:ARG:NH2	3:B:457:HOH:O	2.31	0.63
1:C:321:ILE:HD13	1:C:340:ARG:HD2	1.80	0.63
1:D:340:ARG:HG2	1:D:341:ALA:N	2.14	0.63
1:C:277:GLY:O	1:C:279:ALA:N	2.31	0.63
1:C:309:ILE:HD12	1:C:341:ALA:HB2	1.81	0.63
1:A:211:CYS:SG	1:A:417:ARG:HD2	2.39	0.62
1:C:155:ILE:HG13	1:C:158:ARG:NH1	2.15	0.62
1:B:233:PRO:HB3	1:B:249:TYR:HB3	1.81	0.62
1:B:413:ARG:HG2	1:B:415:TRP:HE3	1.64	0.62
1:B:117:HIS:H	1:B:117:HIS:CD2	2.17	0.62
1:C:353:LEU:O	1:C:357:PHE:HB2	2.00	0.62
1:A:438:LYS:HE2	2:A:451:RVB:C2	2.30	0.61
1:A:367:LYS:O	1:A:371:VAL:HG23	2.00	0.61
1:C:292:SER:O	1:C:296:VAL:HG23	2.00	0.61
1:D:20:MET:HE1	1:D:24:VAL:CG2	2.31	0.61
1:B:20:MET:CE	1:B:148:ILE:HG12	2.29	0.61
1:D:193:VAL:O	1:D:197:GLU:HG3	2.01	0.61
1:B:43:GLU:HG2	1:B:59:GLY:HA2	1.83	0.61
1:C:284:ALA:O	1:C:288:LEU:N	2.30	0.61
1:D:283:LEU:C	1:D:285:ARG:N	2.53	0.61
1:B:325:THR:HG22	1:B:326:VAL:N	2.16	0.61
1:C:258:ARG:NH2	1:C:260:ASP:OD2	2.33	0.60
1:B:182:ASP:OD2	1:B:183:ASP:N	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:ASN:OD1	1:C:441:THR:CG2	2.49	0.60
1:A:115:GLY:HA3	1:A:358:PRO:HD3	1.84	0.60
1:B:26:PRO:HB2	1:B:54:TRP:CZ3	2.37	0.60
1:D:291:ASN:ND2	1:D:294:GLU:HG2	2.14	0.59
1:A:193:VAL:O	1:A:197:GLU:HG3	2.02	0.59
1:D:283:LEU:O	1:D:284:ALA:CB	2.39	0.59
1:B:292:SER:O	1:B:296:VAL:HG23	2.03	0.59
1:D:226:LEU:HG	1:D:445:TYR:HB3	1.84	0.59
1:B:32:GLU:OE2	1:B:225:ARG:NH1	2.34	0.59
1:B:20:MET:HE1	1:B:143:VAL:HG13	1.84	0.59
1:A:116:VAL:HG21	1:A:125:LEU:HD11	1.84	0.59
1:D:362:ALA:HB1	1:D:386:SER:HB2	1.84	0.59
1:D:189:ARG:O	1:D:193:VAL:HG23	2.03	0.59
1:C:277:GLY:C	1:C:279:ALA:H	2.05	0.58
1:C:362:ALA:HB1	1:C:386:SER:HB2	1.85	0.58
1:C:115:GLY:HA3	1:C:358:PRO:HD3	1.83	0.58
1:B:430:ARG:O	1:B:430:ARG:HD2	2.03	0.58
1:B:233:PRO:CG	1:B:249:TYR:HB3	2.32	0.58
1:B:226:LEU:HG	1:B:445:TYR:HB3	1.84	0.58
1:A:186:GLY:O	1:A:190:ARG:HG3	2.04	0.58
1:A:80:ARG:HH21	1:A:81:ARG:H	1.50	0.58
1:D:20:MET:HE1	1:D:24:VAL:HG22	1.85	0.57
1:C:296:VAL:HG12	1:C:300:ILE:HD12	1.86	0.57
1:D:191:VAL:HG13	1:D:422:ILE:HD12	1.85	0.57
1:A:37:VAL:O	1:A:41:VAL:HG12	2.05	0.57
1:C:440:SER:HA	1:C:443:THR:OG1	2.04	0.57
