



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2017 – 01:58 AM EDT

PDB ID : 2PG8
Title : Crystal structure of R254K mutant of DpgC with bound substrate analog
Authors : Fielding, E.N.
Deposited on : unknown
Resolution : 3.00 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

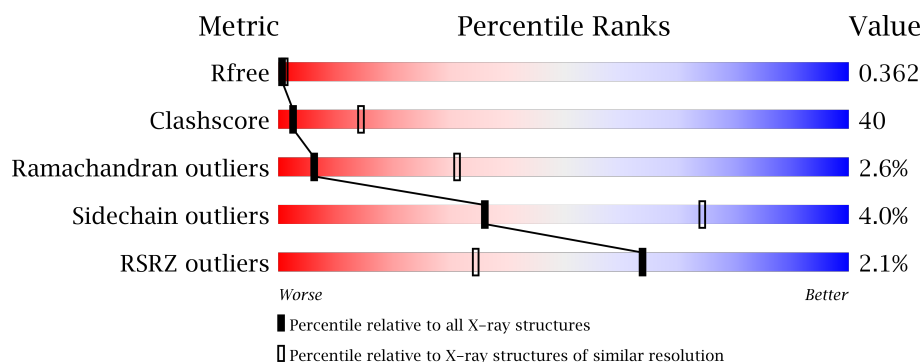
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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 $\leq 5\%$. 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	417	<div> <div>3%</div> <div>43%</div> <div>50%</div> <div>6%</div> </div>
1	B	417	<div> <div>2%</div> <div>50%</div> <div>47%</div> </div>
1	C	417	<div> <div>%</div> <div>53%</div> <div>43%</div> </div>

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	YE1	A	997	-	-	-	X
2	YE1	B	998	-	-	-	X
3	OXY	C	2	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9923 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.

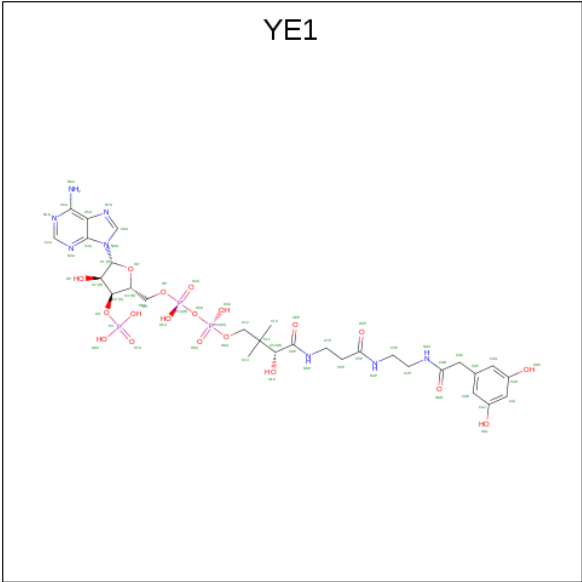
- Molecule 1 is a protein called DpgC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3186	2003	588	585	10			
1	B	417	Total	C	N	O	S	0	0	0
			3232	2029	600	593	10			
1	C	415	Total	C	N	O	S	0	0	0
			3201	2010	594	587	10			

There are 3 discrepancies between the modelled and reference sequences:

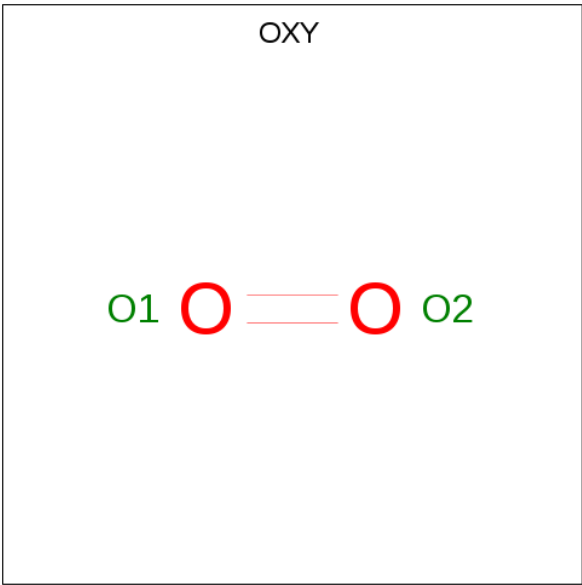
Chain	Residue	Modelled	Actual	Comment	Reference
A	254	LYS	ARG	ENGINEERED	UNP Q8KLK7
B	254	LYS	ARG	ENGINEERED	UNP Q8KLK7
C	254	LYS	ARG	ENGINEERED	UNP Q8KLK7

- Molecule 2 is [(2R,3S,4R,5R)-5-(6-AMINO-9H-PURIN-9-YL)-4-HYDROXY-3-(PHOSPHONOXY)TETRAHYDROFURAN-2-YL]METHYL (3R)-4-({3-[(2-{[(3,5-DIHYDROXYPHENYL)ACETYL]AMINO}ETHYL)AMINO]-3-OXOPROPYL}AMINO)-3-HYDROXY-2,2-DIMETHYL-4-OXOBUTYL DIHYDROGEN DIPHOSPHATE (three-letter code: YE1) (formula: C₂₉H₄₃N₈O₁₉P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			59	29	8	19	3		
2	B	1	Total	C	N	O	P	0	0
			59	29	8	19	3		
2	C	1	Total	C	N	O	P	0	0
			59	29	8	19	3		

- Molecule 3 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	O	0	0
			2	2		

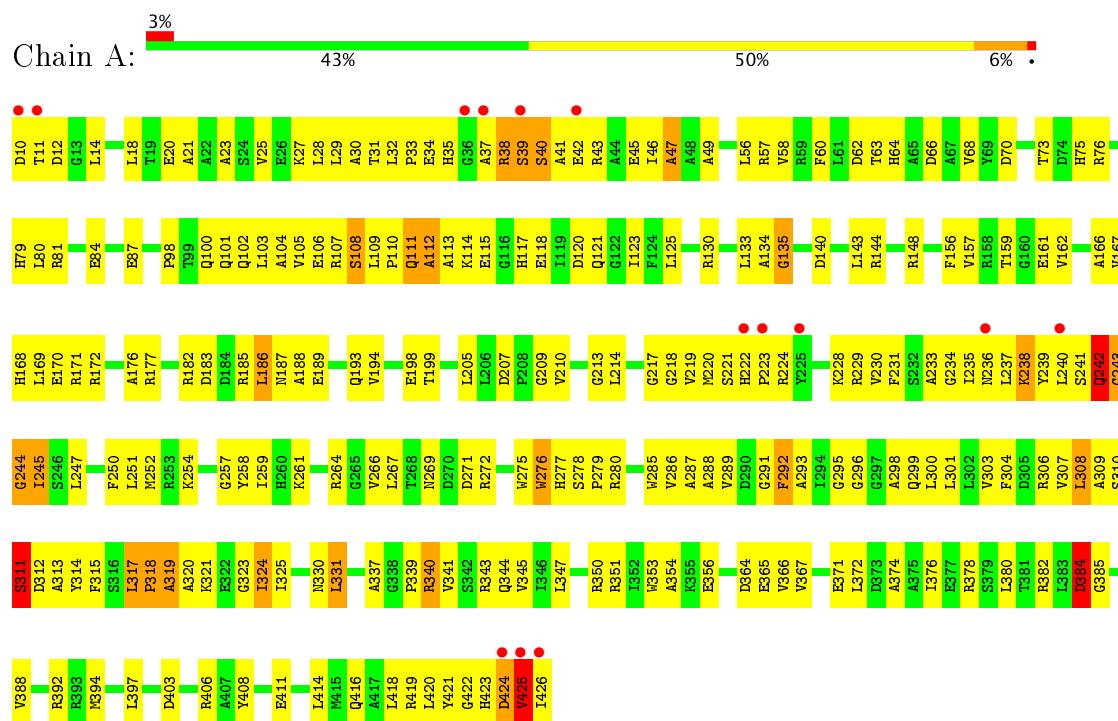
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	44	Total	O	0	0
			44	44		
4	B	43	Total	O	0	0
			43	43		
4	C	36	Total	O	0	0
			36	36		

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 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: DpgC



S342	S343	Q344	V345	I346	L347	E348	G349	R350	R351	P357	E358	A359	R360	L361	L362	V363	V366	D370	E371	L372	I376	E377	R378	S379	L380	D384	G385	D386	A387	V388	L389	A390	R391	R392	L395	R396	L397	A398	D399	E400	R406	A407	Y408	M415	Q416	R419	L420	Y421	G422	H423
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D924	V425	I426
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● Molecule 1: DpgC



ASP	THR	D12	G13	L14	W15	A16	A17	L18	T19	E20	A104	A21	A22	A23	S24	V25	E26	P110	Q111	A112	L28	L29	A30	T31	L32	I119	P33	E34	H35	G36	A37	L125	R38	S39	S40	A41	E42	R43	I46	A47	A48	A49	R148	R57	V58	D62	T63	H64	V68	V69	D70	R71	L72	T73	D74	H75	R76	H79	R80	R81
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L82	A88	P98	T99	Q100	Q101	L103	A104	V105	E106	R107	S108	L109	P110	Q111	A112	A113	R114	E118	I119	D120	I123	F124	L125	R126	R130	L139	R144	P145	T146	P147	R148	A149	V58	L152	L153	P154	E155	F156	V162	E170	R171	R172	D173	R182	D183	D184	R185	L186
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N187	A188	E189	D190	G191	Q192	Q193	V194	M197	E198	V201	L205	L214	L215	R216	G217	N220	S221	H222	P223	R224	L235	N236	L237	K238	Y239	L240	S241	Q242	G243	P250	L251	K254	E255	L256	G257	Y258	I259	L262	V263	R264	G265	V266	L267	T268	N269	D270	D271	R272	H277
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S278	T281	E282	E283	P284	E285	V286	G295	Q299	L300	L301	L302	V303	F304	D305	R306	V307	L308	A309	S310	F315	S316	L317	P318	A319	A320	K321	E322	G323	I324	R335	F336	A337	R340	V341	S342	R343	Q344	L347	R350	R351	I352	W353	E356	A359	R360	L361	L362	V363	D364
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E365	V366	V367	E371	L372	D373	I376	E377	R378	S379	R382	V388	L389	A390	N391	R392	L395	N396	L397	E400	F412	A413	L414	M415	Q416	A417	L420	Y421	V425	I426
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4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	139.05Å 155.31Å 169.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 49.54 – 3.00	Depositor EDS
% Data completeness (in resolution range)	61.2 (50.00-3.00) 93.6 (49.54-3.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.66 (at 3.01Å)	Xtriage
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.331 , 0.367 0.330 , 0.362	Depositor DCC
R_{free} test set	7013 reflections (10.14%)	DCC
Wilson B-factor (Å ²)	55.9	Xtriage
Anisotropy	0.730	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 56.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	9923	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.94 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.3135e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: YE1, OXY

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	0.43	0/3245	0.64	1/4403 (0.0%)
1	B	0.44	0/3292	0.67	1/4462 (0.0%)
1	C	0.44	0/3261	0.66	0/4419
All	All	0.44	0/9798	0.66	2/13284 (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	9
1	B	0	2
1	C	0	4
All	All	0	15

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	SER	N-CA-CB	-5.62	102.07	110.50
1	B	242	GLN	O-C-N	-5.07	114.57	123.20

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	242	GLN	Peptide
1	A	243	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	A	292	PHE	Peptide
1	A	317	LEU	Peptide
1	A	37	ALA	Peptide
1	A	384	ASP	Peptide
1	A	39	SER	Peptide
1	A	40	SER	Peptide
1	A	41	ALA	Peptide
1	B	241	SER	Mainchain
1	B	242	GLN	Mainchain
1	C	184	ASP	Peptide
1	C	317	LEU	Peptide
1	C	39	SER	Peptide
1	C	40	SER	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	3186	0	3176	327	0
1	B	3232	0	3244	244	0
1	C	3201	0	3201	221	0
2	A	59	0	37	20	0
2	B	59	0	37	13	0
2	C	59	0	37	12	0
3	A	2	0	0	1	0
3	C	2	0	0	0	0
4	A	44	0	0	4	0
4	B	43	0	0	2	0
4	C	36	0	0	2	0
All	All	9923	0	9732	784	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 40.

