Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:36 PM GMT

PDB ID	:	1PTJ
Title	:	Crystal structure analysis of the DI and DIII complex of transhydrogenase with a thio-nicotinamide nucleotide analogue
Authors	:	Singh, A.; Venning, J.D.; Quirk, P.G.; van Boxel, G.I.; Rodrigues, D.J.; White, S.A.; Jackson, J.B.
Deposited on	:	2003-06-23
Resolution	:	2.61 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:

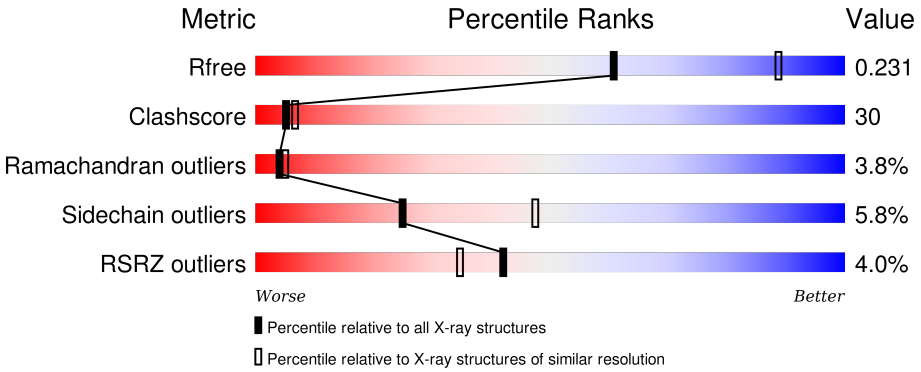
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.61 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	2700 (2.64-2.60)
Clashscore	102246	3065 (2.64-2.60)
Ramachandran outliers	100387	3015 (2.64-2.60)
Sidechain outliers	100360	3015 (2.64-2.60)
RSRZ outliers	91569	2706 (2.64-2.60)

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 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	381	4% 52% 39% • • 5%
1	B	381	3% 61% 31% • • •
2	C	174	5% 36% 54% 10%

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
5	GOL	A	402	-	X	-	X
5	GOL	A	403	-	X	-	-
5	GOL	B	401	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6932 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.

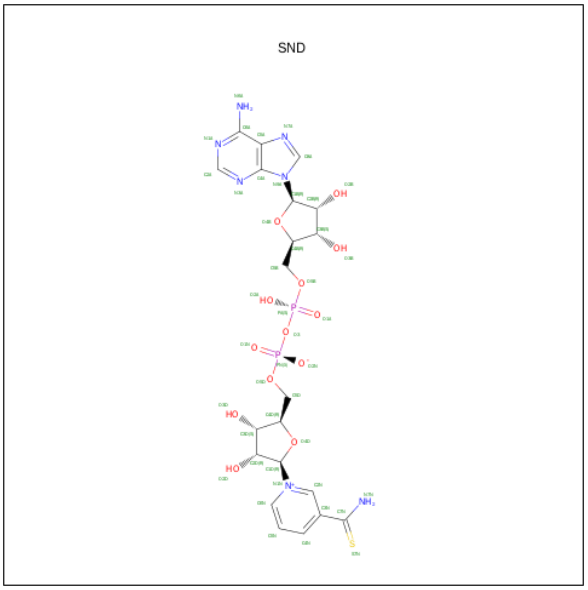
- Molecule 1 is a protein called NAD(P) transhydrogenase subunit alpha part 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	1	0
			2674	1690	461	506	17			
1	B	366	Total	C	N	O	S	0	0	0
			2691	1700	464	510	17			

- Molecule 2 is a protein called NAD(P) transhydrogenase subunit beta.

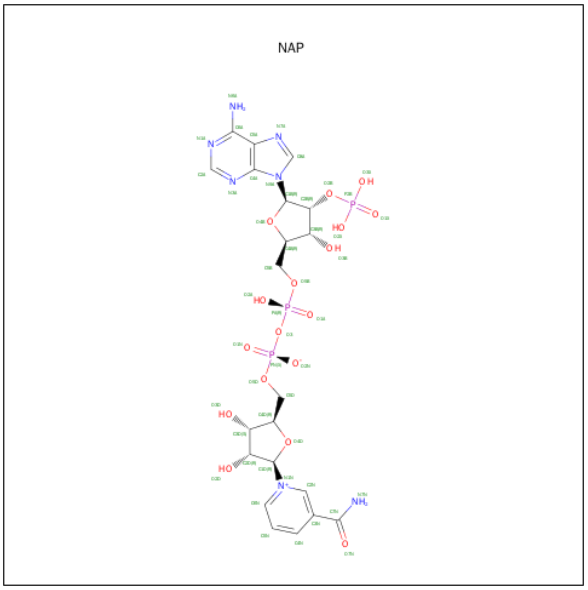
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	174	Total	C	N	O	S	0	0	0
			1311	830	217	253	11			

- Molecule 3 is THIONICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: SND) (formula: $C_{21}H_{27}N_7O_{13}P_2S$).



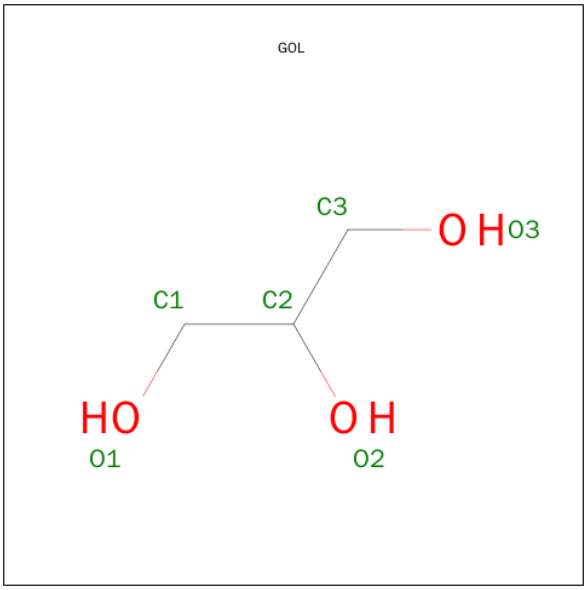
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			44	21	7	13	2	1		

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

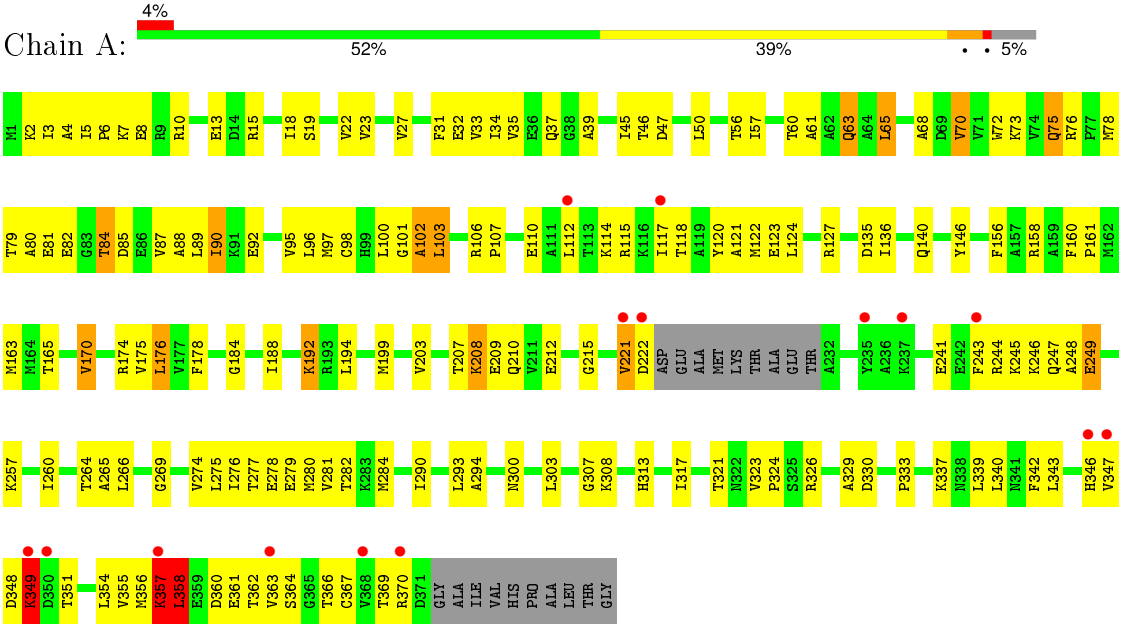
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	42	Total O 42 42	0	0
6	B	79	Total O 79 79	0	0
6	C	25	Total O 25 25	0	0

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.