1:D:20:MET:CE	1:D:24:VAL:CG2	2.81	0.57
1:C:270:GLY:O	1:C:271:THR:CG2	2.50	0.57
1:B:358:PRO:O	1:B:367:LYS:HE2	2.05	0.57
1:B:32:GLU:HG3	1:B:169:VAL:HG12	1.85	0.57
1:C:49:GLU:HB2	1:C:54:TRP:NE1	2.19	0.57
1:C:419:GLY:N	2:C:451:RVB:OA	2.37	0.56
1:D:283:LEU:O	1:D:285:ARG:N	2.35	0.56
1:A:220:PHE:CD2	1:A:247:LEU:HD23	2.40	0.56
1:A:326:VAL:HA	1:A:334:HIS:O	2.05	0.56
1:C:307:GLU:O	1:C:310:THR:HB	2.06	0.56
1:A:80:ARG:HD3	1:A:80:ARG:C	2.26	0.56
1:C:19:PRO:O	1:C:21:PRO:HD3	2.05	0.56
1:D:124:ARG:NH2	1:D:372:GLU:OE2	2.38	0.56
1:A:84:TRP:HH2	1:A:117[B]:HIS:CE1	2.23	0.56
1:A:379:GLU:HG3	3:A:548:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:443:THR:N	1:D:444:PRO:CD	2.69	0.55
1:C:309:ILE:HG22	1:C:356:LEU:HD21	1.88	0.55
1:B:385:TYR:CG	1:B:417:ARG:HD3	2.41	0.55
1:C:36:VAL:HG12	1:C:37:VAL:H	1.65	0.55
1:D:118:ARG:NH2	1:D:118:ARG:HG3	2.21	0.54
1:B:126:ALA:O	1:B:129:THR:OG1	2.22	0.54
1:B:233:PRO:CB	1:B:249:TYR:HB3	2.38	0.54
1:C:285:ARG:O	1:C:289:GLU:HB2	2.08	0.54
1:C:33:LEU:HD11	1:C:161:ILE:HG12	1.88	0.54
1:B:57:ALA:HB1	1:B:137:PRO:HB3	1.90	0.54
1:A:189:ARG:HH21	1:C:118:ARG:HA	1.72	0.54
1:D:156:ARG:HG2	1:D:157:HIS:H	1.72	0.53
1:A:113:GLU:HA	1:A:116:VAL:HG13	1.91	0.53
1:C:277:GLY:C	1:C:279:ALA:N	2.62	0.53
1:D:62:ALA:HB3	1:D:99:LEU:HD22	1.89	0.53
1:A:433:GLU:O	1:A:437:GLU:HG3	2.08	0.53
1:A:157:HIS:O	1:A:161:ILE:HG13	2.08	0.53
1:D:349:ARG:HG3	1:D:350:MET:N	2.23	0.53
1:B:394:ALA:HB1	1:C:189:ARG:HD3	1.92	0.52
1:C:142:MET:HG3	1:C:151:PHE:HE2	1.75	0.52
1:B:159:GLU:O	1:B:163:ARG:HG3	2.09	0.52
1:D:186:GLY:O	1:D:190:ARG:HG3	2.09	0.52
1:A:322:ASP:O	1:A:337:SER:HA	2.10	0.52
1:C:247:LEU:O	1:C:406:ALA:HA	2.10	0.52
1:B:26:PRO:HG3	1:B:145:GLU:HA	1.92	0.51
1:B:433:GLU:O	1:B:436:CYS:HB2	2.10	0.51
1:C:334:HIS:ND1	1:C:334:HIS:N	2.57	0.51
1:B:361:THR:CG2	2:B:451:RVB:H10	2.35	0.51
1:B:49:GLU:HB2	1:B:54:TRP:CD1	2.45	0.51
1:A:189:ARG:NH2	1:C:118:ARG:HA	2.25	0.51
1:A:80:ARG:HD3	1:A:81:ARG:N	2.26	0.51
1:D:443:THR:N	1:D:444:PRO:HD3	2.26	0.51
1:C:309:ILE:CG2	1:C:356:LEU:HD21	2.41	0.51
1:D:260:ASP:OD1	1:D:262:VAL:HG23	2.10	0.51
2:D:451:RVB:H10	2:D:451:RVB:C3	2.38	0.51