All (784) 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:230:VAL:HG11	1:A:292:PHE:CE2	1.49	1.47
1:B:183:ASP:HA	1:B:220:MET:SD	1.55	1.45
1:B:337:ALA:CB	1:B:341:VAL:HG11	1.51	1.37
1:A:230:VAL:CG1	1:A:292:PHE:CE2	2.24	1.18
1:C:266:VAL:HG23	1:C:281:ILE:HG22	1.24	1.16
1:B:337:ALA:HB1	1:B:341:VAL:HG11	1.23	1.14
1:C:99:THR:HG23	1:C:102:GLN:HE21	0.96	1.12
1:C:99:THR:HG23	1:C:102:GLN:NE2	1.66	1.10
1:C:182:ARG:HH11	1:C:185:ARG:HD2	1.02	1.09
1:A:230:VAL:HG11	1:A:292:PHE:CZ	1.89	1.08
1:A:111:GLN:HA	1:A:114:LYS:HD2	1.18	1.07
1:C:111:GLN:HG2	1:C:243:GLY:HA2	1.37	1.07
1:B:337:ALA:CB	1:B:341:VAL:CG1	2.32	1.06
1:B:337:ALA:HB1	1:B:341:VAL:CG1	1.85	1.05
1:A:38:ARG:CG	1:A:38:ARG:HH11	1.67	1.05
1:C:266:VAL:CG2	1:C:281:ILE:CG2	2.35	1.03
1:B:139:LEU:CD2	1:B:256:LEU:HD22	1.87	1.03
1:B:183:ASP:CA	1:B:220:MET:SD	2.49	1.00
1:C:182:ARG:NH1	1:C:185:ARG:HD2	1.77	0.99
1:C:266:VAL:HG23	1:C:281:ILE:CG2	1.93	0.97
1:C:266:VAL:CG2	1:C:281:ILE:HG22	1.96	0.94
1:A:110:PRO:HG2	1:A:113:ALA:HB3	1.48	0.94
1:A:425:VAL:O	1:A:426:ILE:HG13	1.65	0.94
1:A:143:LEU:HD13	1:A:280:ARG:CD	1.97	0.94
1:C:191:GLY:HA2	1:C:250:PHE:HD1	1.33	0.93
1:A:12:ASP:OD2	1:A:14:LEU:HB2	1.69	0.93
1:A:183:ASP:HA	1:A:220:MET:SD	2.09	0.92
1:A:308:LEU:HD13	1:A:365:GLU:HB2	1.52	0.92
1:C:286:VAL:HG22	1:C:306:ARG:HB3	1.49	0.91
1:B:254:LYS:NZ	1:B:259:ILE:HD11	1.86	0.91
1:A:308:LEU:N	1:A:308:LEU:HD22	1.85	0.90
1:B:194:VAL:HG21	1:B:250:PHE:CD1	2.06	0.90
1:A:38:ARG:HG3	1:A:38:ARG:HH11	1.36	0.90
1:B:254:LYS:HZ3	1:B:259:ILE:HD11	1.38	0.89
1:C:186:LEU:HA	1:C:220:MET:HE2	1.51	0.89
1:B:183:ASP:HB2	1:B:221:SER:N	1.87	0.89
1:A:308:LEU:CD2	1:A:308:LEU:N	2.35	0.88
1:B:337:ALA:HB1	1:B:341:VAL:CB	2.02	0.88
1:C:308:LEU:HD23	1:C:365:GLU:HB3	1.55	0.88
1:B:337:ALA:HB3	1:B:341:VAL:HG11	1.54	0.88
1:B:423:HIS:HD2	4:B:1027:HOH:O	1.58	0.87
1:C:254:LYS:HE3	2:C:999:YE1:OAL	1.72	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:THR:H	1:B:102:GLN:HE21	1.19	0.87
1:A:112:ALA:HB2	1:A:426:ILE:HG21	1.55	0.87
1:B:214:LEU:HD12	1:B:380:LEU:HD21	1.54	0.87
1:B:176:ALA:HB2	1:B:210:VAL:HG11	1.55	0.86
1:B:337:ALA:HB1	1:B:341:VAL:HG21	1.55	0.86
1:C:20:GLU:O	1:C:23:ALA:HB3	1.74	0.86
1:A:238:LYS:O	1:A:242:GLN:HG2	1.76	0.86
1:A:143:LEU:CD1	1:A:280:ARG:HD3	2.05	0.85
1:C:39:SER:H	1:C:42:GLU:HB2	1.41	0.85
1:A:337:ALA:HB1	1:A:341:VAL:HG11	1.54	0.85
1:A:38:ARG:O	1:A:40:SER:HA	1.76	0.85
1:A:319:ALA:HB1	1:A:323:GLY:HA3	1.57	0.85
1:A:183:ASP:HB2	1:A:221:SER:N	1.92	0.84
1:A:254:LYS:HE2	2:A:997:YE1:HAI	1.57	0.84
1:A:38:ARG:HG2	1:A:38:ARG:HH11	1.43	0.83
1:B:235:ILE:HD11	1:B:245:ILE:HD12	1.60	0.83
1:A:143:LEU:HD13	1:A:280:ARG:HD2	1.58	0.83
1:A:40:SER:N	1:A:42:GLU:H	1.76	0.83
1:C:186:LEU:CA	1:C:220:MET:HE2	2.07	0.83
1:C:99:THR:OG1	1:C:102:GLN:HG3	1.79	0.83
1:A:111:GLN:CA	1:A:114:LYS:HD2	2.07	0.83
1:B:337:ALA:HB1	1:B:341:VAL:CG2	2.09	0.82
1:A:108:SER:O	1:A:109:LEU:HD23	1.81	0.81
1:A:337:ALA:CB	1:A:341:VAL:HG11	2.11	0.81
1:B:286:VAL:HG22	1:B:306:ARG:HB3	1.63	0.80
1:C:39:SER:N	1:C:42:GLU:HB2	1.95	0.80
1:A:183:ASP:HB2	1:A:221:SER:H	1.45	0.80
1:C:39:SER:H	1:C:42:GLU:CB	1.94	0.80
1:A:230:VAL:CG1	1:A:292:PHE:CZ	2.58	0.80
1:A:287:ALA:HB2	1:A:304:PHE:CE1	2.17	0.80
1:B:236:ASN:HA	2:B:998:YE1:N1A	1.97	0.79
1:B:139:LEU:HD21	1:B:256:LEU:HD22	1.63	0.79
1:C:186:LEU:H	1:C:220:MET:CE	1.95	0.79
1:A:106:GLU:OE1	1:A:114:LYS:HB3	1.83	0.79
1:B:272:ARG:HH11	1:B:272:ARG:CG	1.95	0.79
1:C:99:THR:CG2	1:C:102:GLN:HE21	1.87	0.78
1:B:147:PRO:O	1:B:151:GLU:HG3	1.82	0.78
1:A:426:ILE:O	1:A:426:ILE:HG22	1.84	0.78
1:A:307:VAL:C	1:A:308:LEU:HD22	2.03	0.78
1:A:143:LEU:CD1	1:A:280:ARG:CD	2.61	0.78
1:A:189:GLU:HB2	1:A:235:ILE:HA	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:VAL:HG12	1:B:168:HIS:N	1.99	0.78
1:A:286:VAL:HG22	1:A:306:ARG:HB3	1.65	0.77
1:C:186:LEU:N	1:C:220:MET:HE2	1.99	0.77
1:A:337:ALA:O	1:A:341:VAL:CG2	2.33	0.77
1:B:139:LEU:CD1	1:B:406:ARG:HG3	2.16	0.76
1:B:388:VAL:HG12	1:B:388:VAL:O	1.84	0.76
1:A:112:ALA:CA	1:A:426:ILE:HD13	2.15	0.76
1:B:139:LEU:HD11	1:B:406:ARG:HG3	1.65	0.76
1:A:109:LEU:HB3	1:A:110:PRO:HD2	1.67	0.76
1:A:29:LEU:HD11	1:A:115:GLU:HG3	1.67	0.76
1:B:214:LEU:HD23	1:B:214:LEU:C	2.06	0.76
1:C:28:LEU:N	1:C:28:LEU:HD12	2.01	0.76
1:B:337:ALA:HB3	1:B:341:VAL:CG1	2.12	0.76
1:B:111:GLN:O	1:B:112:ALA:CB	2.33	0.76
1:C:18:LEU:HD11	1:C:57:ARG:HG2	1.67	0.75
1:A:231:PHE:HB3	1:A:292:PHE:O	1.87	0.75
1:A:39:SER:C	1:A:42:GLU:H	1.90	0.75
1:B:139:LEU:HD23	1:B:256:LEU:HD22	1.68	0.75
1:C:182:ARG:HH11	1:C:185:ARG:CD	1.92	0.75
1:C:266:VAL:HG22	1:C:281:ILE:CG2	2.15	0.75
1:A:337:ALA:O	1:A:341:VAL:HG21	1.87	0.75
1:B:126:ARG:O	1:B:130:ARG:HG3	1.87	0.74
1:A:425:VAL:O	1:A:426:ILE:CG1	2.36	0.74
1:A:384:ASP:HB2	1:C:321:LYS:NZ	2.03	0.74
1:A:353:TRP:O	1:A:356:GLU:HG2	1.87	0.74
1:C:322:GLU:O	1:C:425:VAL:HG22	1.87	0.74
1:A:46:ILE:HG23	1:A:47:ALA:H	1.52	0.74
1:C:186:LEU:H	1:C:220:MET:HE2	1.49	0.74
1:B:82:LEU:HD11	1:B:256:LEU:HD12	1.68	0.74
1:B:361:LEU:O	1:B:362:LEU:HD23	1.88	0.74
1:B:167:VAL:HG12	1:B:168:HIS:H	1.52	0.73
1:B:423:HIS:CD2	4:B:1027:HOH:O	2.36	0.73
1:B:223:PRO:HA	1:B:226:ARG:HG3	1.69	0.73
1:B:419:ARG:O	1:B:425:VAL:HG21	1.87	0.73
1:B:291:GLY:O	1:B:313:ALA:HA	1.89	0.73
1:A:135:GLY:HA3	1:A:406:ARG:HD2	1.70	0.73
2:A:997:YE1:O9A	2:A:997:YE1:O2'	2.04	0.73
1:A:112:ALA:HB2	1:A:426:ILE:HD13	1.71	0.73
1:C:18:LEU:O	1:C:21:ALA:HB3	1.89	0.73
1:A:189:GLU:HB3	1:A:250:PHE:HZ	1.54	0.72
1:C:343:ARG:HH11	1:C:343:ARG:HG3	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:HIS:O	1:B:226:ARG:HG2	1.89	0.72
1:B:324:ILE:HD11	2:B:998:YE1:HAC1	1.72	0.72
1:A:143:LEU:HD12	1:A:280:ARG:HD3	1.71	0.72
1:B:101:GLN:O	1:B:104:ALA:HB3	1.90	0.72
1:B:186:LEU:HD11	1:B:225:TYR:CD1	2.24	0.72