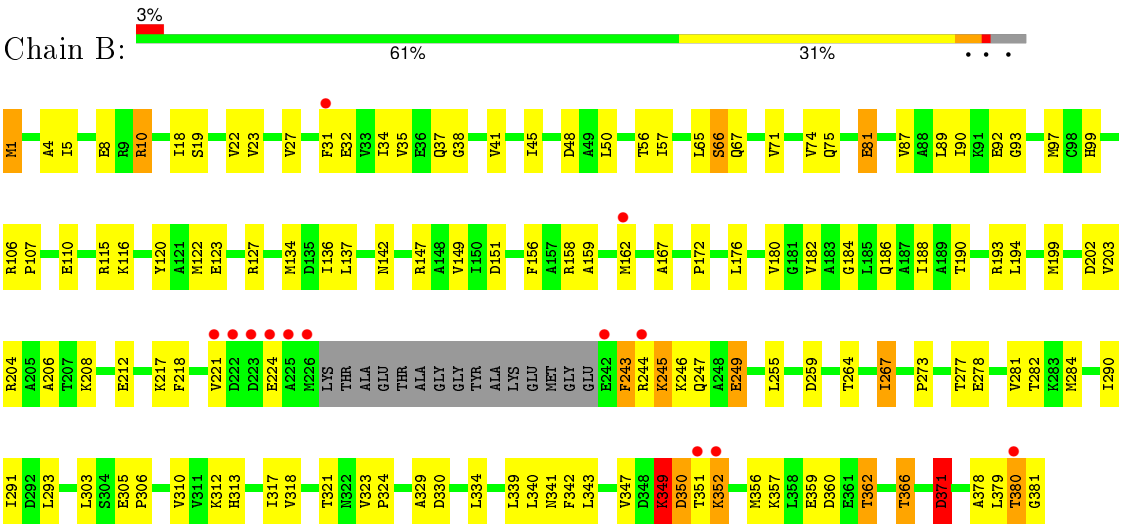
• Molecule 1: NAD(P) transhydrogenase subunit alpha part 1

Chain A:



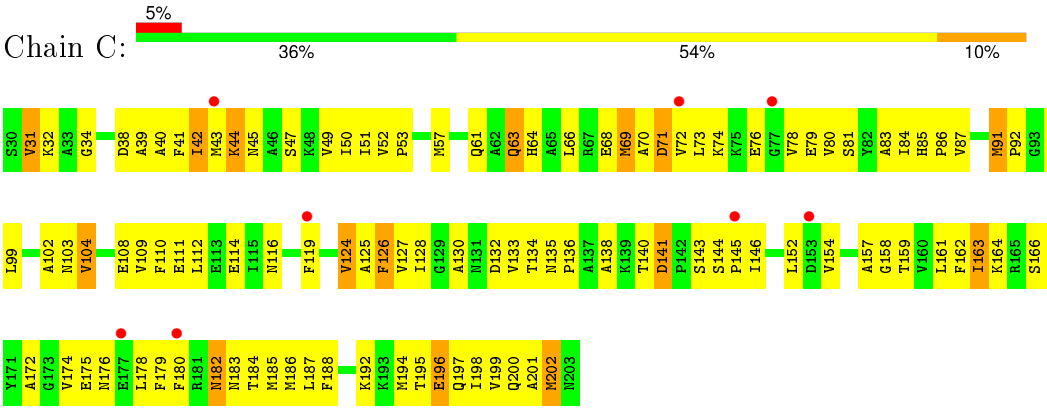
• Molecule 1: NAD(P) transhydrogenase subunit alpha part 1

Chain B:



• Molecule 2: NAD(P) transhydrogenase subunit beta

Chain C:


5%
36%
54%
10%
S30 V31 K32 A33 G34 D38 A39 A40 F41 I42 M43 K44 N45 A46 S47 K48 V49 I50 I51 V52 P53 M57 Q61 A62 Q63 H64 A65 L66 R67 E68 M69 A70 D71 V72 L73 K74 K75 E76 G77 V78 E79 V80 S81 Y82 A83 I84 H85 P86 V87 M91 P92 G93 H94 M95 L98
L99 A102 N103 V104 E108 V109 F110 E111 L112 E113 E114 I115 N116 F119 V124 A125 F126 V127 I128 G129 A130 N131 D132 V133 T134 N135 P136 A137 A138 K139 T140 D141 P142 S143 S144 P145 I146 L152 D153 V154 A157 G158 T159 V160 L161 F162 I163 K164 R165 S166 M167 A168 S169 G170
Y171 A172 G173 V174 E175 N176 E177 L178 F179 F180 R181 M182 N183 T184 M185 M186 L187 F188 K192 K193 M194 T195 E196 Q197 I198 V199 Q200 A201 M202 N203

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.09Å 74.70Å 205.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.26 – 2.61 42.26 – 2.61	Depositor EDS
% Data completeness (in resolution range)	98.4 (42.26-2.61) 97.9 (42.26-2.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	3.35 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.234 , 0.287 0.244 , 0.231	Depositor DCC
R_{free} test set	1955 reflections (5.80%)	DCC
Wilson B-factor (Å^2)	65.3	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 38.0	EDS
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 34103 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6932	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% 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: GOL, NAP, SND

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	0.99	3/2708 (0.1%)	1.10	6/3667 (0.2%)
1	B	1.29	1/2726 (0.0%)	0.73	4/3695 (0.1%)
2	C	0.38	0/1334	0.59	0/1803
All	All	1.04	4/6768 (0.1%)	0.88	10/9165 (0.1%)

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	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	352	LYS	CA-CB	64.02	2.94	1.53
1	A	358[A]	LEU	C-N	-33.09	0.57	1.34
1	A	358[B]	LEU	C-N	-33.09	0.57	1.34
1	A	349	LYS	C-N	-9.90	1.11	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	349	LYS	O-C-N	-40.96	57.16	122.70
1	A	349	LYS	CA-C-N	19.00	158.99	117.20
1	A	358[A]	LEU	O-C-N	-18.92	92.42	122.70
1	A	358[B]	LEU	O-C-N	-18.92	92.42	122.70
1	B	352	LYS	N-CA-CB	-15.52	82.66	110.60
1	A	349	LYS	C-N-CA	14.12	157.00	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	352	LYS	CA-CB-CG	11.34	138.35	113.40
1	B	352	LYS	CB-CA-C	5.85	122.11	110.40
1	A	357	LYS	O-C-N	-5.43	114.01	122.70
1	B	32	GLU	N-CA-C	-5.26	96.81	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	349	LYS	Mainchain,Peptide
1	A	357	LYS	Mainchain
1	A	358[A]	LEU	Mainchain,Peptide

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	2674	0	2803	178	0
1	B	2691	0	2817	119	0
2	C	1311	0	1303	130	0
3	A	44	0	23	1	0
4	C	48	0	25	3	0
5	A	12	0	8	0	0
5	B	6	0	4	0	0
6	A	42	0	0	6	0
6	B	79	0	0	11	0
6	C	25	0	0	18	0
All	All	6932	0	6983	420	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 30.