1:D:33:LEU:HD11	1:D:161:ILE:HG12	1.92	0.51
1:C:360:VAL:CG2	1:C:367:LYS:HE3	2.36	0.51
1:C:61:GLN:HE21	1:C:75:ARG:NH1	2.08	0.51
1:B:382:ARG:HG2	1:B:385:TYR:HD2	1.76	0.50
1:D:149:ARG:C	1:D:150:LEU:HD23	2.31	0.50
1:D:332:VAL:HG22	1:D:333:GLN:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:ASN:OD1	1:C:441:THR:HG22	2.12	0.50
1:B:233:PRO:HB3	1:B:249:TYR:CB	2.41	0.50
1:A:251:PRO:HB2	2:A:451:RVB:H11A	1.93	0.50
1:A:37:VAL:O	1:A:41:VAL:CG1	2.59	0.50
1:B:437:GLU:O	1:B:440:SER:OG	2.30	0.50
1:C:32:GLU:HG3	1:C:169:VAL:HB	1.92	0.50
1:C:66:LEU:HD13	1:C:71:LEU:HD13	1.94	0.50
1:B:298:HIS:CD2	1:B:324:MET:HG3	2.46	0.50
1:D:180:VAL:HG12	1:D:212:VAL:HG11	1.94	0.50
1:B:233:PRO:HB2	1:B:235:ARG:O	2.12	0.49
1:A:405:ARG:HH11	1:A:405:ARG:HG2	1.77	0.49
1:C:372:GLU:O	1:C:375:PHE:HB2	2.12	0.49
1:B:123[B]:GLN:H	1:B:123[B]:GLN:CD	2.16	0.49
1:A:353:LEU:O	1:A:357:PHE:HB2	2.12	0.49
1:A:378:ASP:OD2	1:A:382:ARG:NH2	2.36	0.49
1:D:353:LEU:O	1:D:357:PHE:HB2	2.12	0.49
1:D:362:ALA:CB	1:D:386:SER:HB2	2.41	0.49
1:A:268:LEU:HD23	2:A:451:RVB:H11B	1.94	0.49
1:A:306:LEU:O	1:A:309:ILE:HG22	2.13	0.49
1:B:328:GLU:OE1	1:B:328:GLU:O	2.30	0.49
1:A:103:THR:HB	3:A:504:HOH:O	2.12	0.49
1:C:283:LEU:O	1:C:287:ASP:HB3	2.13	0.49
1:D:21:PRO:O	1:D:24:VAL:HG13	2.13	0.49
1:A:433:GLU:O	1:A:436:CYS:HB2	2.12	0.49
1:A:361:THR:HG21	2:A:451:RVB:H10B	1.80	0.49
1:C:49:GLU:HB2	1:C:54:TRP:CD1	2.47	0.48
1:C:41:VAL:HG22	1:C:156:ARG:CZ	2.43	0.48
1:D:24:VAL:HG21	1:D:29:LEU:HB2	1.94	0.48
1:B:325:THR:CG2	1:B:326:VAL:N	2.75	0.48
1:B:75:ARG:O	1:B:76:ASP:HB2	2.12	0.48
1:A:253:LEU:HD12	1:A:400:ALA:O	2.13	0.48
1:B:25:ASN:ND2	3:B:547:HOH:O	2.33	0.48
1:D:21:PRO:O	1:D:24:VAL:CG1	2.61	0.48
1:D:437:GLU:O	1:D:440:SER:OG	2.30	0.48
1:C:288:LEU:HD21	1:C:334:HIS:HA	1.96	0.48
1:C:344:ASP:OD1	1:C:346:SER:OG	2.30	0.48
1:B:117:HIS:CD2	1:B:117:HIS:N	2.81	0.47
1:D:305:SER:HB2	1:D:339:ILE:HD13	1.96	0.47
1:D:305:SER:HB2	1:D:339:ILE:CD1	2.45	0.47
1:C:322:ASP:OD2	1:C:325:THR:HB	2.13	0.47
1:A:405:ARG:NH1	1:A:441:THR:HG21	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:CYS:SG	1:D:417:ARG:CD	3.03	0.47