1:B:272:ARG:HB2	1:B:273:PRO:HD2	1.70	0.72
1:A:14:LEU:HD23	1:A:60:PHE:HA	1.70	0.72
1:B:237:LEU:O	1:B:240:LEU:N	2.20	0.72
1:B:189:GLU:OE2	1:B:254:LYS:HE3	1.90	0.71
1:A:261:LYS:HD3	1:A:266:VAL:HG12	1.69	0.71
1:A:254:LYS:HE2	2:A:997:YE1:CAI	2.20	0.71
1:A:98:PRO:CG	1:A:117:HIS:HB3	2.20	0.71
1:C:39:SER:H	1:C:42:GLU:CG	2.03	0.71
1:B:130:ARG:HG2	1:B:130:ARG:HH11	1.56	0.71
1:B:272:ARG:HG2	1:B:272:ARG:HH11	1.56	0.71
1:C:262:LEU:O	1:C:392:ARG:NH2	2.24	0.71
1:B:182:ARG:HB2	1:B:187:ASN:OD1	1.90	0.70
1:B:194:VAL:CG2	1:B:250:PHE:CE1	2.74	0.70
1:A:230:VAL:CG1	1:A:292:PHE:CD2	2.74	0.70
1:C:130:ARG:HG2	1:C:130:ARG:HH11	1.56	0.70
1:C:281:ILE:HG23	1:C:281:ILE:O	1.90	0.70
1:A:217:GLY:O	1:A:229:ARG:HD3	1.89	0.70
1:B:99:THR:N	1:B:102:GLN:HE21	1.89	0.70
2:B:998:YE1:O2'	2:B:998:YE1:O9A	2.08	0.70
1:A:111:GLN:HA	1:A:114:LYS:CD	2.11	0.70
1:C:182:ARG:O	1:C:184:ASP:N	2.22	0.70
1:B:139:LEU:HD21	1:B:256:LEU:CD2	2.21	0.69
1:A:257:GLY:O	1:A:261:LYS:HG3	1.91	0.69
1:A:422:GLY:O	1:A:425:VAL:HG12	1.93	0.69
1:B:296:GLY:O	1:B:299:GLN:HB2	1.92	0.69
1:A:46:ILE:HG23	1:A:47:ALA:N	2.06	0.69
1:B:194:VAL:CG2	1:B:250:PHE:CD1	2.76	0.69
1:C:182:ARG:HB2	1:C:187:ASN:HA	1.75	0.69
1:C:57:ARG:HD2	1:C:120:ASP:OD1	1.93	0.69
1:B:235:ILE:CD1	1:B:250:PHE:HE2	2.05	0.69
1:B:337:ALA:O	1:B:341:VAL:CG2	2.40	0.69
1:A:73:THR:HG22	1:A:80:LEU:HD12	1.75	0.69
1:A:98:PRO:HG3	1:A:117:HIS:HB3	1.75	0.69
1:A:425:VAL:HG13	1:A:425:VAL:O	1.93	0.68
1:A:343:ARG:O	1:A:347:LEU:HB2	1.93	0.68
1:B:99:THR:HG23	1:B:102:GLN:NE2	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:LEU:CD2	1:B:256:LEU:CD2	2.69	0.68
1:A:311:SER:O	1:A:354:ALA:HB3	1.92	0.68
1:C:39:SER:O	1:C:42:GLU:HG3	1.94	0.68
1:B:166:ALA:HB1	1:B:193:GLN:OE1	1.93	0.68
1:A:112:ALA:CB	1:A:426:ILE:HD13	2.24	0.68
1:A:43:ARG:O	1:A:46:ILE:HG22	1.92	0.68
1:A:87:GLU:OE2	1:A:100:GLN:HB2	1.94	0.68
1:C:12:ASP:CG	1:C:13:GLY:H	1.97	0.68
1:B:317:LEU:HD12	1:B:346:ILE:HG12	1.76	0.68
1:C:182:ARG:HB3	1:C:185:ARG:HG2	1.76	0.68
1:B:186:LEU:HA	1:B:220:MET:CE	2.25	0.67
1:B:99:THR:H	1:B:102:GLN:NE2	1.92	0.67
1:B:325:ILE:O	2:B:998:YE1:HAG	1.94	0.67
1:A:169:LEU:HD12	1:A:170:GLU:H	1.59	0.67
1:B:73:THR:HG22	1:B:80:LEU:HD12	1.75	0.67
1:A:354:ALA:HB1	1:A:366:VAL:CG1	2.23	0.67
1:A:343:ARG:HG3	1:A:343:ARG:HH11	1.60	0.67
1:C:222:HIS:CE1	1:C:224:ARG:H	2.13	0.66
2:C:999:YE1:HAE	2:C:999:YE1:OAD	1.95	0.66
1:A:414:LEU:O	1:A:418:LEU:HG	1.96	0.66
1:B:194:VAL:HG23	1:B:250:PHE:CE1	2.30	0.66
1:A:38:ARG:HG2	1:A:38:ARG:NH1	2.06	0.66
1:B:254:LYS:NZ	1:B:259:ILE:CD1	2.58	0.66
2:A:997:YE1:HAE	2:A:997:YE1:OAD	1.95	0.66
1:C:371:GLU:HG3	1:C:371:GLU:O	1.95	0.66
1:C:186:LEU:CD1	1:C:220:MET:HE2	2.25	0.66
1:C:282:GLU:OE1	1:C:392:ARG:NH1	2.29	0.66
1:B:337:ALA:HB2	1:B:341:VAL:HG11	1.72	0.66
1:A:39:SER:HA	1:A:40:SER:HB3	1.78	0.65
1:B:183:ASP:OD2	1:B:221:SER:HB3	1.96	0.65
2:B:998:YE1:OAD	2:B:998:YE1:HAE	1.95	0.65
1:C:235:ILE:HB	2:C:999:YE1:HAE	1.78	0.65
1:B:170:GLU:OE1	1:B:172:ARG:HD3	1.96	0.65
1:A:110:PRO:O	1:A:111:GLN:C	2.35	0.65
1:A:185:ARG:O	1:A:186:LEU:HB2	1.95	0.65
1:A:39:SER:O	1:A:42:GLU:N	2.30	0.65
1:C:103:LEU:O	1:C:106:GLU:HB2	1.97	0.65
1:A:304:PHE:O	1:C:340:ARG:NH2	2.29	0.65
1:A:43:ARG:CA	1:A:46:ILE:HG22	2.27	0.65
1:C:216:ARG:HG2	1:C:217:GLY:H	1.62	0.65
1:A:287:ALA:HB2	1:A:304:PHE:CD1	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:ARG:O	1:B:173:ASP:HB2	1.97	0.65
1:A:425:VAL:CG1	1:A:425:VAL:O	2.44	0.65
1:A:397:LEU:HD23	1:A:397:LEU:O	1.97	0.64
1:B:237:LEU:O	1:B:239:TYR:N	2.30	0.64
1:A:112:ALA:HA	1:A:426:ILE:CD1	2.28	0.64
1:A:267:LEU:HA	1:A:280:ARG:HG2	1.80	0.64
1:B:98:PRO:HG3	1:B:117:HIS:HB3	1.79	0.64
1:A:318:PRO:O	1:A:320:ALA:N	2.30	0.64
1:C:191:GLY:HA2	1:C:250:PHE:CD1	2.23	0.64
1:A:143:LEU:HD13	1:A:280:ARG:HD3	1.71	0.64
1:B:272:ARG:NH1	1:B:272:ARG:CG	2.59	0.64
1:C:111:GLN:HB2	1:C:241:SER:O	1.98	0.64
1:A:112:ALA:HA	1:A:426:ILE:HD13	1.80	0.64
1:B:176:ALA:HB2	1:B:210:VAL:CG1	2.27	0.64
1:A:239:TYR:O	1:A:244:GLY:N	2.31	0.63
1:A:367:VAL:CG1	1:A:372:LEU:HD13	2.28	0.63
1:C:35:HIS:CE1	1:C:113:ALA:HA	2.33	0.63
1:A:275:TRP:CD1	1:A:279:PRO:HA	2.33	0.63
1:C:28:LEU:HD12	1:C:28:LEU:H	1.62	0.63
1:C:266:VAL:HG22	1:C:281:ILE:HG23	1.80	0.63
1:C:372:LEU:O	1:C:376:ILE:HG13	1.98	0.63
1:A:264:ARG:HG2	1:A:264:ARG:HH11	1.63	0.63
1:C:73:THR:HG22	1:C:80:LEU:HD12	1.81	0.63
1:A:111:GLN:HB2	1:A:243:GLY:CA	2.28	0.63
1:B:305:ASP:OD2	1:B:392:ARG:NH1	2.32	0.63
1:C:308:LEU:HD21	1:C:365:GLU:OE1	1.99	0.63
1:A:111:GLN:HB2	1:A:243:GLY:HA2	1.80	0.63
1:C:82:LEU:HB2	4:C:1007:HOH:O	1.97	0.63
1:A:118:GLU:HB2	1:A:421:TYR:HE2	1.63	0.63
1:B:357:PRO:HA	1:B:360:ARG:NH1	2.14	0.62
1:A:46:ILE:CG2	1:A:47:ALA:H	2.12	0.62
1:B:309:ALA:HB3	1:B:363:VAL:HG11	1.80	0.62
1:A:38:ARG:CG	1:A:38:ARG:NH1	2.39	0.62
1:A:411:GLU:HG2	4:A:1020:HOH:O	2.00	0.62
1:A:254:LYS:NZ	1:A:259:ILE:HD11	2.15	0.62
1:A:319:ALA:CB	1:A:323:GLY:HA3	2.29	0.62
1:C:111:GLN:HG3	1:C:240:LEU:O	1.99	0.62
1:A:170:GLU:OE2	1:A:172:ARG:HD3	2.00	0.62
1:B:99:THR:HG23	1:B:102:GLN:HE21	1.63	0.61
1:A:354:ALA:HB1	1:A:366:VAL:HG13	1.82	0.61
1:B:337:ALA:CB	1:B:341:VAL:CB	2.72	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:LEU:O	1:B:376:ILE:HG13	2.00	0.61
1:C:186:LEU:HD12	1:C:220:MET:HE2	1.81	0.61
1:A:314:TYR:CG	1:A:351:ARG:HD2	2.35	0.61
2:A:997:YE1:HC8	2:A:997:YE1:O10	2.01	0.61
1:A:374:ALA:HB1	1:A:378:ARG:HH12	1.66	0.61
1:B:176:ALA:CB	1:B:210:VAL:HG11	2.30	0.61
2:C:999:YE1:O10	2:C:999:YE1:HC8	2.01	0.61
1:A:235:ILE:H	2:A:997:YE1:HC22	1.66	0.60
1:A:27:LYS:O	1:A:30:ALA:N	2.34	0.60
1:A:296:GLY:O	1:A:299:GLN:HB2	2.00	0.60
1:A:343:ARG:HB3	1:A:347:LEU:HD12	1.83	0.60
1:C:222:HIS:CG	1:C:223:PRO:HD2	2.36	0.60
1:B:166:ALA:HB1	1:B:193:GLN:CD	2.22	0.60
1:B:376:ILE:O	1:B:380:LEU:HG	2.01	0.60