All (420) 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:358[A]:LEU:HD21	1:A:370:ARG:HH12	1.06	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358[A]:LEU:HD11	1:A:370:ARG:NH2	1.74	1.01
1:A:3:ILE:HG13	1:A:70:VAL:HG22	1.42	0.99
1:B:362:THR:HG21	6:B:408:HOH:O	1.62	0.97
2:C:50:ILE:HG22	2:C:81:SER:HB2	1.44	0.97
1:A:276:ILE:HA	1:A:280:MET:HE3	1.46	0.96
1:A:265:ALA:HB3	1:A:300:ASN:HD21	1.29	0.96
1:A:358[A]:LEU:HD11	1:A:370:ARG:CZ	1.95	0.96
2:C:159:THR:HA	6:C:307:HOH:O	1.71	0.91
1:B:71:VAL:HA	6:B:409:HOH:O	1.70	0.89
2:C:85:HIS:CE1	2:C:87:VAL:HG22	2.08	0.87
2:C:49:VAL:HA	6:C:304:HOH:O	1.73	0.87
2:C:162:PHE:O	2:C:163:ILE:HG13	1.75	0.86
1:A:221:VAL:HG13	1:A:222:ASP:H	1.40	0.85
1:A:10:ARG:HA	1:A:78:MET:HE3	1.60	0.84
2:C:141:ASP:HB3	6:C:322:HOH:O	1.79	0.82
1:A:265:ALA:HB3	1:A:300:ASN:ND2	1.94	0.82
2:C:63:GLN:HG2	2:C:98:LEU:HB3	1.62	0.81
1:A:45:ILE:HG22	1:A:50:LEU:HD11	1.61	0.81
1:A:356:MET:HB3	1:A:363:VAL:HG11	1.62	0.81
1:A:358[A]:LEU:HD21	1:A:370:ARG:NH1	1.92	0.80
1:B:134:MET:HE2	1:B:342:PHE:HA	1.63	0.80
2:C:124:VAL:HG23	6:C:304:HOH:O	1.81	0.80
2:C:43:MET:HE2	6:C:305:HOH:O	1.82	0.78
1:A:358[A]:LEU:CD2	1:A:370:ARG:HH12	1.92	0.78
1:A:7:LYS:HG2	1:A:39:ALA:HA	1.65	0.77
1:A:103:LEU:H	1:A:103:LEU:HD12	1.49	0.77
1:A:329:ALA:HB3	1:B:158:ARG:HG3	1.67	0.77
6:A:508:HOH:O	1:B:193:ARG:HB2	1.85	0.77
1:A:10:ARG:NH1	1:A:78:MET:HG2	2.01	0.75
1:B:134:MET:CE	1:B:342:PHE:HA	2.16	0.75
1:A:158:ARG:HG2	1:B:329:ALA:HB3	1.67	0.75
2:C:119:PHE:CD2	2:C:154:VAL:HA	2.22	0.74
2:C:182:ASN:HA	6:C:321:HOH:O	1.88	0.73
1:A:60:THR:HG23	1:A:63:GLN:HB2	1.69	0.73
2:C:140:THR:HG22	2:C:141:ASP:H	1.50	0.73
1:A:60:THR:HG22	1:A:63:GLN:HE21	1.51	0.73
1:B:349:LYS:HB3	6:B:454:HOH:O	1.88	0.72
1:B:10:ARG:HH11	1:B:10:ARG:HG3	1.54	0.72
1:A:281:VAL:HG11	1:A:303:LEU:HD11	1.72	0.72
1:A:347:VAL:O	1:A:349:LYS:NZ	2.21	0.71
1:B:4:ALA:O	6:B:409:HOH:O	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:ASN:HD21	1:B:186:GLN:HE21	1.39	0.70
2:C:49:VAL:HG13	2:C:124:VAL:HG23	1.73	0.70
1:A:2:LYS:HG2	1:A:32:GLU:HB2	1.74	0.70
2:C:183:ASN:HB3	6:C:307:HOH:O	1.91	0.70
1:A:294:ALA:HB3	1:A:300:ASN:OD1	1.92	0.69
1:A:264:THR:HG22	1:A:293:LEU:HD12	1.72	0.69
1:B:349:LYS:O	1:B:351:THR:N	2.26	0.69
1:B:291:ILE:HD13	1:B:318:VAL:HB	1.76	0.68
2:C:47:SER:HB2	6:C:318:HOH:O	1.92	0.68
1:A:61:ALA:O	1:A:65:LEU:HD22	1.93	0.68
2:C:52:VAL:HG22	2:C:83:ALA:HB3	1.76	0.68
1:A:45:ILE:CG2	1:A:50:LEU:HD11	2.24	0.68
1:A:118:THR:HG23	1:A:370:ARG:HA	1.77	0.67
1:A:346:HIS:HB3	1:A:355:VAL:O	1.94	0.67
1:A:96:LEU:HD11	1:A:98:CYS:SG	2.35	0.67
1:A:330:ASP:O	1:A:333:PRO:HD2	1.95	0.67
2:C:66:LEU:HD12	2:C:128:ILE:HD13	1.76	0.67
2:C:195:THR:O	2:C:199:VAL:HG23	1.94	0.67
1:B:37:GLN:HG2	6:B:451:HOH:O	1.93	0.67
1:A:112:LEU:HD22	1:A:117:ILE:HG21	1.75	0.67
1:A:107:PRO:O	1:A:110:GLU:HG2	1.95	0.66
1:A:346:HIS:HD2	1:A:357:LYS:H	1.43	0.66
2:C:61:GLN:HA	2:C:63:GLN:OE1	1.96	0.66
1:A:72:TRP:HE1	1:A:97:MET:HE3	1.59	0.66
2:C:40:ALA:O	2:C:44:LYS:HB2	1.95	0.66
1:A:349:LYS:HA	1:A:349:LYS:HE3	1.77	0.65
1:A:247:GLN:C	1:A:249:GLU:H	1.97	0.65
1:B:134:MET:HE3	1:B:341:ASN:O	1.95	0.65
1:A:80:ALA:HB2	1:A:85:ASP:OD2	1.96	0.65
1:A:87:VAL:HG13	1:A:112:LEU:HD23	1.79	0.64
1:A:136:ILE:O	1:A:140:GLN:HG2	1.97	0.64
1:A:279:GLU:O	1:A:282:THR:HG22	1.97	0.64
2:C:43:MET:HB3	6:C:305:HOH:O	1.97	0.64
1:A:60:THR:HG23	1:A:63:GLN:H	1.63	0.64
2:C:40:ALA:HB3	6:C:303:HOH:O	1.96	0.64
1:A:244:ARG:HG2	1:A:244:ARG:HH11	1.61	0.64
1:A:22:VAL:HG13	1:A:340:LEU:HD22	1.81	0.64
2:C:31:VAL:CG2	2:C:180:PHE:HB3	2.28	0.63
1:B:221:VAL:HG13	1:B:247:GLN:HG3	1.80	0.63
1:B:8:GLU:OE1	1:B:74:VAL:HG22	1.99	0.63
1:A:276:ILE:CA	1:A:280:MET:HE3	2.27	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:119:PHE:CE2	2:C:154:VAL:HG12	2.34	0.62
2:C:69:MET:O	2:C:69:MET:HG2	1.98	0.62
1:A:60:THR:CG2	1:A:63:GLN:HB2	2.28	0.62
1:A:367:CYS:SG	1:A:370:ARG:HB3	2.39	0.62
2:C:198:ILE:O	2:C:202:MET:HB2	2.00	0.62
1:B:4:ALA:HA	1:B:34:ILE:O	2.00	0.62
2:C:57:MET:HE3	2:C:66:LEU:HD13	1.82	0.62
2:C:175:GLU:HG3	6:C:313:HOH:O	1.98	0.61
1:B:380:THR:HG22	1:B:380:THR:O	1.99	0.61
1:A:337:LYS:HD2	1:B:167:ALA:O	1.99	0.61
1:B:371:ASP:HB2	6:B:452:HOH:O	1.99	0.61
1:A:7:LYS:CG	1:A:39:ALA:HA	2.31	0.61
1:B:19:SER:OG	1:B:22:VAL:HG23	2.01	0.61
2:C:185:MET:O	2:C:186:MET:HE2	2.00	0.61
2:C:200:GLN:C	2:C:202:MET:H	2.04	0.61
1:A:106:ARG:N	1:A:107:PRO:HD2	2.15	0.60
1:A:275:LEU:CD1	1:A:300:ASN:HD22	2.14	0.60
2:C:85:HIS:ND1	2:C:87:VAL:HG22	2.15	0.60
1:B:99:HIS:CD2	1:B:123:GLU:HB3	2.36	0.60
1:B:4:ALA:N	6:B:409:HOH:O	2.16	0.60
2:C:187:LEU:HD12	2:C:187:LEU:N	2.17	0.60