1:A:437:GLU:O	1:A:440:SER:OG	2.29	0.47
1:D:59:GLY:O	1:D:137:PRO:HA	2.15	0.47
1:A:268:LEU:HD23	2:A:451:RVB:C11	2.44	0.47
1:B:20:MET:CE	1:B:148:ILE:CD1	2.74	0.47
1:B:295:ILE:HG23	1:B:324:MET:HE1	1.95	0.47
1:C:98:ARG:N	1:C:98:ARG:HD3	2.30	0.47
1:D:118:ARG:HH21	1:D:118:ARG:CG	2.23	0.47
1:D:327:ARG:NH2	1:D:327:ARG:HG3	2.21	0.47
1:C:186:GLY:O	1:C:190:ARG:HG3	2.15	0.47
1:B:327:ARG:O	1:B:334:HIS:N	2.38	0.47
1:C:94:GLU:O	1:C:98:ARG:HG2	2.14	0.47
1:B:370:GLY:O	1:B:374:ILE:HG13	2.15	0.47
1:A:440:SER:HA	1:A:443:THR:OG1	2.15	0.47
1:D:37:VAL:O	1:D:41:VAL:HG22	2.15	0.47
1:C:323:PHE:CE2	1:C:324:MET:HE2	2.49	0.47
1:C:211:CYS:SG	1:C:417:ARG:HD2	2.55	0.46
1:D:75:ARG:CG	1:D:76:ASP:OD2	2.57	0.46
1:D:385:TYR:CG	1:D:417:ARG:HD3	2.50	0.46
1:C:321:ILE:CD1	1:C:340:ARG:HD2	2.44	0.46
1:C:155:ILE:HG13	1:C:158:ARG:HH12	1.80	0.46
1:C:245:ARG:HB2	1:C:409:GLN:HB3	1.98	0.46
1:C:433:GLU:O	1:C:436:CYS:HB2	2.15	0.46
1:A:266:GLU:OE1	1:A:327:ARG:NH1	2.47	0.46
1:B:443:THR:N	1:B:444:PRO:CD	2.79	0.46
1:A:358:PRO:O	1:A:367:LYS:HE2	2.09	0.46
1:B:334:HIS:CE1	2:B:451:RVB:H11	2.51	0.46
1:C:321:ILE:HD13	1:C:340:ARG:CD	2.46	0.46
1:C:314:GLU:HG3	1:C:344:ASP:HA	1.97	0.46
1:C:124:ARG:NH2	1:C:372:GLU:OE2	2.49	0.46
1:D:360:VAL:HG23	1:D:367:LYS:HE2	1.97	0.46
1:A:251:PRO:HB2	2:A:451:RVB:C11	2.46	0.46
1:D:258:ARG:HB2	1:D:260:ASP:OD1	2.16	0.46
1:C:183:ASP:N	1:C:184:PRO:CD	2.79	0.46
1:B:285:ARG:CB	1:B:333:GLN:OE1	2.58	0.46
1:B:286:ASP:O	1:B:290:SER:OG	2.30	0.46
1:D:332:VAL:HG22	1:D:333:GLN:N	2.31	0.45
1:A:296:VAL:O	1:A:300:ILE:HG13	2.16	0.45
2:D:451:RVB:O2	2:D:451:RVB:OB	2.32	0.45
1:A:119:TYR:OH	1:A:367:LYS:HD2	2.16	0.45
1:D:253:LEU:CD1	1:D:400:ALA:O	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:GLU:CD	1:C:54:TRP:CZ2	2.89	0.45
2:A:451:RVB:O2	2:A:451:RVB:OA	2.30	0.45
1:D:329:ARG:HA	1:D:330:GLY:HA2	1.50	0.45
1:C:272:ARG:HA	1:C:272:ARG:HD3	1.55	0.45
1:B:107:PHE:N	1:B:107:PHE:CD2	2.85	0.45
1:B:253:LEU:HD12	1:B:400:ALA:O	2.17	0.45
1:A:25:ASN:HB3	1:A:28:ASP:OD2	2.17	0.45
1:D:251:PRO:HB2	2:D:451:RVB:H10B	2.00	0.44
1:C:258:ARG:HB2	1:C:260:ASP:OD1	2.18	0.44