1:A:106:GLU:CD	1:A:114:LYS:HB3	2.21	0.60
1:B:167:VAL:CG1	1:B:168:HIS:H	2.14	0.60
2:C:999:YE1:HO10	2:C:999:YE1:C8A	2.15	0.60
1:A:109:LEU:HB3	1:A:110:PRO:CD	2.32	0.59
1:A:10:ASP:O	1:A:12:ASP:N	2.34	0.59
1:B:194:VAL:HG23	1:B:250:PHE:HE1	1.67	0.59
1:A:241:SER:O	1:A:243:GLY:N	2.34	0.59
1:B:109:LEU:HB3	1:B:110:PRO:HD2	1.84	0.59
1:B:111:GLN:O	1:B:112:ALA:HB2	2.01	0.59
1:C:397:LEU:HD23	1:C:397:LEU:O	2.02	0.59
1:B:157:VAL:HA	1:B:171:ARG:NH2	2.17	0.59
1:B:226:ARG:HH11	1:B:226:ARG:HG3	1.67	0.59
1:C:307:VAL:HG12	1:C:363:VAL:HG13	1.83	0.59
1:A:272:ARG:NH2	1:A:278:SER:O	2.35	0.59
1:B:343:ARG:HH11	1:B:343:ARG:HG3	1.66	0.59
1:A:189:GLU:OE1	2:A:997:YE1:HAE	2.02	0.59
1:C:350:ARG:HG2	1:C:351:ARG:N	2.17	0.59
1:A:39:SER:O	1:A:42:GLU:CA	2.50	0.59
1:B:325:ILE:HD11	1:C:390:ALA:HB1	1.82	0.59
1:A:310:SER:O	1:A:311:SER:C	2.41	0.59
1:B:357:PRO:HA	1:B:360:ARG:HH11	1.67	0.59
1:A:12:ASP:OD2	1:A:14:LEU:CB	2.48	0.59
1:A:166:ALA:HB1	1:A:193:GLN:OE1	2.03	0.59
1:B:11:THR:C	1:B:13:GLY:H	2.07	0.58
1:B:318:PRO:O	1:B:320:ALA:N	2.34	0.58
1:C:324:ILE:HB	1:C:416:GLN:HE22	1.67	0.58
1:A:364:ASP:OD2	1:C:340:ARG:NH1	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:ILE:H	2:C:999:YE1:HC22	1.69	0.58
1:B:16:ALA:O	1:B:20:GLU:HB2	2.03	0.58
1:B:340:ARG:NH2	1:C:301:LEU:O	2.36	0.58
1:A:183:ASP:HA	1:A:220:MET:CE	2.33	0.58
2:A:997:YE1:C8A	2:A:997:YE1:O10	2.51	0.58
1:C:263:VAL:CG2	1:C:303:VAL:HG13	2.34	0.58
1:A:222:HIS:CG	1:A:223:PRO:HD2	2.39	0.58
1:C:21:ALA:O	1:C:25:VAL:HG23	2.03	0.58
1:A:205:LEU:HD12	1:A:266:VAL:HG13	1.85	0.58
1:B:194:VAL:HG21	1:B:250:PHE:CE1	2.38	0.58
1:A:230:VAL:HG11	1:A:292:PHE:HE2	1.53	0.57
1:A:254:LYS:CE	2:A:997:YE1:HAI	2.32	0.57
1:A:40:SER:N	1:A:42:GLU:N	2.50	0.57
1:A:236:ASN:OD1	1:A:238:LYS:CB	2.52	0.57
1:C:216:ARG:HG2	1:C:217:GLY:N	2.19	0.57
1:C:310:SER:HB3	1:C:372:LEU:HD22	1.86	0.57
1:A:35:HIS:HA	1:A:38:ARG:HG2	1.86	0.57
1:B:348:GLU:HG3	1:C:306:ARG:NH1	2.19	0.57
2:B:998:YE1:HO10	2:B:998:YE1:C8A	2.18	0.57
1:C:281:ILE:HD11	4:C:1023:HOH:O	2.04	0.57
1:B:235:ILE:HD11	1:B:250:PHE:CE2	2.39	0.57
1:A:312:ASP:O	1:A:312:ASP:CG	2.42	0.57
2:A:997:YE1:C8A	2:A:997:YE1:HO10	2.18	0.57
1:C:14:LEU:O	1:C:17:ALA:HB3	2.04	0.57
1:A:218:GLY:O	1:A:220:MET:HE2	2.04	0.57
1:C:269:ASN:HB2	1:C:271:ASP:OD2	2.05	0.57
1:C:343:ARG:HG3	1:C:343:ARG:NH1	2.20	0.57
1:A:254:LYS:HD2	4:A:1006:HOH:O	2.04	0.56
1:C:111:GLN:HA	1:C:114:LYS:HE3	1.87	0.56
1:A:235:ILE:HB	2:A:997:YE1:CAB	2.34	0.56
1:A:308:LEU:CD1	1:A:365:GLU:HB2	2.31	0.56
1:C:222:HIS:CD2	2:C:999:YE1:H4'	2.40	0.56
1:C:28:LEU:H	1:C:28:LEU:CD1	2.18	0.56
1:A:125:LEU:CD1	1:A:252:MET:HG3	2.36	0.56
1:A:222:HIS:CE1	1:A:224:ARG:H	2.23	0.56
1:B:206:LEU:O	1:B:208:PRO:HD3	2.06	0.56
1:A:46:ILE:CG2	1:A:47:ALA:N	2.68	0.56
1:B:28:LEU:O	1:B:32:LEU:HB2	2.05	0.56
1:C:146:THR:O	1:C:149:ALA:HB3	2.04	0.56
1:C:182:ARG:C	1:C:184:ASP:H	2.07	0.56
1:C:284:PRO:HA	1:C:305:ASP:OD2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:999:YE1:O10	2:C:999:YE1:C8A	2.53	0.56
1:B:254:LYS:HZ2	1:B:259:ILE:CD1	2.19	0.56
1:A:35:HIS:HA	1:A:38:ARG:NH1	2.20	0.56
1:B:153:LEU:N	1:B:154:PRO:HD2	2.21	0.56
1:A:110:PRO:O	1:A:112:ALA:N	2.38	0.56
1:A:272:ARG:HG2	1:A:272:ARG:NH1	2.21	0.56
1:A:378:ARG:O	1:A:382:ARG:HG3	2.06	0.56
1:C:39:SER:N	1:C:42:GLU:OE1	2.38	0.55
1:A:186:LEU:HD12	1:A:220:MET:HG3	1.87	0.55
1:B:314:TYR:CD2	1:B:351:ARG:HD2	2.41	0.55
1:B:235:ILE:HD11	1:B:250:PHE:HE2	1.71	0.55
1:C:28:LEU:N	1:C:28:LEU:CD1	2.68	0.55
1:B:207:ASP:OD2	1:B:210:VAL:HG23	2.07	0.55
1:A:222:HIS:CD2	2:A:997:YE1:H4'	2.42	0.55
1:A:272:ARG:HG2	1:A:272:ARG:HH11	1.71	0.55
1:A:110:PRO:O	1:A:113:ALA:N	2.39	0.55
1:A:230:VAL:HG13	1:A:292:PHE:CE2	2.33	0.55
1:A:384:ASP:HB2	1:C:321:LYS:HZ1	1.67	0.55
1:A:29:LEU:HD21	1:A:115:GLU:CD	2.27	0.55
1:A:123:ILE:HD11	1:B:276:TRP:CZ3	2.42	0.55
1:C:103:LEU:O	1:C:107:ARG:HG3	2.07	0.55
1:A:384:ASP:HB2	1:C:321:LYS:HZ2	1.69	0.55
1:C:186:LEU:H	1:C:220:MET:HE1	1.72	0.55
1:A:18:LEU:HD11	1:A:57:ARG:HG2	1.89	0.54
1:C:39:SER:H	1:C:42:GLU:CD	2.11	0.54
1:C:189:GLU:HA	1:C:193:GLN:OE1	2.07	0.54
1:C:239:TYR:CD1	1:C:239:TYR:N	2.73	0.54
1:A:254:LYS:HE2	2:A:997:YE1:OAL	2.08	0.54
1:A:169:LEU:HD12	1:A:170:GLU:N	2.23	0.54
1:A:425:VAL:O	1:A:426:ILE:CB	2.55	0.54
1:C:172:ARG:HG2	1:C:173:ASP:OD2	2.08	0.54
1:A:354:ALA:HB1	1:A:366:VAL:HG11	1.90	0.54
1:C:182:ARG:NH1	1:C:185:ARG:CD	2.62	0.54
1:C:295:GLY:O	1:C:299:GLN:HG3	2.08	0.54
1:A:236:ASN:HA	2:A:997:YE1:N1A	2.23	0.53
1:A:27:LYS:O	1:A:28:LEU:C	2.45	0.53
1:C:317:LEU:O	1:C:319:ALA:N	2.42	0.53
2:B:998:YE1:O10	2:B:998:YE1:C8A	2.57	0.53
1:A:372:LEU:O	1:A:376:ILE:HG13	2.08	0.53
1:A:39:SER:C	1:A:42:GLU:N	2.61	0.53
1:A:176:ALA:HB2	1:A:210:VAL:HG11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:ASP:HB2	1:B:221:SER:CB	2.38	0.53
1:B:214:LEU:HD23	1:B:214:LEU:O	2.08	0.53
1:A:101:GLN:O	1:A:104:ALA:HB3	2.08	0.53
1:A:219:VAL:HG13	1:A:228:LYS:O	2.09	0.53
1:C:281:ILE:CG2	1:C:281:ILE:O	2.57	0.53
1:A:238:LYS:O	1:A:242:GLN:CG	2.54	0.53
1:B:197:MET:O	1:B:201:VAL:HG23	2.08	0.53
1:B:226:ARG:NH1	1:B:226:ARG:HG3	2.24	0.53
1:B:239:TYR:HB3	1:B:244:GLY:HA3	1.90	0.53
1:A:222:HIS:CE1	1:A:223:PRO:HG2	2.44	0.53
1:A:343:ARG:NH2	1:B:399:ASP:OD2	2.30	0.53
1:A:231:PHE:CD2	1:A:293:ALA:HB2	2.44	0.53
1:C:186:LEU:CD1	1:C:220:MET:CE	2.87	0.53
1:B:139:LEU:HD12	1:B:406:ARG:HG3	1.91	0.52
1:A:230:VAL:HG13	1:A:292:PHE:CD2	2.44	0.52
1:A:321:LYS:NZ	1:B:384:ASP:HB2	2.24	0.52
2:B:998:YE1:O10	2:B:998:YE1:HC8	2.09	0.52
1:A:103:LEU:HD11	1:A:121:GLN:NE2	2.23	0.52
1:A:189:GLU:CB	1:A:235:ILE:HA	2.38	0.52
1:A:235:ILE:HD11	1:A:245:ILE:HG21	1.90	0.52
1:A:183:ASP:HA	1:A:220:MET:HE1	1.92	0.52
1:B:130:ARG:HG2	1:B:130:ARG:NH1	2.22	0.52
1:C:250:PHE:O	1:C:254:LYS:HB2	2.10	0.52