2:C:51:ILE:HD13	2:C:66:LEU:HD21	1.82	0.60
1:A:361:GLU:HA	1:A:364:SER:OG	2.02	0.60
2:C:66:LEU:HD23	2:C:66:LEU:C	2.22	0.60
1:B:310:VAL:CG2	1:B:317:ILE:HB	2.32	0.60
1:A:8:GLU:HA	6:A:513:HOH:O	2.01	0.59
2:C:110:PHE:HB3	2:C:114:GLU:HG3	1.83	0.59
2:C:116:ASN:OD1	2:C:152:LEU:HA	2.02	0.59
1:A:47:ASP:HB3	1:A:57:ILE:CD1	2.32	0.59
1:A:244:ARG:HG2	1:A:244:ARG:NH1	2.16	0.59
1:B:74:VAL:CG2	1:B:75:GLN:N	2.65	0.59
2:C:43:MET:HE1	2:C:126:PHE:CG	2.38	0.59
1:A:87:VAL:HG13	1:A:112:LEU:CD2	2.33	0.58
1:A:356:MET:HB3	1:A:363:VAL:CG1	2.33	0.58
1:A:47:ASP:HB3	1:A:57:ILE:HD13	1.84	0.58
1:B:127:ARG:HG2	1:B:127:ARG:HH11	1.68	0.58
1:A:281:VAL:HG11	1:A:303:LEU:CD1	2.34	0.58
2:C:71:ASP:HA	2:C:74:LYS:HG2	1.86	0.58
1:B:74:VAL:HG23	1:B:75:GLN:N	2.18	0.57
2:C:140:THR:HG22	2:C:141:ASP:N	2.19	0.57
2:C:91:MET:HA	4:C:300:NAP:O7N	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358[A]:LEU:CD1	1:A:370:ARG:NH2	2.61	0.57
2:C:49:VAL:HG23	2:C:78:VAL:HG11	1.87	0.57
1:B:93:GLY:HA2	1:B:116:LYS:O	2.05	0.57
1:B:162:MET:HB2	1:B:172:PRO:HD3	1.86	0.57
1:A:10:ARG:NH2	1:A:76:ARG:HH12	2.03	0.57
1:A:247:GLN:O	1:A:249:GLU:N	2.38	0.57
1:B:284:MET:CE	1:B:290:ILE:HD11	2.35	0.56
1:A:275:LEU:HD12	1:A:300:ASN:HD22	1.70	0.56
1:B:343:LEU:O	1:B:343:LEU:HD12	2.04	0.56
1:A:68:ALA:HB3	6:A:533:HOH:O	2.05	0.56
2:C:66:LEU:CD1	2:C:128:ILE:HG21	2.36	0.56
1:A:103:LEU:H	1:A:103:LEU:CD1	2.19	0.56
1:A:45:ILE:HG22	1:A:50:LEU:CD1	2.35	0.56
2:C:31:VAL:HG22	2:C:180:PHE:HB3	1.87	0.56
1:B:97:MET:HB3	1:B:122:MET:HE3	1.88	0.56
2:C:69:MET:HE1	2:C:126:PHE:CD2	2.40	0.56
1:B:244:ARG:C	1:B:246:LYS:H	2.08	0.56
1:A:358[A]:LEU:HD11	1:A:370:ARG:NH1	2.21	0.55
1:B:120:TYR:OH	1:B:356:MET:HG3	2.05	0.55
1:A:221:VAL:HG13	1:A:222:ASP:N	2.15	0.55
1:A:317:ILE:N	1:A:317:ILE:HD12	2.21	0.55
1:B:90:ILE:O	1:B:115:ARG:NH1	2.39	0.55
1:B:106:ARG:O	1:B:110:GLU:HG3	2.05	0.55
2:C:124:VAL:HG13	2:C:159:THR:HG23	1.88	0.55
2:C:66:LEU:HD12	2:C:128:ILE:HG21	1.88	0.55
2:C:76:GLU:HG3	6:C:324:HOH:O	2.05	0.55
2:C:57:MET:CE	2:C:66:LEU:HD13	2.36	0.55
1:A:342:PHE:CE1	1:A:362:THR:HG22	2.41	0.55
1:A:3:ILE:CG1	1:A:70:VAL:HG22	2.27	0.55
2:C:68:GLU:C	2:C:70:ALA:H	2.10	0.55
2:C:42:ILE:HG21	2:C:161:LEU:HD11	1.87	0.55
1:A:35:VAL:HG21	1:A:50:LEU:HD23	1.89	0.55
1:B:35:VAL:HG21	1:B:50:LEU:HD23	1.89	0.55
1:A:31:PHE:HE2	1:A:70:VAL:HG11	1.72	0.54
1:A:277:THR:H	1:A:280:MET:CE	2.21	0.54
1:A:97:MET:HG2	1:A:120:TYR:HB2	1.89	0.54
1:B:127:ARG:HG2	1:B:127:ARG:NH1	2.21	0.54
1:A:278:GLU:HA	1:A:281:VAL:HG12	1.89	0.54
1:A:75:GLN:HG3	6:A:505:HOH:O	2.08	0.54
1:B:244:ARG:HG2	1:B:244:ARG:O	2.08	0.54
2:C:192:LYS:O	2:C:196:GLU:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:MET:HE3	1:B:290:ILE:HD11	1.89	0.54
1:A:23:VAL:O	1:A:27:VAL:HG23	2.08	0.54
1:B:1:MET:CE	1:B:1:MET:H3	2.20	0.54
2:C:63:GLN:CG	2:C:98:LEU:HB3	2.35	0.53
1:A:356:MET:O	1:A:358[B]:LEU:N	2.41	0.53
1:B:92:GLU:HB2	6:B:472:HOH:O	2.09	0.53
1:A:360:ASP:OD2	1:A:362:THR:HB	2.08	0.53
2:C:85:HIS:CD2	2:C:112:LEU:HD12	2.44	0.53
2:C:125:ALA:O	2:C:127:VAL:HG23	2.09	0.53
1:A:174:ARG:HD3	1:A:257:LYS:O	2.08	0.53
1:B:31:PHE:HE1	1:B:347:VAL:HG21	1.73	0.53
1:B:310:VAL:HG23	1:B:317:ILE:HB	1.90	0.53
1:A:79:THR:OG1	1:A:82:GLU:HG3	2.08	0.53
2:C:112:LEU:O	2:C:116:ASN:HB2	2.09	0.53
1:A:76:ARG:CB	1:A:100:LEU:HD12	2.38	0.53
2:C:161:LEU:HA	2:C:185:MET:HB2	1.91	0.53
2:C:41:PHE:HB3	6:C:306:HOH:O	2.09	0.53
1:A:60:THR:CG2	1:A:63:GLN:HE21	2.20	0.53
1:A:118:THR:HA	1:A:369:THR:O	2.09	0.52
1:A:46:THR:O	1:A:50:LEU:HD13	2.09	0.52
1:A:158:ARG:HB3	1:B:330:ASP:OD2	2.09	0.52
2:C:132:ASP:O	2:C:146:ILE:HD11	2.09	0.52
1:A:6:PRO:HD2	1:A:72:TRP:O	2.09	0.52
2:C:111:GLU:HG2	2:C:114:GLU:HG2	1.91	0.52
1:A:121:ALA:HB1	1:A:123:GLU:OE2	2.09	0.52
1:A:343:LEU:C	1:A:343:LEU:HD23	2.30	0.52
2:C:112:LEU:HG	2:C:152:LEU:HD23	1.91	0.52
1:A:127:ARG:HH11	1:A:127:ARG:HG2	1.75	0.52
2:C:194:MET:SD	6:C:315:HOH:O	2.59	0.52
1:A:241:GLU:OE2	1:A:245:LYS:HG3	2.10	0.52
2:C:53:PRO:HG2	2:C:95:MET:HG2	1.92	0.52
1:B:81:GLU:HA	1:B:81:GLU:OE1	2.10	0.51
1:A:358[A]:LEU:HD11	1:A:370:ARG:HH22	1.69	0.51
2:C:170:GLY:HA3	4:C:300:NAP:O1A	2.11	0.51
1:A:221:VAL:HG22	1:A:222:ASP:N	2.26	0.51
2:C:66:LEU:HD23	2:C:66:LEU:O	2.10	0.51
1:A:76:ARG:HB3	1:A:100:LEU:HA	1.90	0.51
1:A:92:GLU:HG3	1:A:115:ARG:O	2.11	0.51
1:A:135:ASP:OD2	3:A:500:SND:H4N	2.11	0.51
1:A:284:MET:SD	1:A:290:ILE:HD11	2.51	0.51
2:C:119:PHE:CE2	2:C:154:VAL:HA	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:68:GLU:O	2:C:70:ALA:N	2.43	0.51
2:C:70:ALA:O	2:C:74:LYS:HG2	2.11	0.51
2:C:144:SER:OG	2:C:146:ILE:HG22	2.11	0.51
1:B:18:ILE:HG13	1:B:19:SER:N	2.26	0.51