1:C:191:VAL:HG13	1:C:422:ILE:HD12	2.00	0.44
1:D:20:MET:HE1	1:D:24:VAL:HG21	1.99	0.44
1:C:438:LYS:HE2	2:C:451:RVB:C'	2.48	0.44
1:C:322:ASP:OD2	1:C:325:THR:CB	2.65	0.44
1:A:122:GLN:N	1:A:122:GLN:OE1	2.30	0.44
1:C:100:LEU:HA	1:C:100:LEU:HD23	1.89	0.44
1:C:422:ILE:CD1	1:C:431:GLU:HG3	2.47	0.44
1:D:327:ARG:HD2	1:D:327:ARG:HA	1.83	0.44
1:C:309:ILE:HG13	1:C:310:THR:N	2.32	0.44
1:C:171:GLU:O	1:C:173:PRO:HD3	2.18	0.44
1:C:25:ASN:HB3	1:C:28:ASP:OD2	2.17	0.44
1:B:49:GLU:OE2	1:B:236:SER:OG	2.27	0.44
1:B:180:VAL:HG11	1:B:443:THR:HG21	1.99	0.44
1:C:272:ARG:HG2	1:C:288:LEU:HD13	2.00	0.44
1:B:43:GLU:HG2	1:B:59:GLY:CA	2.47	0.44
1:A:18:ILE:O	1:A:18:ILE:HG13	2.18	0.44
1:A:207:ILE:HG13	1:A:421:GLY:HA2	2.00	0.43
1:A:140:ARG:HB2	1:A:151:PHE:HB2	1.99	0.43
1:B:297:GLU:HA	1:B:297:GLU:OE1	2.17	0.43
1:B:202:ARG:HG2	1:B:203:TYR:CD2	2.53	0.43
1:D:24:VAL:CG2	1:D:29:LEU:HB2	2.48	0.43
1:A:117[B]:HIS:CD2	1:A:117[B]:HIS:H	2.35	0.43
1:C:274:LEU:HA	1:C:281:ASP:OD2	2.19	0.43
1:B:288:LEU:HD12	1:B:294:GLU:HG3	2.00	0.43
1:B:211:CYS:SG	1:B:417:ARG:HD2	2.59	0.43
1:D:150:LEU:HD23	1:D:150:LEU:N	2.33	0.43
1:C:245:ARG:HH21	1:C:409:GLN:HE22	1.65	0.43
1:C:182:ASP:HB3	1:C:184:PRO:HD3	2.00	0.43
1:C:256:ALA:HB3	1:C:264:ILE:HB	2.00	0.43
1:C:432:PHE:CD2	1:C:432:PHE:C	2.91	0.43
1:C:180:VAL:O	1:C:180:VAL:HG23	2.19	0.43
1:C:300:ILE:CG2	1:C:365:ILE:HD13	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:ARG:N	1:A:334:HIS:O	2.38	0.43
1:D:327:ARG:O	1:D:328:GLU:CB	2.65	0.43
1:C:155:ILE:CG1	1:C:158:ARG:NH1	2.82	0.43
1:D:210:ARG:O	1:D:210:ARG:HG3	2.19	0.43
1:A:138:ARG:NH2	1:D:39:GLU:OE2	2.39	0.43
1:C:270:GLY:O	1:C:271:THR:CB	2.67	0.42
1:D:182:ASP:CG	1:D:184:PRO:HD3	2.40	0.42
1:B:253:LEU:HD21	1:B:256:ALA:HB2	2.01	0.42
1:C:63:MET:HE1	1:C:241:LEU:HD11	2.01	0.42
1:B:207:ILE:HG13	1:B:421:GLY:HA2	2.01	0.42
1:B:332:VAL:HG12	3:B:452:HOH:O	2.19	0.42
1:D:433:GLU:O	1:D:436:CYS:HB2	2.19	0.42
1:A:83:GLN:NE2	1:A:85:SER:OG	2.49	0.42
1:A:233:PRO:CB	1:A:249:TYR:HB3	2.50	0.42
1:D:328:GLU:O	1:D:329:ARG:CB	2.66	0.42
1:D:211:CYS:SG	1:D:417:ARG:CG	3.06	0.42