1:A:324:ILE:HG12	3:A:3:OXY:O1	2.10	0.52
1:A:426:ILE:CG2	1:A:426:ILE:O	2.56	0.52
1:B:54:ARG:NH1	1:B:119:ILE:HD12	2.25	0.52
1:B:388:VAL:CG1	1:B:388:VAL:O	2.54	0.52
1:C:316:SER:OG	1:C:318:PRO:HD3	2.10	0.52
1:A:421:TYR:O	1:A:422:GLY:C	2.48	0.52
1:B:196:ASP:N	1:B:196:ASP:OD1	2.42	0.52
1:B:234:GLY:HA3	2:B:998:YE1:HPN4	1.75	0.52
1:C:201:VAL:HG21	1:C:258:TYR:HB2	1.92	0.52
1:A:340:ARG:NH2	1:B:304:PHE:O	2.42	0.52
1:A:331:LEU:HD13	1:A:408:TYR:HB2	1.92	0.52
1:B:180:MET:SD	1:B:215:LEU:HD11	2.50	0.52
1:B:185:ARG:HG3	1:B:188:ALA:H	1.75	0.52
1:A:419:ARG:HH12	1:B:386:ASP:CB	2.23	0.52
4:A:1011:HOH:O	1:C:415:MET:HE1	2.10	0.52
1:A:275:TRP:O	1:A:276:TRP:C	2.48	0.52
1:A:337:ALA:HB1	1:A:341:VAL:CG1	2.35	0.52
1:C:148:ARG:O	1:C:152:LEU:HG	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:VAL:HG23	1:C:303:VAL:CG1	2.39	0.52
1:C:27:LYS:C	1:C:29:LEU:H	2.13	0.52
1:C:353:TRP:O	1:C:356:GLU:HG2	2.10	0.52
1:C:186:LEU:HD12	1:C:220:MET:CE	2.39	0.51
1:C:263:VAL:HG12	1:C:264:ARG:HG3	1.92	0.51
1:A:111:GLN:HE21	1:A:426:ILE:CG1	2.23	0.51
2:C:999:YE1:O2'	2:C:999:YE1:O9A	2.23	0.51
1:C:190:ASP:O	1:C:192:GLN:N	2.43	0.51
1:C:272:ARG:O	1:C:272:ARG:HG2	2.08	0.51
1:C:340:ARG:O	1:C:344:GLN:HG3	2.11	0.51
1:C:417:ALA:O	1:C:420:LEU:HB2	2.10	0.51
1:A:106:GLU:OE2	1:A:114:LYS:HB3	2.10	0.51
1:A:275:TRP:O	1:A:277:HIS:N	2.44	0.51
1:B:178:LEU:HD13	1:B:285:TRP:HZ3	1.75	0.51
1:B:235:ILE:HD11	1:B:245:ILE:CD1	2.38	0.51
1:A:254:LYS:HZ2	1:A:259:ILE:HD11	1.74	0.51
1:B:327:GLY:C	1:B:329:ALA:H	2.14	0.51
1:B:343:ARG:HG3	1:B:343:ARG:NH1	2.24	0.51
1:B:425:VAL:HG12	1:B:426:ILE:N	2.24	0.51
1:B:106:GLU:O	1:B:114:LYS:HE3	2.10	0.51
1:B:167:VAL:CG1	1:B:168:HIS:N	2.67	0.51
1:B:309:ALA:CB	1:B:363:VAL:HG11	2.40	0.51
1:B:333:LEU:CD2	1:B:342:SER:HA	2.41	0.51
1:B:335:ARG:NH2	1:B:400:GLU:OE1	2.38	0.51
1:C:82:LEU:HD11	1:C:256:LEU:HD12	1.92	0.51
1:A:394:MET:HE2	1:C:412:PHE:HA	1.93	0.51
1:B:189:GLU:O	1:B:236:ASN:HB2	2.11	0.51
1:C:214:LEU:HD12	1:C:286:VAL:O	2.11	0.51
1:B:223:PRO:HA	1:B:226:ARG:CG	2.39	0.51
1:B:235:ILE:CD1	1:B:250:PHE:CE2	2.90	0.51
1:C:156:PHE:CD1	1:C:162:VAL:HG23	2.46	0.51
1:C:191:GLY:CA	1:C:250:PHE:HD1	2.13	0.51
1:C:337:ALA:O	1:C:341:VAL:HB	2.11	0.51
1:A:275:TRP:NE1	1:A:279:PRO:HA	2.25	0.51
1:A:314:TYR:CD2	1:A:351:ARG:HD2	2.45	0.51
1:B:186:LEU:HA	1:B:220:MET:HE3	1.93	0.51
1:A:108:SER:C	1:A:109:LEU:HD23	2.32	0.51
1:A:240:LEU:HA	1:A:245:ILE:HG12	1.93	0.51
1:B:219:VAL:HA	1:B:229:ARG:HA	1.93	0.51
1:B:377:GLU:HA	1:B:380:LEU:HD12	1.91	0.51
1:B:424:ASP:CG	1:B:425:VAL:H	2.15	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:LEU:HD21	1:C:256:LEU:HD22	1.93	0.51
1:C:266:VAL:CG2	1:C:281:ILE:HG21	2.34	0.51
1:C:31:THR:OG1	1:C:32:LEU:HD13	2.10	0.51
1:A:239:TYR:HA	1:A:242:GLN:HG3	1.93	0.50
1:C:235:ILE:HB	2:C:999:YE1:CAE	2.41	0.50
1:C:303:VAL:O	1:C:303:VAL:HG12	2.10	0.50
1:A:186:LEU:HB3	1:A:233:ALA:HB2	1.93	0.50
1:B:186:LEU:HD12	1:B:230:VAL:HG11	1.94	0.50
1:B:269:ASN:C	1:B:271:ASP:OD1	2.50	0.50
1:C:263:VAL:HG23	1:C:303:VAL:HG13	1.94	0.50
1:C:70:ASP:OD1	1:C:75:HIS:HA	2.12	0.50
1:A:58:VAL:HG12	1:A:62:ASP:OD2	2.11	0.50
1:C:15:TRP:O	1:C:18:LEU:HB3	2.12	0.50
1:A:40:SER:CA	1:A:42:GLU:H	2.24	0.50
1:C:101:GLN:O	1:C:104:ALA:HB3	2.12	0.50
1:A:32:LEU:HB3	1:A:33:PRO:HD2	1.94	0.50
1:A:331:LEU:HD13	1:A:408:TYR:CB	2.42	0.50
1:A:43:ARG:O	1:A:47:ALA:N	2.43	0.50
1:C:106:GLU:OE1	1:C:114:LYS:HB3	2.12	0.50
1:C:58:VAL:HG22	1:C:123:ILE:HG23	1.93	0.50
1:C:111:GLN:CG	1:C:243:GLY:HA2	2.24	0.50
1:C:58:VAL:HG12	1:C:62:ASP:OD2	2.11	0.50
1:A:98:PRO:HG2	1:A:117:HIS:HB3	1.94	0.50
1:B:111:GLN:O	1:B:112:ALA:HB3	2.11	0.50
1:B:98:PRO:HD3	1:B:120:ASP:HB2	1.93	0.50
1:B:98:PRO:CG	1:B:117:HIS:HB3	2.42	0.49
1:C:269:ASN:O	1:C:271:ASP:CG	2.50	0.49
1:C:46:ILE:O	1:C:49:ALA:HB3	2.11	0.49
1:A:207:ASP:C	1:A:209:GLY:H	2.15	0.49
1:A:331:LEU:HA	1:B:398:ALA:CB	2.43	0.49
1:C:315:PHE:N	1:C:315:PHE:CD1	2.80	0.49
1:A:213:GLY:HA3	1:A:285:TRP:CE3	2.47	0.49
1:B:239:TYR:O	1:B:243:GLY:N	2.36	0.49
1:B:264:ARG:HH11	1:B:264:ARG:HG2	1.77	0.49
1:B:272:ARG:HB2	1:B:273:PRO:CD	2.42	0.49
1:B:337:ALA:O	1:B:341:VAL:HG21	2.10	0.49
1:A:230:VAL:HG21	1:A:292:PHE:CZ	2.47	0.49
1:A:167:VAL:CG1	1:A:168:HIS:N	2.75	0.49
1:A:38:ARG:HG3	1:A:38:ARG:NH1	2.14	0.49
1:C:352:ILE:HG21	1:C:359:ALA:HA	1.93	0.49
1:B:11:THR:C	1:B:13:GLY:N	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:ARG:HG3	1:B:272:ARG:NH1	2.27	0.49
1:A:207:ASP:OD1	1:A:209:GLY:N	2.42	0.49
1:B:221:SER:O	1:B:226:ARG:NE	2.45	0.49
1:A:110:PRO:CG	1:A:113:ALA:HB3	2.32	0.49
1:B:214:LEU:C	1:B:214:LEU:CD2	2.80	0.49
1:C:12:ASP:CG	1:C:13:GLY:N	2.65	0.49
1:A:176:ALA:HB2	1:A:210:VAL:CG1	2.43	0.49
1:A:264:ARG:NH1	1:A:264:ARG:HG2	2.25	0.49
1:B:419:ARG:NH2	1:B:424:ASP:OD2	2.46	0.49
1:A:111:GLN:O	1:A:114:LYS:HG3	2.13	0.48
1:B:424:ASP:CG	1:B:425:VAL:N	2.66	0.48
1:C:197:MET:O	1:C:201:VAL:HG23	2.13	0.48
1:A:66:ASP:OD1	1:A:133:LEU:HB2	2.14	0.48
1:B:284:PRO:HA	1:B:305:ASP:OD2	2.13	0.48
1:A:251:LEU:HD13	1:A:416:GLN:CG	2.44	0.48
1:B:183:ASP:HB2	1:B:221:SER:H	1.73	0.48
1:B:343:ARG:O	1:B:347:LEU:HB2	2.13	0.48
1:C:236:ASN:HA	2:C:999:YE1:N1A	2.27	0.48
1:A:29:LEU:CD1	1:A:115:GLU:HG3	2.41	0.48
1:A:198:GLU:HA	1:A:258:TYR:HB3	1.94	0.48
1:A:235:ILE:HB	2:A:997:YE1:HAE	1.94	0.48
1:A:384:ASP:H	1:C:321:LYS:NZ	2.11	0.48
1:C:46:ILE:HG23	1:C:47:ALA:N	2.28	0.48
1:A:308:LEU:HD23	1:A:308:LEU:N	2.25	0.48
1:C:79:HIS:CD2	1:C:144:ARG:HD2	2.49	0.48
1:A:98:PRO:HD3	1:A:120:ASP:HB2	1.96	0.48
1:B:58:VAL:HG12	1:B:62:ASP:OD2	2.14	0.48
1:C:139:LEU:CD2	1:C:256:LEU:HD22	2.43	0.48
1:A:171:ARG:HH11	1:A:171:ARG:HG2	1.79	0.48
1:A:189:GLU:HB3	1:A:250:PHE:CZ	2.40	0.48
1:A:339:PRO:O	1:A:343:ARG:HG3	2.14	0.48
1:B:271:ASP:OD1	1:B:271:ASP:N	2.36	0.48
1:A:105:VAL:O	1:A:109:LEU:HG	2.14	0.48