1:B:379:LEU:O	1:B:381:GLY:N	2.43	0.51
1:A:76:ARG:HB2	1:A:100:LEU:HD12	1.92	0.50
2:C:99:LEU:HB3	2:C:104:VAL:CG1	2.42	0.50
1:A:192:LYS:HE2	1:A:215:GLY:HA3	1.93	0.50
1:A:246:LYS:O	1:A:249:GLU:HB2	2.11	0.50
1:A:247:GLN:C	1:A:249:GLU:N	2.64	0.50
1:A:161:PRO:HB3	1:A:194:LEU:O	2.11	0.50
2:C:49:VAL:HG13	2:C:124:VAL:CG2	2.39	0.50
2:C:69:MET:O	2:C:73:LEU:HB2	2.11	0.50
2:C:127:VAL:HG13	2:C:130:ALA:HB3	1.93	0.50
1:B:278:GLU:O	1:B:281:VAL:HG22	2.12	0.50
1:A:34:ILE:HD12	1:A:34:ILE:N	2.27	0.50
2:C:187:LEU:N	2:C:187:LEU:CD1	2.75	0.50
1:A:120:TYR:OH	1:A:356:MET:HG3	2.12	0.50
1:A:330:ASP:CG	1:B:158:ARG:HG2	2.31	0.50
1:A:10:ARG:HH11	1:A:78:MET:HG2	1.72	0.50
1:B:8:GLU:CD	1:B:74:VAL:HG22	2.32	0.50
1:A:120:TYR:CE2	1:A:363:VAL:HG13	2.47	0.49
2:C:112:LEU:C	2:C:112:LEU:HD23	2.32	0.49
2:C:128:ILE:O	2:C:128:ILE:HG23	2.12	0.49
1:B:18:ILE:HG13	1:B:19:SER:H	1.77	0.49
1:A:56:THR:HG22	1:A:57:ILE:N	2.27	0.49
1:B:31:PHE:CE1	1:B:347:VAL:HG21	2.47	0.49
2:C:145:PRO:HD2	2:C:174:VAL:HG11	1.93	0.49
2:C:172:ALA:HB3	6:C:311:HOH:O	2.13	0.49
2:C:49:VAL:O	2:C:80:VAL:HA	2.11	0.49
1:A:5:ILE:HD12	1:A:5:ILE:N	2.27	0.49
2:C:49:VAL:HG23	2:C:78:VAL:CG1	2.43	0.49
2:C:133:VAL:CG1	2:C:133:VAL:O	2.60	0.49
1:A:70:VAL:HB	1:A:95:VAL:CG2	2.43	0.49
1:B:349:LYS:N	1:B:349:LYS:HD2	2.28	0.49
1:B:156:PHE:CE2	1:B:158:ARG:HB2	2.48	0.48
1:A:323:VAL:O	1:A:326:ARG:HB2	2.12	0.48
1:A:178:PHE:CE2	1:A:276:ILE:HD11	2.47	0.48
1:B:247:GLN:C	1:B:249:GLU:H	2.15	0.48
1:A:343:LEU:HD21	1:A:354:LEU:HD21	1.95	0.48
1:A:175:VAL:HG22	1:A:260:ILE:HB	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ARG:HG3	6:A:512:HOH:O	2.14	0.48
1:A:121:ALA:O	1:A:366:THR:HG23	2.12	0.48
2:C:178:LEU:O	2:C:184:THR:HG21	2.13	0.48
1:A:207:THR:HA	1:A:210:GLN:HE21	1.79	0.48
1:B:264:THR:HG22	1:B:293:LEU:HD12	1.95	0.48
1:A:158:ARG:HG2	1:B:329:ALA:CB	2.42	0.48
2:C:44:LYS:HG3	2:C:202:MET:CE	2.44	0.48
2:C:111:GLU:O	2:C:114:GLU:HG2	2.14	0.47
2:C:68:GLU:C	2:C:70:ALA:N	2.65	0.47
1:A:156:PHE:CE2	1:A:158:ARG:HB2	2.50	0.47
1:A:369:THR:O	1:A:369:THR:HG23	2.14	0.47
1:A:307:GLY:N	1:A:321:THR:HG23	2.29	0.47
1:A:156:PHE:CZ	1:A:158:ARG:HB2	2.50	0.47
1:A:278:GLU:HA	1:A:281:VAL:CG1	2.45	0.47
2:C:68:GLU:HA	2:C:71:ASP:OD1	2.15	0.47
2:C:78:VAL:HG12	2:C:79:GLU:N	2.30	0.46
1:B:106:ARG:NH1	1:B:110:GLU:OE2	2.48	0.46
1:A:146:TYR:CE2	1:B:159:ALA:HA	2.49	0.46
1:B:10:ARG:NH1	1:B:10:ARG:HG3	2.27	0.46
1:B:208:LYS:HG2	1:B:212:GLU:OE2	2.15	0.46
2:C:34:GLY:HA3	2:C:185:MET:CE	2.45	0.46
1:B:321:THR:HA	6:B:471:HOH:O	2.15	0.46
1:B:303:LEU:O	1:B:310:VAL:HG21	2.16	0.46
1:A:184:GLY:O	1:A:188:ILE:HG13	2.15	0.46
1:A:277:THR:H	1:A:280:MET:HE2	1.80	0.46
1:B:243:PHE:CE1	1:B:245:LYS:HB2	2.51	0.46
1:B:281:VAL:HG21	1:B:303:LEU:CD1	2.46	0.46
1:B:199:MET:SD	1:B:217:LYS:HB3	2.56	0.46
2:C:140:THR:O	2:C:141:ASP:C	2.55	0.46
2:C:187:LEU:H	2:C:187:LEU:CD1	2.29	0.46
1:B:106:ARG:N	1:B:107:PRO:CD	2.78	0.46
1:B:312:LYS:HG2	1:B:313:HIS:CD2	2.51	0.46
1:A:170:VAL:O	1:A:170:VAL:HG22	2.14	0.46
1:A:120:TYR:HE2	1:A:363:VAL:HG13	1.81	0.46
1:B:74:VAL:CG2	1:B:75:GLN:H	2.28	0.46
2:C:91:MET:O	2:C:94:HIS:HB2	2.15	0.46
1:A:163:MET:HB2	1:A:170:VAL:HG13	1.97	0.46
1:A:97:MET:O	1:A:98:CYS:HB3	2.16	0.45
1:A:19:SER:HA	1:A:45:ILE:HD13	1.98	0.45
1:B:180:VAL:O	1:B:180:VAL:HG12	2.15	0.45
1:B:99:HIS:HD2	1:B:123:GLU:HB3	1.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:300:NAP:PN	6:C:309:HOH:O	2.75	0.45
1:A:84:THR:HG23	1:A:84:THR:O	2.17	0.45
1:A:122:MET:HG3	1:A:339:LEU:CD2	2.46	0.45
1:B:23:VAL:O	1:B:27:VAL:HG23	2.16	0.45
2:C:140:THR:CG2	2:C:141:ASP:H	2.19	0.45
1:B:352:LYS:CB	1:B:352:LYS:CA	2.94	0.45
2:C:40:ALA:HA	2:C:202:MET:HE3	1.98	0.45
1:A:73:LYS:HE3	1:A:75:GLN:O	2.17	0.45
1:A:63:GLN:HB2	1:A:63:GLN:HE21	1.54	0.45
1:B:122:MET:HB3	1:B:136:ILE:HD13	1.98	0.45
1:B:184:GLY:O	1:B:188:ILE:HG13	2.15	0.45
1:B:244:ARG:C	1:B:246:LYS:N	2.70	0.45
1:A:323:VAL:HG13	1:A:326:ARG:HD3	1.99	0.45
1:B:357:LYS:HB3	1:B:359:GLU:OE1	2.17	0.45
1:A:357:LYS:HB3	1:A:360:ASP:HB3	1.99	0.45
1:A:178:PHE:HE2	1:A:276:ILE:HD11	1.81	0.45
1:A:3:ILE:HG23	1:A:33:VAL:HG13	1.98	0.45
1:A:60:THR:HG22	1:A:63:GLN:NE2	2.25	0.45
2:C:166:SER:O	2:C:188:PHE:HE1	1.98	0.45
1:B:182:VAL:HG23	6:B:457:HOH:O	2.17	0.45
1:A:18:ILE:HG13	1:A:19:SER:H	1.82	0.44
1:B:349:LYS:C	1:B:351:THR:N	2.70	0.44
2:C:176:ASN:HB3	2:C:179:PHE:CD2	2.52	0.44
2:C:102:ALA:O	2:C:103:ASN:HB2	2.18	0.44
1:B:282:THR:HG22	1:B:313:HIS:CE1	2.52	0.44
1:B:35:VAL:HG21	1:B:50:LEU:CD2	2.47	0.44
1:B:194:LEU:HD23	1:B:194:LEU:HA	1.88	0.44
1:A:313:HIS:CD2	1:A:313:HIS:N	2.86	0.44
1:A:13:GLU:OE2	1:A:15:ARG:HB2	2.17	0.44
2:C:134:THR:HB	2:C:154:VAL:HG21	1.99	0.44