1:D:322:ASP:O	1:D:337:SER:HA	2.20	0.42
1:A:305:SER:HB2	1:A:339:ILE:HD13	2.00	0.42
1:D:105:GLN:HA	1:D:392:LEU:O	2.20	0.42
1:A:344:ASP:OD1	1:A:346:SER:OG	2.30	0.42
1:A:405:ARG:HH11	1:A:441:THR:HG21	1.85	0.42
1:C:36:VAL:HG12	1:C:37:VAL:HG13	2.01	0.42
1:C:32:GLU:HB3	1:C:164:LEU:HD11	2.01	0.42
1:A:18:ILE:CG1	1:A:18:ILE:O	2.68	0.42
1:D:20:MET:HE3	1:D:24:VAL:CG2	2.49	0.41
1:C:116:VAL:HB	1:C:121:LEU:HB2	2.02	0.41
1:B:213:GLU:OE1	1:B:413:ARG:NE	2.36	0.41
1:D:41:VAL:HG11	1:D:156:ARG:HG3	2.01	0.41
1:A:80:ARG:HD2	1:B:83:GLN:HG2	2.03	0.41
1:A:349:ARG:HD2	1:A:392:LEU:HD23	2.02	0.41
1:C:287:ASP:O	1:C:291:ASN:HB2	2.21	0.41
1:A:344:ASP:HA	1:A:345:PRO:HD3	1.89	0.41
1:B:140:ARG:HB2	1:B:151:PHE:HB2	2.03	0.41
1:A:22:ALA:O	3:A:453:HOH:O	2.22	0.41
1:C:309:ILE:HD11	1:C:318:ALA:HB1	2.01	0.41
1:B:326:VAL:HG12	3:B:544:HOH:O	2.19	0.41
1:D:232:THR:HA	1:D:233:PRO:HD2	1.85	0.41
1:A:66:LEU:HD13	1:A:71:LEU:HD12	2.01	0.41
1:A:32:GLU:HG3	1:A:169:VAL:HG12	2.02	0.41
1:C:178:VAL:HG22	1:C:179:ASP:N	2.36	0.41
1:B:157:HIS:O	1:B:161:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ARG:HB3	1:A:354:GLU:OE1	2.20	0.41
1:B:245:ARG:HB2	1:B:409:GLN:HB3	2.02	0.41
1:A:172:VAL:HA	1:A:173:PRO:HD3	1.92	0.41
1:B:328:GLU:OE1	1:B:328:GLU:C	2.59	0.40
1:B:413:ARG:NH2	3:B:567:HOH:O	2.30	0.40
1:A:189:ARG:O	1:A:193:VAL:HG23	2.21	0.40
1:A:113:GLU:HA	1:A:116:VAL:CG1	2.51	0.40
1:A:41:VAL:O	1:A:41:VAL:CG2	2.68	0.40
1:D:434:GLU:O	1:D:438:LYS:HG3	2.20	0.40
1:D:20:MET:HE3	1:D:24:VAL:HG13	2.03	0.40
1:C:271:THR:O	1:C:272:ARG:NH1	2.54	0.40
1:D:268:LEU:HB2	2:D:451:RVB:C11	2.51	0.40
1:C:41:VAL:O	1:C:41:VAL:CG1	2.68	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	412/450 (92%)	405 (98%)	4 (1%)	3 (1%)	26	46
1	B	420/450 (93%)	411 (98%)	9 (2%)	0	100	100
1	C	427/450 (95%)	421 (99%)	4 (1%)	2 (0%)	34	55
1	D	424/450 (94%)	415 (98%)	7 (2%)	2 (0%)	34	55
All	All	1683/1800 (94%)	1652 (98%)	24 (1%)	7 (0%)	39	61

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	271	THR
1	D	329	ARG

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Mol	Chain	Res	Type
1	A	19	PRO
1	C	278	PRO