1:A:237:LEU:O	1:A:238:LYS:C	2.52	0.48
1:A:251:LEU:HD13	1:A:416:GLN:HG2	1.96	0.48
1:B:182:ARG:HD2	1:B:184:ASP:OD1	2.13	0.48
1:B:415:MET:O	1:B:419:ARG:HG2	2.14	0.48
1:A:296:GLY:O	1:A:300:LEU:HD22	2.14	0.47
1:C:215:LEU:HD23	1:C:304:PHE:CZ	2.49	0.47
1:B:179:THR:HA	1:B:216:ARG:O	2.13	0.47
1:B:238:LYS:O	1:B:242:GLN:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:SER:O	1:C:42:GLU:N	2.30	0.47
1:B:157:VAL:HA	1:B:171:ARG:HH22	1.79	0.47
1:B:333:LEU:HD23	1:B:342:SER:HA	1.97	0.47
1:B:343:ARG:HG2	1:C:395:LEU:HD13	1.96	0.47
1:A:114:LYS:HD3	1:A:421:TYR:HE1	1.79	0.47
1:A:134:ALA:O	1:A:135:GLY:C	2.52	0.47
1:C:376:ILE:O	1:C:379:SER:HB3	2.15	0.47
1:A:25:VAL:HG22	1:A:49:ALA:HB1	1.95	0.47
1:C:12:ASP:O	1:C:13:GLY:C	2.52	0.47
1:C:184:ASP:OD2	1:C:185:ARG:NE	2.43	0.47
1:C:43:ARG:O	1:C:46:ILE:HG22	2.14	0.47
1:A:130:ARG:HG2	1:A:130:ARG:HH11	1.79	0.47
1:A:31:THR:OG1	1:A:32:LEU:N	2.47	0.47
1:B:262:LEU:O	1:B:392:ARG:NH2	2.42	0.47
1:B:287:ALA:HB2	1:B:304:PHE:CE2	2.50	0.47
1:B:315:PHE:CZ	1:B:363:VAL:HG21	2.49	0.47
1:B:309:ALA:O	1:B:366:VAL:HA	2.15	0.47
1:C:236:ASN:OD1	1:C:238:LYS:HB2	2.15	0.47
1:C:335:ARG:NH2	1:C:400:GLU:HB2	2.30	0.47
1:A:231:PHE:HD2	1:A:293:ALA:HB2	1.79	0.47
1:B:116:GLY:HA2	1:B:421:TYR:CE1	2.50	0.47
1:B:57:ARG:HD2	1:B:120:ASP:OD1	2.15	0.47
1:C:27:LYS:C	1:C:29:LEU:N	2.69	0.47
1:A:109:LEU:CB	1:A:110:PRO:CD	2.93	0.47
1:A:343:ARG:HG2	1:B:395:LEU:HD13	1.96	0.47
1:A:241:SER:C	1:A:243:GLY:N	2.69	0.47
1:B:269:ASN:O	1:B:271:ASP:OD1	2.31	0.47
1:A:156:PHE:CE1	1:A:169:LEU:HG	2.50	0.46
1:A:287:ALA:HB2	1:A:304:PHE:CZ	2.50	0.46
1:C:343:ARG:HB3	1:C:347:LEU:HD12	1.96	0.46
1:C:352:ILE:HD12	1:C:352:ILE:N	2.29	0.46
1:C:126:ARG:O	1:C:130:ARG:HG3	2.16	0.46
1:B:285:TRP:O	1:B:305:ASP:HB2	2.15	0.46
1:C:112:ALA:HA	1:C:426:ILE:HG21	1.96	0.46
1:B:347:LEU:HD22	1:C:388:VAL:HG13	1.97	0.46
2:A:997:YE1:CAE	2:A:997:YE1:OAD	2.62	0.46
1:A:367:VAL:HG22	1:A:371:GLU:HB2	1.97	0.46
1:A:388:VAL:O	1:A:392:ARG:HB2	2.16	0.46
1:B:397:LEU:HD23	1:B:397:LEU:O	2.16	0.46
1:C:130:ARG:CG	1:C:130:ARG:HH11	2.28	0.46
1:A:240:LEU:HB2	1:A:245:ILE:CG1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:SER:HA	1:A:366:VAL:CG1	2.46	0.46
1:A:38:ARG:HD3	1:A:38:ARG:HA	1.53	0.46
1:B:264:ARG:NH1	1:B:264:ARG:HG2	2.31	0.46
1:B:70:ASP:OD1	1:B:75:HIS:HA	2.15	0.46
1:A:159:THR:HG22	1:A:161:GLU:N	2.31	0.46
1:A:324:ILE:HB	1:A:325:ILE:H	1.56	0.46
1:B:192:GLN:NE2	1:B:195:ASP:HB3	2.31	0.46
1:B:419:ARG:HH22	1:B:424:ASP:CG	2.19	0.46
1:C:416:GLN:O	1:C:417:ALA:C	2.54	0.46
1:A:419:ARG:NH1	1:B:386:ASP:HB3	2.31	0.46
1:B:214:LEU:HD12	1:B:380:LEU:CD2	2.36	0.45
1:B:64:HIS:O	1:B:68:VAL:HG23	2.16	0.45
1:B:286:VAL:HG13	1:B:308:LEU:HD23	1.98	0.45
1:A:241:SER:C	1:A:243:GLY:H	2.19	0.45
1:A:298:ALA:HA	1:A:301:LEU:HG	1.99	0.45
1:A:341:VAL:O	1:A:344:GLN:HB2	2.17	0.45
1:A:254:LYS:HE2	2:A:997:YE1:CAJ	2.45	0.45
1:C:186:LEU:HD13	1:C:220:MET:HE2	1.97	0.45
1:C:239:TYR:N	1:C:239:TYR:HD1	2.14	0.45
1:C:308:LEU:CD2	1:C:365:GLU:OE1	2.64	0.45
1:C:38:ARG:HB3	1:C:42:GLU:HB3	1.98	0.45
1:A:157:VAL:HA	1:A:171:ARG:HH21	1.82	0.45
1:A:156:PHE:O	1:A:171:ARG:NH2	2.49	0.45
1:A:303:VAL:O	1:A:303:VAL:CG1	2.65	0.45
1:B:178:LEU:HD13	1:B:285:TRP:CZ3	2.51	0.45
1:C:153:LEU:HB3	1:C:154:PRO:CD	2.46	0.45
1:A:222:HIS:CD2	1:A:223:PRO:HD2	2.50	0.45
1:C:222:HIS:CE1	1:C:223:PRO:HG2	2.52	0.45
1:C:118:GLU:HB2	1:C:421:TYR:HE2	1.81	0.45
1:B:111:GLN:HB3	1:B:426:ILE:HD11	1.97	0.45
1:B:183:ASP:OD2	1:B:221:SER:CB	2.62	0.45
1:A:207:ASP:C	1:A:209:GLY:N	2.70	0.45
1:A:295:GLY:HA3	2:A:997:YE1:HC21	1.98	0.45
1:A:291:GLY:O	1:A:313:ALA:CB	2.65	0.45
1:A:319:ALA:HB3	4:A:1028:HOH:O	2.15	0.45
1:C:110:PRO:O	1:C:112:ALA:N	2.50	0.45
1:A:172:ARG:HB3	1:A:177:ARG:HE	1.82	0.45
1:A:189:GLU:HG3	1:A:234:GLY:O	2.17	0.45
1:A:289:VAL:HB	1:A:309:ALA:CB	2.47	0.45
1:B:222:HIS:C	1:B:226:ARG:HG2	2.37	0.45
1:C:412:PHE:O	1:C:413:ALA:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:VAL:HG12	1:A:168:HIS:N	2.30	0.45
1:B:11:THR:O	1:B:13:GLY:N	2.50	0.45
1:B:337:ALA:O	1:B:341:VAL:HG23	2.16	0.45
1:C:58:VAL:HG22	1:C:123:ILE:CG2	2.47	0.45
1:B:222:HIS:CD2	2:B:998:YE1:H4'	2.52	0.44
1:B:237:LEU:N	2:B:998:YE1:N1A	2.63	0.44
1:A:21:ALA:HB2	1:A:56:LEU:HD12	1.98	0.44
1:A:219:VAL:HA	1:A:229:ARG:HB3	1.99	0.44
1:A:318:PRO:HG2	1:A:319:ALA:H	1.81	0.44
1:B:350:ARG:NH2	1:B:358:GLU:OE1	2.46	0.44
1:C:194:VAL:HG12	1:C:194:VAL:O	2.16	0.44
1:C:337:ALA:CB	1:C:361:LEU:HD13	2.47	0.44
1:B:233:ALA:HB2	1:B:292:PHE:HE2	1.82	0.44
1:C:64:HIS:O	1:C:68:VAL:HG23	2.17	0.44
1:A:106:GLU:C	1:A:108:SER:H	2.21	0.44
1:B:115:GLU:HB2	1:B:117:HIS:CE1	2.52	0.44
1:B:150:LEU:HA	1:B:150:LEU:HD23	1.85	0.44
1:C:182:ARG:C	1:C:184:ASP:N	2.70	0.44
1:A:111:GLN:C	1:A:113:ALA:H	2.20	0.44
1:A:220:MET:HA	1:A:220:MET:CE	2.47	0.44
1:A:125:LEU:HD13	1:A:252:MET:HG3	2.00	0.44
1:B:16:ALA:O	1:B:20:GLU:CB	2.66	0.44
1:C:363:VAL:HG12	1:C:364:ASP:N	2.32	0.44
1:A:156:PHE:HD1	1:A:162:VAL:HG23	1.82	0.44
1:A:296:GLY:O	1:A:300:LEU:CD2	2.65	0.44
1:A:384:ASP:H	1:C:321:LYS:HZ2	1.66	0.44
1:C:319:ALA:HB1	1:C:323:GLY:HA3	2.00	0.44
1:A:189:GLU:CG	1:A:235:ILE:HA	2.48	0.44
1:A:70:ASP:OD1	1:A:75:HIS:HA	2.17	0.44
1:A:236:ASN:ND2	2:A:997:YE1:HC2	2.33	0.44
1:C:377:GLU:C	1:C:379:SER:N	2.71	0.44
1:C:343:ARG:O	1:C:347:LEU:HB2	2.17	0.43
1:A:11:THR:O	1:A:12:ASP:C	2.57	0.43
1:A:337:ALA:CB	1:A:341:VAL:CG1	2.91	0.43
1:C:277:HIS:CE1	1:C:278:SER:HG	2.31	0.43
1:A:117:HIS:O	1:A:120:ASP:HB2	2.17	0.43
1:A:148:ARG:HD3	1:A:199:THR:OG1	2.18	0.43
2:B:998:YE1:OAD	2:B:998:YE1:CAE	2.62	0.43
1:C:130:ARG:NH1	1:C:130:ARG:HG2	2.29	0.43
1:A:20:GLU:O	1:A:23:ALA:HB3	2.19	0.43
1:A:416:GLN:HA	1:A:416:GLN:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ARG:C	1:A:46:ILE:HG22	2.38	0.43