2:C:84:ILE:HG13	2:C:109:VAL:CG1	2.48	0.44
2:C:124:VAL:HA	2:C:159:THR:O	2.18	0.44
1:A:203:VAL:HG12	1:A:243:PHE:CE2	2.53	0.44
2:C:164:LYS:HE2	2:C:166:SER:O	2.18	0.44
1:A:357:LYS:HG2	1:A:360:ASP:HB2	2.00	0.43
2:C:187:LEU:C	2:C:194:MET:HE3	2.39	0.43
1:B:1:MET:CE	1:B:1:MET:N	2.81	0.43
1:A:89:LEU:O	1:A:90:ILE:C	2.56	0.43
2:C:69:MET:SD	2:C:126:PHE:CE2	3.11	0.43
1:B:5:ILE:HG12	1:B:18:ILE:HB	2.01	0.43
1:B:360:ASP:OD1	1:B:362:THR:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:85:HIS:CD2	2:C:133:VAL:HG13	2.54	0.43
1:B:255:LEU:HD21	1:B:284:MET:HE2	2.01	0.43
1:B:180:VAL:HG23	1:B:202:ASP:HB2	2.01	0.43
1:B:349:LYS:CD	1:B:350:ASP:H	2.32	0.43
1:A:342:PHE:HE1	1:A:362:THR:O	2.00	0.43
1:A:76:ARG:HD3	1:A:100:LEU:O	2.19	0.43
1:A:103:LEU:N	1:A:103:LEU:HD12	2.26	0.43
1:B:330:ASP:O	1:B:334:LEU:HG	2.19	0.43
2:C:200:GLN:C	2:C:202:MET:N	2.72	0.43
1:B:27:VAL:HG22	6:B:475:HOH:O	2.18	0.43
2:C:42:ILE:CG2	2:C:159:THR:HG21	2.48	0.43
2:C:84:ILE:HD11	2:C:99:LEU:HD11	2.01	0.43
1:A:96:LEU:HD13	1:A:96:LEU:C	2.39	0.43
1:A:274:VAL:O	1:A:274:VAL:HG13	2.19	0.43
1:A:323:VAL:N	1:A:324:PRO:CD	2.81	0.42
1:B:342:PHE:CZ	1:B:366:THR:HG21	2.54	0.42
1:B:5:ILE:HD12	1:B:5:ILE:N	2.33	0.42
1:B:277:THR:O	1:B:281:VAL:HG13	2.18	0.42
1:B:343:LEU:C	1:B:343:LEU:HD12	2.38	0.42
2:C:41:PHE:CB	6:C:306:HOH:O	2.67	0.42
2:C:39:ALA:CB	2:C:187:LEU:HD21	2.49	0.42
2:C:51:ILE:HG22	2:C:53:PRO:HD3	2.01	0.42
1:A:342:PHE:CD1	1:A:362:THR:HG22	2.54	0.42
2:C:34:GLY:HA3	2:C:185:MET:HE1	2.01	0.42
1:B:351:THR:O	1:B:352:LYS:CB	2.68	0.42
2:C:52:VAL:HG12	2:C:52:VAL:O	2.20	0.42
1:A:122:MET:HG3	1:A:339:LEU:HD21	2.02	0.42
1:A:346:HIS:CD2	1:A:357:LYS:H	2.31	0.42
1:A:96:LEU:HD13	1:A:97:MET:N	2.35	0.42
1:A:330:ASP:C	1:A:333:PRO:HD2	2.39	0.42
2:C:64:HIS:O	2:C:68:GLU:HG2	2.20	0.42
1:B:208:LYS:HG3	1:B:218:PHE:CB	2.50	0.42
2:C:68:GLU:O	2:C:72:VAL:HG13	2.19	0.42
1:B:203:VAL:HG23	1:B:204:ARG:N	2.35	0.42
1:B:38:GLY:HA2	1:B:41:VAL:HG23	2.00	0.42
1:A:207:THR:O	1:A:208:LYS:C	2.58	0.42
1:A:207:THR:O	1:A:209:GLU:N	2.53	0.42
1:B:208:LYS:HB2	1:B:218:PHE:CD2	2.55	0.42
1:A:3:ILE:HA	1:A:70:VAL:O	2.20	0.42
1:A:65:LEU:HB3	6:A:533:HOH:O	2.19	0.42
2:C:197:GLN:O	2:C:200:GLN:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:164:LYS:O	2:C:188:PHE:HA	2.20	0.42
2:C:135:ASN:HA	2:C:136:PRO:HD3	1.91	0.42
1:B:349:LYS:O	1:B:350:ASP:C	2.59	0.41
2:C:38:ASP:O	2:C:41:PHE:HB2	2.20	0.41
2:C:176:ASN:OD1	2:C:178:LEU:HB2	2.19	0.41
1:A:165:THR:HG22	2:C:92:PRO:HB3	2.02	0.41
1:A:85:ASP:CG	1:A:88:ALA:HB2	2.41	0.41
1:B:74:VAL:O	1:B:99:HIS:HB3	2.20	0.41
1:B:317:ILE:N	1:B:317:ILE:HD12	2.35	0.41
1:A:176:LEU:HA	1:A:199:MET:O	2.20	0.41
1:B:156:PHE:CZ	1:B:259:ASP:HB3	2.55	0.41
1:B:142:ASN:HD21	1:B:186:GLN:NE2	2.13	0.41
1:A:178:PHE:HB3	1:A:275:LEU:HD13	2.03	0.41
2:C:162:PHE:HB3	2:C:163:ILE:H	1.59	0.41
1:A:343:LEU:O	1:A:343:LEU:HD23	2.20	0.41
1:B:56:THR:O	1:B:57:ILE:HD13	2.20	0.41
1:A:110:GLU:O	1:A:114:LYS:HD3	2.20	0.41
1:A:121:ALA:HB3	1:A:124:LEU:HD12	2.01	0.41
2:C:99:LEU:HB3	2:C:104:VAL:HG13	2.02	0.41
1:A:208:LYS:HG2	1:A:212:GLU:OE2	2.20	0.41
1:A:101:GLY:O	1:A:102:ALA:C	2.59	0.41
1:B:147:ARG:HD2	1:B:151:ASP:OD1	2.20	0.41
1:B:342:PHE:HE1	1:B:362:THR:HG23	1.86	0.41
1:A:265:ALA:CB	1:A:275:LEU:HD11	2.51	0.41
1:B:323:VAL:N	1:B:324:PRO:CD	2.83	0.41
2:C:162:PHE:O	2:C:163:ILE:CG1	2.58	0.41
1:B:305:GLU:OE2	1:B:310:VAL:HG11	2.21	0.41
1:B:45:ILE:CG2	1:B:50:LEU:HD13	2.51	0.41
1:A:4:ALA:HA	1:A:34:ILE:O	2.21	0.41
1:A:357:LYS:O	1:A:358[B]:LEU:HB2	2.21	0.41
1:B:360:ASP:CG	1:B:362:THR:HG22	2.41	0.41
1:A:277:THR:H	1:A:280:MET:HE3	1.85	0.41
2:C:111:GLU:O	2:C:112:LEU:C	2.60	0.41
1:B:267:ILE:HD11	1:B:273:PRO:HD3	2.03	0.41
2:C:167:MET:O	2:C:168:ALA:C	2.60	0.41
1:B:65:LEU:O	1:B:66:SER:C	2.60	0.41
2:C:44:LYS:HG3	2:C:202:MET:HE2	2.01	0.40
2:C:157:ALA:O	2:C:158:GLY:C	2.60	0.40
1:A:207:THR:HA	1:A:210:GLN:NE2	2.36	0.40
1:A:95:VAL:HA	1:A:118:THR:O	2.22	0.40
2:C:133:VAL:O	2:C:133:VAL:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:146:ILE:O	2:C:146:ILE:HG12	2.22	0.40
1:B:120:TYR:HD1	1:B:366:THR:HG23	1.87	0.40
1:B:22:VAL:HG13	1:B:340:LEU:HD22	2.03	0.40
2:C:39:ALA:HB2	2:C:187:LEU:HD21	2.03	0.40
2:C:186:MET:HG3	6:C:316:HOH:O	2.21	0.40
1:B:293:LEU:CD2	1:B:323:VAL:HG21	2.52	0.40
2:C:136:PRO:C	2:C:138:ALA:H	2.25	0.40
1:B:149:VAL:HG21	1:B:190:THR:HB	2.04	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	359/381 (94%)	316 (88%)	31 (9%)	12 (3%)	5	7
1	B	362/381 (95%)	329 (91%)	23 (6%)	10 (3%)	6	9
2	C	172/174 (99%)	132 (77%)	28 (16%)	12 (7%)	1	1
All	All	893/936 (95%)	777 (87%)	82 (9%)	34 (4%)	4	5