1	A	271	THR
1	D	233	PRO
1	A	233	PRO

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	324/358 (90%)	318 (98%)	6 (2%)	65	87
1	B	332/358 (93%)	327 (98%)	5 (2%)	72	91
1	C	332/358 (93%)	325 (98%)	7 (2%)	61	85
1	D	329/358 (92%)	326 (99%)	3 (1%)	84	95
All	All	1317/1432 (92%)	1296 (98%)	21 (2%)	70	90

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	ARG
1	A	82	GLN
1	A	249	TYR
1	A	309	ILE
1	A	326	VAL
1	A	405	ARG
1	B	80	ARG
1	B	268	LEU
1	B	285	ARG
1	B	340	ARG
1	B	367	LYS
1	C	258	ARG
1	C	285	ARG
1	C	300	ILE
1	C	334	HIS
1	C	405	ARG

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Mol	Chain	Res	Type
1	C	431	GLU
1	C	434	GLU
1	D	24	VAL
1	D	156	ARG
1	D	327	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	230	HIS
1	A	291	ASN
1	B	25	ASN
1	B	83	GLN
1	B	117	HIS
1	B	230	HIS
1	B	334	HIS
1	C	61	GLN
1	C	230	HIS
1	C	291	ASN
1	C	409	GLN
1	D	230	HIS
1	D	291	ASN
1	D	333	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

4 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	RVB	A	451	-	12,19,19	1.23	1 (8%)	14,26,26	2.19	2 (14%)
2	RVB	B	451	-	12,19,19	1.37	1 (8%)	14,26,26	2.01	1 (7%)
2	RVB	C	451	-	12,19,19	1.32	2 (16%)	14,26,26	1.49	1 (7%)
2	RVB	D	451	-	12,19,19	1.27	2 (16%)	14,26,26	1.10	1 (7%)

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	RVB	A	451	-	-	0/8/16/16	0/1/1/1
2	RVB	B	451	-	-	0/8/16/16	0/1/1/1
2	RVB	C	451	-	-	0/8/16/16	0/1/1/1
2	RVB	D	451	-	-	0/8/16/16	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	451	RVB	O3-C3	-3.12	1.34	1.41
2	B	451	RVB	O3-C3	-2.90	1.35	1.41
2	A	451	RVB	C3-C2	-2.72	1.36	1.40
2	D	451	RVB	O3-C3	-2.68	1.35	1.41
2	D	451	RVB	C3-C2	-2.16	1.37	1.40
2	C	451	RVB	C3-C2	-2.01	1.37	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	451	RVB	C1-C2-C3	2.41	121.56	120.28
2	A	451	RVB	O3-C3-C4	3.36	127.46	118.77
2	C	451	RVB	C1-C2-C3	4.58	122.70	120.28
2	A	451	RVB	C1-C2-C3	6.48	123.71	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	451	RVB	C1-C2-C3	6.56	123.75	120.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	451	RVB	11	0
2	B	451	RVB	4	0
2	C	451	RVB	2	0