1:C:124:PHE:O	1:C:126:ARG:N	2.52	0.43
1:C:184:ASP:CG	1:C:185:ARG:HE	2.20	0.43
1:A:194:VAL:HG23	1:A:250:PHE:CE1	2.53	0.43
1:A:242:GLN:H	1:A:242:GLN:HG2	1.41	0.43
1:A:64:HIS:O	1:A:68:VAL:HG23	2.18	0.43
1:C:259:ILE:HG12	1:C:300:LEU:HD23	2.01	0.43
1:A:367:VAL:HG12	1:A:372:LEU:HD13	1.98	0.43
1:B:237:LEU:HD11	2:B:998:YE1:HC71	1.99	0.43
1:A:242:GLN:HB2	1:A:243:GLY:O	2.18	0.43
1:B:223:PRO:HA	1:B:226:ARG:NH1	2.34	0.43
1:A:185:ARG:HG3	1:A:188:ALA:H	1.84	0.43
1:B:99:THR:OG1	1:B:102:GLN:HG3	2.19	0.43
1:B:205:LEU:CD1	1:B:266:VAL:HG13	2.49	0.43
1:B:326:PRO:HD2	1:C:391:ASN:OD1	2.18	0.43
1:A:207:ASP:O	1:A:209:GLY:N	2.52	0.42
1:A:79:HIS:CD2	1:A:144:ARG:HD2	2.53	0.42
1:B:238:LYS:O	1:B:242:GLN:CG	2.67	0.42
1:B:250:PHE:O	1:B:254:LYS:HB3	2.18	0.42
1:B:331:LEU:HB2	1:B:408:TYR:CD1	2.53	0.42
2:C:999:YE1:OAD	2:C:999:YE1:CAE	2.62	0.42
1:A:343:ARG:HG3	1:A:343:ARG:NH1	2.29	0.42
1:B:103:LEU:HD11	1:B:121:GLN:HE22	1.84	0.42
1:C:99:THR:HG1	1:C:102:GLN:HG3	1.80	0.42
1:C:106:GLU:OE1	1:C:106:GLU:HA	2.18	0.42
1:C:109:LEU:HB3	1:C:110:PRO:HD2	2.01	0.42
1:C:111:GLN:OE1	1:C:421:TYR:CE1	2.72	0.42
1:A:111:GLN:O	1:A:113:ALA:N	2.52	0.42
1:A:66:ASP:CG	1:A:133:LEU:HD12	2.40	0.42
1:A:318:PRO:O	1:A:319:ALA:C	2.57	0.42
1:A:350:ARG:HG2	1:A:351:ARG:N	2.33	0.42
1:A:424:ASP:CG	1:A:425:VAL:N	2.73	0.42
1:B:148:ARG:HD3	1:B:199:THR:HG21	1.99	0.42
1:A:177:ARG:HG2	1:A:214:LEU:HD23	2.00	0.42
1:A:374:ALA:HB1	1:A:378:ARG:NH1	2.32	0.42
1:A:81:ARG:HB2	1:A:84:GLU:OE1	2.19	0.42
1:B:174:GLY:HA2	1:B:209:GLY:O	2.19	0.42
1:C:316:SER:HB3	1:C:351:ARG:HB3	2.00	0.42
1:A:214:LEU:HD22	1:A:380:LEU:HD11	2.01	0.42
1:A:235:ILE:N	2:A:997:YE1:HC22	2.34	0.42
1:B:340:ARG:O	1:B:344:GLN:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:414:LEU:O	1:C:415:MET:C	2.57	0.42
1:A:144:ARG:NH2	1:A:269:ASN:OD1	2.53	0.42
1:A:247:LEU:HB2	1:A:420:LEU:HD23	2.02	0.42
1:C:170:GLU:OE2	1:C:172:ARG:NH1	2.52	0.42
1:C:186:LEU:HA	1:C:220:MET:CE	2.38	0.42
1:C:215:LEU:HD23	1:C:304:PHE:HZ	1.84	0.42
1:A:388:VAL:HG13	1:C:347:LEU:HD22	2.00	0.42
1:B:235:ILE:HD12	1:B:250:PHE:HE2	1.83	0.42
1:B:205:LEU:HD12	1:B:266:VAL:HG13	2.00	0.42
1:A:331:LEU:HA	1:B:398:ALA:HB1	2.02	0.42
1:C:309:ALA:O	1:C:366:VAL:HA	2.19	0.42
1:A:340:ARG:O	1:A:344:GLN:HG3	2.19	0.42
1:A:419:ARG:HD3	1:B:390:ALA:CB	2.49	0.42
1:A:183:ASP:CA	1:A:220:MET:HE1	2.49	0.42
1:A:240:LEU:HB2	1:A:245:ILE:HG13	2.02	0.42
1:A:311:SER:HA	1:A:366:VAL:HG12	2.01	0.42
1:B:416:GLN:O	1:B:420:LEU:HD13	2.20	0.42
1:A:330:ASN:HB2	1:A:408:TYR:OH	2.20	0.42
1:B:54:ARG:NH2	1:B:116:GLY:O	2.53	0.42
1:A:43:ARG:C	1:A:45:GLU:N	2.73	0.41
1:B:172:ARG:O	1:B:173:ASP:CB	2.64	0.41
1:C:378:ARG:HG2	1:C:382:ARG:NH1	2.35	0.41
1:A:18:LEU:CD1	1:A:57:ARG:HG2	2.49	0.41
1:B:254:LYS:HG3	1:B:259:ILE:CD1	2.50	0.41
1:A:75:HIS:O	1:A:76:ARG:C	2.59	0.41
1:B:162:VAL:HG21	1:B:203:LEU:CD1	2.50	0.41
1:B:223:PRO:HD3	1:B:226:ARG:NH2	2.35	0.41
1:B:239:TYR:HB3	1:B:244:GLY:CA	2.50	0.41
1:B:231:PHE:HB3	1:B:292:PHE:O	2.20	0.41
1:B:377:GLU:O	1:B:380:LEU:N	2.52	0.41
1:B:425:VAL:HG12	1:B:426:ILE:HG13	2.02	0.41
1:C:27:LYS:O	1:C:29:LEU:N	2.54	0.41
1:C:378:ARG:HG2	1:C:382:ARG:HH12	1.85	0.41
1:A:384:ASP:N	1:C:321:LYS:HZ2	2.18	0.41
1:A:58:VAL:HG22	1:A:123:ILE:HG23	2.01	0.41
1:B:156:PHE:CD1	1:B:162:VAL:HG23	2.56	0.41
1:B:326:PRO:HG3	1:B:346:ILE:HG23	2.02	0.41
1:C:119:ILE:HA	1:C:417:ALA:HB1	2.01	0.41
1:A:247:LEU:O	1:A:252:MET:HG2	2.20	0.41
1:A:337:ALA:HB1	1:A:341:VAL:HG21	2.02	0.41
1:A:341:VAL:O	1:A:345:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ARG:O	1:A:45:GLU:N	2.54	0.41
1:A:70:ASP:OD1	1:A:76:ARG:NH1	2.53	0.41
1:B:34:GLU:O	1:B:35:HIS:C	2.59	0.41
1:B:79:HIS:HD2	1:B:144:ARG:CZ	2.33	0.41
1:C:35:HIS:ND1	1:C:113:ALA:HA	2.36	0.41
1:A:111:GLN:HB2	1:A:243:GLY:N	2.35	0.41
1:B:111:GLN:HB3	1:B:111:GLN:HE21	1.64	0.41
1:B:153:LEU:N	1:B:154:PRO:CD	2.84	0.41
1:A:308:LEU:HD23	1:A:308:LEU:H	1.84	0.41
1:A:343:ARG:HH11	1:A:343:ARG:CG	2.31	0.41
1:C:111:GLN:HG2	1:C:243:GLY:CA	2.27	0.41
1:C:198:GLU:CG	1:C:198:GLU:O	2.68	0.41
1:B:162:VAL:HG21	1:B:203:LEU:HD13	2.02	0.41
1:B:337:ALA:CB	1:B:341:VAL:HB	2.51	0.41
1:B:81:ARG:HB2	1:B:84:GLU:OE1	2.20	0.41
1:C:308:LEU:HD13	1:C:376:ILE:HG12	2.03	0.41
1:C:72:LEU:HD22	1:C:88:ALA:HB1	2.02	0.41
1:A:182:ARG:HB2	1:A:187:ASN:HA	2.03	0.41
1:A:250:PHE:O	1:A:254:LYS:HB2	2.21	0.41
1:A:230:VAL:CG2	1:A:292:PHE:CZ	3.04	0.41
1:C:139:LEU:HA	1:C:139:LEU:HD23	1.93	0.41
1:C:205:LEU:HD12	1:C:266:VAL:HG13	2.02	0.41
1:B:18:LEU:HD11	1:B:57:ARG:HG2	2.03	0.41
1:C:310:SER:HA	1:C:367:VAL:O	2.21	0.41
1:C:119:ILE:O	1:C:123:ILE:HG13	2.21	0.40
1:C:317:LEU:N	1:C:318:PRO:HD3	2.36	0.40
1:C:251:LEU:HD13	1:C:416:GLN:CG	2.51	0.40
1:A:111:GLN:HE21	1:A:426:ILE:HG12	1.86	0.40
1:A:288:ALA:HA	1:A:308:LEU:O	2.21	0.40
1:B:166:ALA:HB3	1:B:196:ASP:OD2	2.21	0.40
1:B:251:LEU:HA	1:B:251:LEU:HD23	1.83	0.40
1:C:145:PRO:HD2	1:C:267:LEU:O	2.20	0.40
1:C:186:LEU:HD13	1:C:220:MET:CE	2.50	0.40
1:C:191:GLY:CA	1:C:250:PHE:CD1	2.96	0.40
1:C:222:HIS:ND1	1:C:224:ARG:N	2.65	0.40
1:C:350:ARG:CG	1:C:351:ARG:N	2.84	0.40
1:C:75:HIS:O	1:C:76:ARG:C	2.59	0.40
1:A:140:ASP:O	1:A:144:ARG:HG3	2.20	0.40
1:A:111:GLN:HG2	1:A:426:ILE:HD11	2.03	0.40
1:B:119:ILE:O	1:B:123:ILE:HG13	2.22	0.40
1:C:216:ARG:CG	1:C:217:GLY:N	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ALA:HB1	1:A:236:ASN:HB2	2.04	0.40
1:B:218:GLY:HA2	1:B:229:ARG:NH1	2.36	0.40
1:B:387:ALA:C	1:B:389:LEU:H	2.23	0.40
1:C:187:ASN:O	1:C:188:ALA:C	2.60	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	415/417 (100%)	350 (84%)	47 (11%)	18 (4%)	3	18
1	B	415/417 (100%)	363 (88%)	45 (11%)	7 (2%)	11	44
1	C	413/417 (99%)	339 (82%)	67 (16%)	7 (2%)	11	44
All	All	1243/1251 (99%)	1052 (85%)	159 (13%)	32 (3%)	6	31