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	ALA
1	A	248	ALA
1	A	357	LYS
1	B	66	SER
1	B	349	LYS
1	B	350	ASP
1	B	380	THR
2	C	108	GLU
2	C	143	SER

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Mol	Chain	Res	Type
2	C	163	ILE
2	C	182	ASN
1	A	103	LEU
1	A	208	LYS
1	B	378	ALA
1	A	221	VAL
1	A	249	GLU
1	B	224	GLU
2	C	69	MET
2	C	168	ALA
1	A	84	THR
1	A	269	GLY
1	A	348	ASP
1	B	206	ALA
1	B	245	LYS
1	B	371	ASP
2	C	31	VAL
2	C	201	ALA
1	A	351	THR
1	B	306	PRO
2	C	126	PHE
2	C	141	ASP
1	A	90	ILE
2	C	42	ILE
2	C	86	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	283/295 (96%)	270 (95%)	13 (5%)	33	60
1	B	285/295 (97%)	268 (94%)	17 (6%)	24	45
2	C	138/138 (100%)	127 (92%)	11 (8%)	15	28
All	All	706/728 (97%)	665 (94%)	41 (6%)	25	47

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	63	GLN
1	A	65	LEU
1	A	70	VAL
1	A	75	GLN
1	A	81	GLU
1	A	160	PHE
1	A	170	VAL
1	A	176	LEU
1	A	192	LYS
1	A	266	LEU
1	A	308	LYS
1	A	349	LYS
1	B	1	MET
1	B	10	ARG
1	B	48	ASP
1	B	67	GLN
1	B	81	GLU
1	B	87	VAL
1	B	89	LEU
1	B	137	LEU
1	B	176	LEU
1	B	243	PHE
1	B	249	GLU
1	B	267	ILE
1	B	339	LEU
1	B	349	LYS
1	B	362	THR
1	B	366	THR
1	B	371	ASP
2	C	32	LYS
2	C	44	LYS
2	C	45	ASN
2	C	63	GLN
2	C	71	ASP
2	C	91	MET
2	C	95	MET
2	C	104	VAL
2	C	124	VAL
2	C	196	GLU
2	C	202	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	75	GLN
1	A	105	ASN
1	A	210	GLN
1	A	247	GLN
1	A	300	ASN
1	A	313	HIS
1	A	320	HIS
1	A	338	ASN
1	A	346	HIS
1	B	67	GLN
1	B	186	GLN
1	B	210	GLN
2	C	61	GLN
2	C	64	HIS
2	C	183	ASN