2	D	451	RVB	6	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	416/450 (92%)	-0.16	9 (2%)	65	69	19, 37, 62, 74	8 (1%)
1	B	423/450 (94%)	-0.13	17 (4%)	42	47	20, 39, 66, 89	8 (1%)
1	C	431/450 (95%)	0.08	26 (6%)	25	28	18, 42, 77, 105	8 (1%)
1	D	428/450 (95%)	0.05	26 (6%)	25	27	22, 44, 74, 88	8 (1%)
All	All	1698/1800 (94%)	-0.04	78 (4%)	36	41	18, 40, 71, 105	32 (1%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	331	SER	6.7
1	C	280	ILE	6.4
1	C	276	ARG	6.1
1	D	79	THR	5.5
1	D	330	GLY	5.1
1	C	275	GLY	4.9
1	B	330	GLY	4.9
1	C	277	GLY	4.5
1	A	272	ARG	4.3
1	D	332	VAL	4.0
1	C	22	ALA	3.9
1	C	274	LEU	3.9
1	C	15	SER	3.9
1	D	166	ALA	3.8
1	B	155	ILE	3.8
1	D	345	PRO	3.7
1	C	279	ALA	3.7
1	D	329	ARG	3.7
1	B	332	VAL	3.6
1	D	155	ILE	3.6
1	C	77	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	23	GLY	3.4
1	B	285	ARG	3.4
1	A	326	VAL	3.3
1	D	22	ALA	3.3
1	B	345	PRO	3.2
1	B	286	ASP	3.2
1	C	278	PRO	3.0
1	B	328	GLU	2.9
1	C	305	SER	2.9
1	D	259	ALA	2.8
1	D	21	PRO	2.8
1	D	283	LEU	2.8
1	B	333	GLN	2.8
1	D	167	THR	2.7
1	D	200	ALA	2.7
1	C	271	THR	2.7
1	D	346	SER	2.7
1	C	281	ASP	2.6
1	B	249	TYR	2.6
1	A	200	ALA	2.6
1	B	14	ALA	2.6
1	D	14	ALA	2.6
1	D	19	PRO	2.6
1	C	78	VAL	2.5
1	D	211	CYS	2.5
1	C	273	ALA	2.5
1	A	115	GLY	2.4
1	D	271	THR	2.4
1	C	167	THR	2.4
1	C	143	VAL	2.4
1	C	346	SER	2.3
1	D	78	VAL	2.3
1	A	271	THR	2.3
1	B	329	ARG	2.3
1	A	315	PRO	2.3
1	C	284	ALA	2.3
1	A	179	ASP	2.3
1	A	249	TYR	2.3
1	D	164	LEU	2.2
1	C	101	LEU	2.2
1	C	283	LEU	2.2
1	C	272	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	198	ILE	2.1
1	D	286	ASP	2.1
1	B	430	ARG	2.1
1	B	411	GLY	2.1
1	B	347	SER	2.1
1	D	331	SER	2.1
1	C	316	GLY	2.1
1	D	81	ARG	2.1
1	D	128	HIS	2.1
1	D	165	LEU	2.1
1	C	16	SER	2.1
1	B	271	THR	2.0
1	C	411	GLY	2.0
1	D	347	SER	2.0
1	B	250	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	RVB	D	451	19/19	0.87	0.25	<mark>3.47</mark>	20,20,20,20	0
2	RVB	A	451	19/19	0.92	0.23	1.58	39,46,64,64	0
2	RVB	C	451	19/19	0.90	0.18	0.39	20,20,20,20	6
2	RVB	B	451	19/19	0.95	0.15	0.33	38,45,62,63	0

6.5 Other polymers (i)

There are no such residues in this entry.