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	ALA
1	A	319	ALA
1	B	112	ALA
1	B	271	ASP
1	C	183	ASP
1	A	107	ARG
1	A	111	GLN
1	A	112	ALA
1	A	135	GLY
1	C	111	GLN
1	C	125	LEU
1	A	34	GLU
1	A	238	LYS

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Mol	Chain	Res	Type
1	A	242	GLN
1	A	276	TRP
1	A	311	SER
1	A	318	PRO
1	A	423	HIS
1	B	12	ASP
1	B	378	ARG
1	C	15	TRP
1	B	425	VAL
1	B	319	ALA
1	C	371	GLU
1	A	385	GLY
1	B	341	VAL
1	C	270	ASP
1	A	425	VAL
1	A	244	GLY
1	A	245	ILE
1	A	324	ILE
1	C	98	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	318/328 (97%)	302 (95%)	16 (5%)	28	67
1	B	327/328 (100%)	317 (97%)	10 (3%)	45	80
1	C	322/328 (98%)	309 (96%)	13 (4%)	36	74
All	All	967/984 (98%)	928 (96%)	39 (4%)	36	74

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	63	THR
1	A	102	GLN

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Mol	Chain	Res	Type
1	A	186	LEU
1	A	242	GLN
1	A	271	ASP
1	A	308	LEU
1	A	311	SER
1	A	315	PHE
1	A	317	LEU
1	A	331	LEU
1	A	340	ARG
1	A	384	ASP
1	A	403	ASP
1	A	424	ASP
1	A	425	VAL
1	B	11	THR
1	B	63	THR
1	B	190	ASP
1	B	196	ASP
1	B	214	LEU
1	B	240	LEU
1	B	254	LYS
1	B	271	ASP
1	B	272	ARG
1	B	370	ASP
1	C	24	SER
1	C	33	PRO
1	C	39	SER
1	C	63	THR
1	C	152	LEU
1	C	183	ASP
1	C	186	LEU
1	C	271	ASP
1	C	272	ARG
1	C	315	PHE
1	C	340	ARG
1	C	367	VAL
1	C	373	ASP

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	100	GLN
1	A	111	GLN

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Mol	Chain	Res	Type
1	A	121	GLN
1	A	168	HIS
1	B	79	HIS
1	B	102	GLN
1	B	111	GLN
1	B	121	GLN
1	B	168	HIS
1	B	423	HIS
1	C	79	HIS
1	C	102	GLN
1	C	299	GLN
1	C	416	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](#)

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
3	OXY	A	3	-	1,1,1	1.31	0	0,0,0	0.00	-
2	YE1	A	997	-	55,62,62	1.83	8 (14%)	66,92,92	2.23	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	YE1	B	998	-	55,62,62	1.84	8 (14%)	66,92,92	2.23	9 (13%)
3	OXY	C	2	-	1,1,1	1.32	0	0,0,0	0.00	-
2	YE1	C	999	-	55,62,62	1.83	8 (14%)	66,92,92	2.22	9 (13%)

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
3	OXY	A	3	-	-	0/0/0/0	0/0/0/0
2	YE1	A	997	-	-	0/51/71/71	0/4/4/4
2	YE1	B	998	-	-	0/51/71/71	0/4/4/4
3	OXY	C	2	-	-	0/0/0/0	0/0/0/0
2	YE1	C	999	-	-	0/51/71/71	0/4/4/4

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	999	YE1	C2P-NAA	-4.69	1.35	1.46
2	A	997	YE1	C2P-NAA	-4.66	1.35	1.46
2	B	998	YE1	C2P-NAA	-4.65	1.35	1.46
2	B	998	YE1	P3'-O3'	-3.59	1.53	1.59
2	A	997	YE1	P3'-O3'	-3.47	1.53	1.59
2	C	999	YE1	P3'-O3'	-3.46	1.53	1.59
2	B	998	YE1	C3P-N4P	-2.47	1.40	1.46
2	A	997	YE1	C3P-N4P	-2.44	1.40	1.46
2	C	999	YE1	C3P-N4P	-2.42	1.40	1.46
2	C	999	YE1	C2A-N1A	2.05	1.37	1.33
2	A	997	YE1	C2A-N1A	2.12	1.37	1.33
2	B	998	YE1	C2A-N1A	2.16	1.38	1.33
2	A	997	YE1	C5P-N4P	2.94	1.40	1.33
2	B	998	YE1	C5P-N4P	2.95	1.40	1.33
2	C	999	YE1	C5P-N4P	3.00	1.40	1.33
2	C	999	YE1	CAB-NAA	3.00	1.40	1.33
2	A	997	YE1	CAB-NAA	3.01	1.40	1.33
2	B	998	YE1	CAB-NAA	3.01	1.40	1.33
2	A	997	YE1	C9P-N8P	3.32	1.40	1.33
2	C	999	YE1	C9P-N8P	3.34	1.40	1.33
2	B	998	YE1	C9P-N8P	3.39	1.40	1.33
2	A	997	YE1	OAD-CAB	9.20	1.42	1.23
2	B	998	YE1	OAD-CAB	9.21	1.42	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	999	YE1	OAD-CAB	9.23	1.42	1.23

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	998	YE1	C2P-NAA-CAB	-7.16	109.09	122.84
2	C	999	YE1	C2P-NAA-CAB	-7.14	109.13	122.84
2	A	997	YE1	C2P-NAA-CAB	-7.11	109.19	122.84
2	B	998	YE1	C7P-N8P-C9P	-7.01	109.53	122.59
2	A	997	YE1	C7P-N8P-C9P	-7.00	109.55	122.59
2	C	999	YE1	C3P-N4P-C5P	-6.97	109.46	122.84
2	B	998	YE1	C3P-N4P-C5P	-6.96	109.48	122.84
2	A	997	YE1	C3P-N4P-C5P	-6.95	109.51	122.84
2	C	999	YE1	C7P-N8P-C9P	-6.93	109.66	122.59
2	B	998	YE1	C6P-C7P-N8P	-6.64	98.13	111.87
2	A	997	YE1	C6P-C7P-N8P	-6.63	98.15	111.87
2	C	999	YE1	C6P-C7P-N8P	-6.61	98.19	111.87
2	A	997	YE1	O6A-P2A-O5A	-6.24	84.08	109.25
2	B	998	YE1	O6A-P2A-O5A	-6.23	84.12	109.25
2	C	999	YE1	O6A-P2A-O5A	-6.21	84.20	109.25
2	A	997	YE1	C7P-C6P-C5P	-4.75	104.58	112.22
2	B	998	YE1	C7P-C6P-C5P	-4.73	104.62	112.22
2	C	999	YE1	C7P-C6P-C5P	-4.70	104.65	112.22
2	C	999	YE1	O9P-C9P-N8P	-2.68	117.90	123.07
2	B	998	YE1	O9P-C9P-N8P	-2.66	117.95	123.07
2	A	997	YE1	O9P-C9P-N8P	-2.66	117.95	123.07
2	A	997	YE1	C4A-C5A-N7A	2.45	111.78	109.41
2	C	999	YE1	C4A-C5A-N7A	2.49	111.81	109.41
2	B	998	YE1	C4A-C5A-N7A	2.52	111.84	109.41
2	B	998	YE1	C14-C11-C10	3.12	114.23	108.82
2	C	999	YE1	C14-C11-C10	3.12	114.23	108.82
2	A	997	YE1	C14-C11-C10	3.12	114.24	108.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3	OXY	1	0
2	A	997	YE1	20	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	998	YE1	13	0
2	C	999	YE1	12	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, 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	417/417 (100%)	-0.00	14 (3%)	46 20	20, 41, 68, 77	0
1	B	417/417 (100%)	-0.10	9 (2%)	62 33	24, 42, 63, 72	0
1	C	415/417 (99%)	-0.07	3 (0%)	87 67	21, 43, 63, 74	0
All	All	1249/1251 (99%)	-0.06	26 (2%)	64 34	20, 42, 64, 77	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	39	SER	4.3
1	A	223	PRO	3.9
1	A	37	ALA	3.2
1	A	426	ILE	3.1
1	A	424	ASP	3.0
1	A	10	ASP	2.9
1	A	225	TYR	2.8
1	B	221	SER	2.6
1	A	11	THR	2.5
1	C	183	ASP	2.5
1	B	227	GLY	2.5
1	A	236	ASN	2.5
1	C	37	ALA	2.5
1	B	224	ARG	2.3
1	A	222	HIS	2.3
1	A	42	GLU	2.3
1	A	425	VAL	2.3
1	B	159	THR	2.3
1	B	236	ASN	2.2
1	B	321	LYS	2.2
1	B	424	ASP	2.2
1	A	240	LEU	2.2
1	B	183	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	36	GLY	2.1
1	C	319	ALA	2.1
1	B	225	TYR	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
3	OXY	C	2	2/2	0.64	0.45	2.29	69,69,69,69	0
2	YE1	B	998	59/59	0.78	0.49	1.79	40,73,105,156	0
2	YE1	A	997	59/59	0.85	0.41	1.43	45,70,105,135	0
2	YE1	C	999	59/59	0.88	0.33	1.21	36,64,86,135	0
3	OXY	A	3	2/2	0.81	0.28	-0.40	69,69,69,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.