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

5 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	$\#\|Z\| > 2$
5	GOL	A	402	-	5,5,5	4.73	5 (100%)	5,5,5	5.70	3 (60%)
5	GOL	A	403	-	5,5,5	4.77	5 (100%)	5,5,5	5.70	3 (60%)
3	SND	A	500	-	38,48,48	3.21	11 (28%)	46,73,73	2.82	17 (36%)
5	GOL	B	401	-	5,5,5	4.86	5 (100%)	5,5,5	5.64	3 (60%)
4	NAP	C	300	-	42,52,52	1.48	7 (16%)	54,80,80	2.48	13 (24%)

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
5	GOL	A	402	-	-	0/4/4/4	0/0/0/0
5	GOL	A	403	-	-	0/4/4/4	0/0/0/0
3	SND	A	500	-	-	0/22/62/62	0/5/5/5
5	GOL	B	401	-	-	0/4/4/4	0/0/0/0
4	NAP	C	300	-	-	0/27/67/67	0/5/5/5

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	SND	O2D-C2D	-12.43	1.13	1.43
5	B	401	GOL	C3-C2	-8.43	1.20	1.52
5	A	402	GOL	C3-C2	-8.09	1.21	1.52
5	A	403	GOL	C3-C2	-8.03	1.21	1.52
3	A	500	SND	C5D-C4D	-7.20	1.28	1.51
3	A	500	SND	C7N-S7N	-3.62	1.62	1.67
5	A	403	GOL	C1-C2	-3.23	1.40	1.52
5	B	401	GOL	C1-C2	-3.14	1.40	1.52
5	A	402	GOL	C1-C2	-2.93	1.41	1.52
5	B	401	GOL	O2-C2	-2.93	1.34	1.43
5	A	403	GOL	O2-C2	-2.81	1.35	1.43
5	A	402	GOL	O2-C2	-2.54	1.35	1.43
3	A	500	SND	PN-O5D	-2.00	1.49	1.59
4	C	300	NAP	P2B-O2B	2.02	1.66	1.60
4	C	300	NAP	O4B-C1B	2.34	1.44	1.41
4	C	300	NAP	C3N-C7N	2.47	1.54	1.50
4	C	300	NAP	C5N-C4N	2.65	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	300	NAP	C4N-C3N	2.85	1.44	1.39
5	B	401	GOL	O3-C3	2.96	1.55	1.42
4	C	300	NAP	C6N-N1N	3.05	1.43	1.35
5	A	402	GOL	O3-C3	3.20	1.56	1.42
3	A	500	SND	C7N-N7N	3.27	1.35	1.32
3	A	500	SND	O4D-C1D	3.28	1.45	1.41
3	A	500	SND	C4A-N3A	3.34	1.40	1.35
5	A	403	GOL	O3-C3	3.47	1.57	1.42
3	A	500	SND	C2A-N1A	3.60	1.40	1.33
4	C	300	NAP	O4D-C1D	4.28	1.46	1.41
5	A	403	GOL	O1-C1	4.36	1.61	1.42
5	B	401	GOL	O1-C1	4.45	1.61	1.42
3	A	500	SND	C4N-C3N	4.59	1.47	1.39
5	A	402	GOL	O1-C1	4.61	1.62	1.42
3	A	500	SND	C6N-N1N	5.40	1.49	1.35
3	A	500	SND	C3N-C7N	7.25	1.58	1.49

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	300	NAP	N3A-C2A-N1A	-13.06	118.89	128.89
3	A	500	SND	C4N-C3N-C7N	-11.66	110.84	120.95
4	C	300	NAP	O3-PA-O5B	-5.12	89.35	102.94
3	A	500	SND	C4B-O4B-C1B	-5.06	104.16	109.72
3	A	500	SND	N3A-C2A-N1A	-4.28	125.61	128.89
4	C	300	NAP	O2A-PA-O3	-3.92	87.33	105.09
3	A	500	SND	C5N-C6N-N1N	-3.68	114.10	120.47
3	A	500	SND	O3-PA-O5B	-3.60	93.40	102.94
3	A	500	SND	S7N-C7N-N7N	-3.26	117.51	122.23
3	A	500	SND	C5N-C4N-C3N	-2.79	116.83	120.33
4	C	300	NAP	C5B-C4B-C3B	-2.68	104.58	115.21
4	C	300	NAP	C1B-N9A-C4A	-2.50	123.17	126.94
3	A	500	SND	C3N-C7N-S7N	-2.30	116.25	120.97
4	C	300	NAP	C3B-C2B-C1B	-2.07	98.72	102.73
3	A	500	SND	C5D-C4D-C3D	-2.04	107.10	115.21
3	A	500	SND	O3B-C3B-C4B	2.10	117.34	111.05
4	C	300	NAP	O2B-C2B-C1B	2.18	118.52	110.02
4	C	300	NAP	C5N-C4N-C3N	2.27	123.19	120.33
4	C	300	NAP	C2B-C3B-C4B	2.39	107.52	101.85
3	A	500	SND	C2B-C1B-N9A	2.39	117.95	114.29
3	A	500	SND	O4D-C1D-N1N	2.40	110.76	108.13
4	C	300	NAP	P2B-O2B-C2B	2.47	127.48	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	500	SND	O2A-PA-O3	2.56	116.70	105.09
3	A	500	SND	C2N-C3N-C4N	2.62	121.21	118.29
5	A	403	GOL	O1-C1-C2	3.14	125.42	110.18
5	B	401	GOL	O1-C1-C2	3.17	125.55	110.18
5	A	402	GOL	O1-C1-C2	3.27	126.03	110.18
4	C	300	NAP	C4B-O4B-C1B	3.32	113.36	109.72
4	C	300	NAP	O2A-PA-O1A	3.36	130.75	112.53
4	C	300	NAP	O4D-C1D-N1N	3.46	111.93	108.13
3	A	500	SND	C6N-C5N-C4N	4.20	125.78	119.44
3	A	500	SND	O5D-C5D-C4D	4.76	126.67	109.12
3	A	500	SND	C3N-C7N-N7N	5.79	125.25	116.78
5	A	402	GOL	O2-C2-C3	6.57	138.80	108.65
5	B	401	GOL	O2-C2-C3	6.59	138.89	108.65
5	A	403	GOL	O2-C2-C3	6.61	138.96	108.65
5	B	401	GOL	O3-C3-C2	10.24	159.86	110.18
5	A	402	GOL	O3-C3-C2	10.39	160.56	110.18
5	A	403	GOL	O3-C3-C2	10.40	160.63	110.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	SND	1	0
4	C	300	NAP	3	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	362/381 (95%)	0.22	15 (4%) 41 34	41, 73, 100, 107	0
1	B	366/381 (96%)	0.16	13 (3%) 46 39	35, 56, 94, 126	0
2	C	174/174 (100%)	0.42	8 (4%) 36 29	48, 78, 92, 98	0
All	All	902/936 (96%)	0.23	36 (3%) 42 35	35, 66, 97, 126	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	226	MET	8.5
1	B	225	ALA	7.9
1	B	222	ASP	5.5
1	B	351	THR	5.3
1	B	242	GLU	4.9
1	B	223	ASP	4.6
1	B	224	GLU	4.4
1	A	350	ASP	4.3
1	A	357	LYS	3.8
1	A	349	LYS	3.7
1	B	244	ARG	3.7
1	A	112	LEU	3.6
2	C	153	ASP	3.6
2	C	43	MET	3.5
1	A	235	TYR	3.3
1	B	221	VAL	3.2
1	A	243	PHE	3.1
1	A	237	LYS	3.0
1	A	363	VAL	2.9
2	C	177	GLU	2.8
1	B	352	LYS	2.8
1	A	368	VAL	2.7
1	A	222	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
2	C	72	VAL	2.6
2	C	77	GLY	2.6
2	C	145	PRO	2.5
1	B	380	THR	2.4
1	B	162	MET	2.3
1	A	347	VAL	2.2
1	B	31	PHE	2.2
1	A	221	VAL	2.2
2	C	119	PHE	2.2
1	A	346	HIS	2.0
1	A	117	ILE	2.0
1	A	370	ARG	2.0
2	C	180	PHE	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
5	GOL	A	402	6/6	0.74	0.33	4.47	82,84,84,85	0
5	GOL	A	403	6/6	0.78	0.15	-0.41	90,92,92,92	0
3	SND	A	500	44/44	0.93	0.17	-0.65	71,77,97,100	0
4	NAP	C	300	48/48	0.95	0.14	-0.80	62,67,75,77	0
5	GOL	B	401	6/6	0.80	0.22	-	79,82,82,83	0

6.5 Other polymers (i)

There are no such residues in this entry.