Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:21 PM GMT

PDB ID	:	1ONP
Title	:	IspC complex with Mn2+ and fosmidomycin
Authors	:	Steinbacher, S.; Kaiser, J.; Eisenreich, W.; Huber, R.; Bacher, A.; Rohdich, F.
Deposited on	:	2003-02-28
Resolution	:	2.50 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:

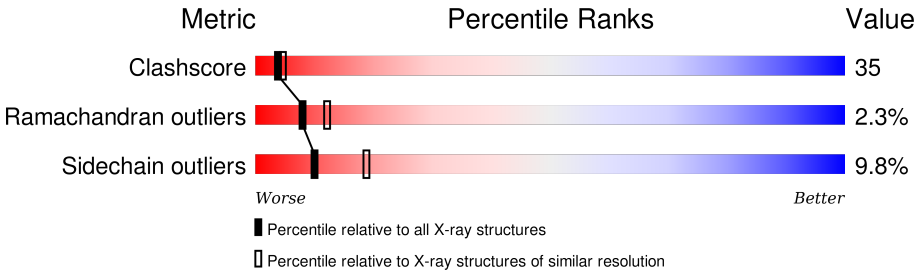
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

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

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	398	50% 42% 6%
1	B	398	46% 46% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6215 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.

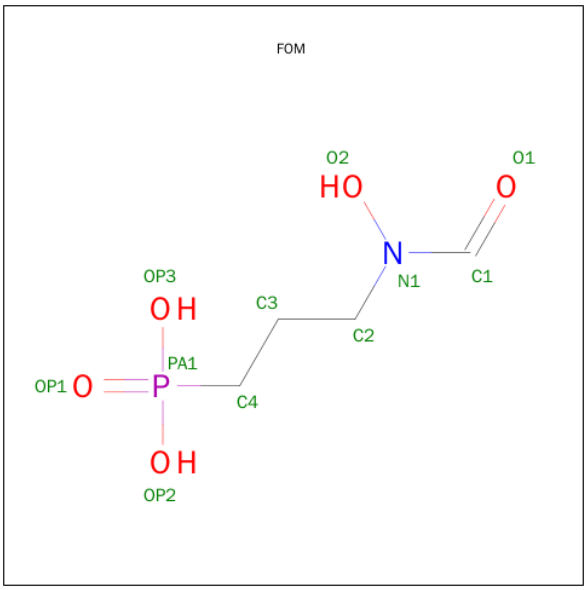
- Molecule 1 is a protein called 1-deoxy-D-xylulose 5-phosphate reductoisomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	0	0
			3023	1889	533	574	27			
1	B	397	Total	C	N	O	S	0	0	0
			3023	1889	533	574	27			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mn	0	0
			1	1		
2	A	1	Total	Mn	0	0
			1	1		

- Molecule 3 is 3-[FORMYL(HYDROXY)AMINO]PROPYLPHOSPHONIC ACID (three-letter code: FOM) (formula: $C_4H_{10}NO_5P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			11	4	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			11	4	1	5	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	83	Total	O	0	0
			83	83		
4	B	62	Total	O	0	0
			62	62		

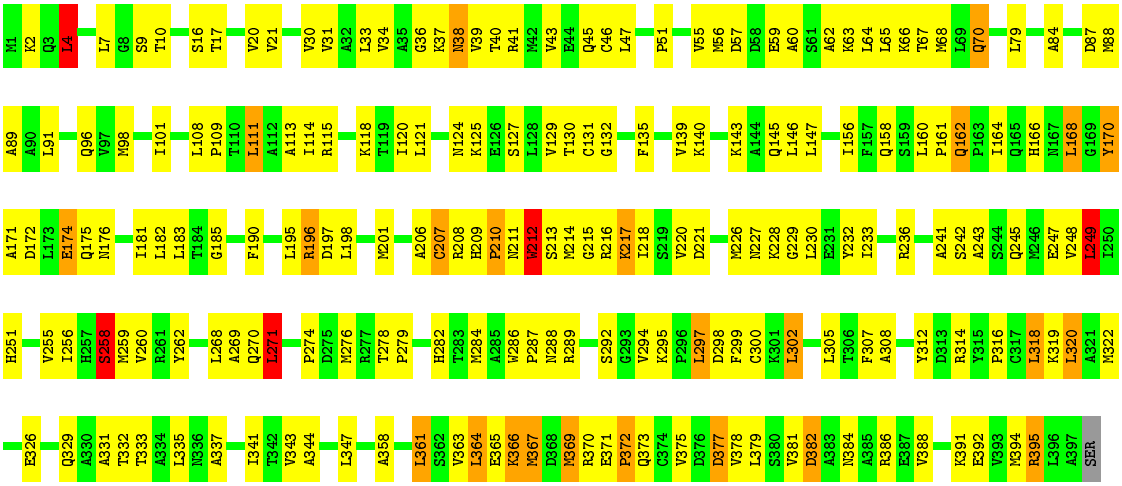
3 Residue-property plots (i)

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.

Note EDS was not executed.

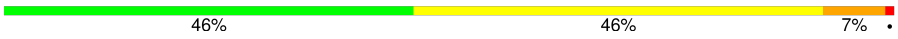
- Molecule 1: 1-deoxy-D-xylulose 5-phosphate reductoisomerase

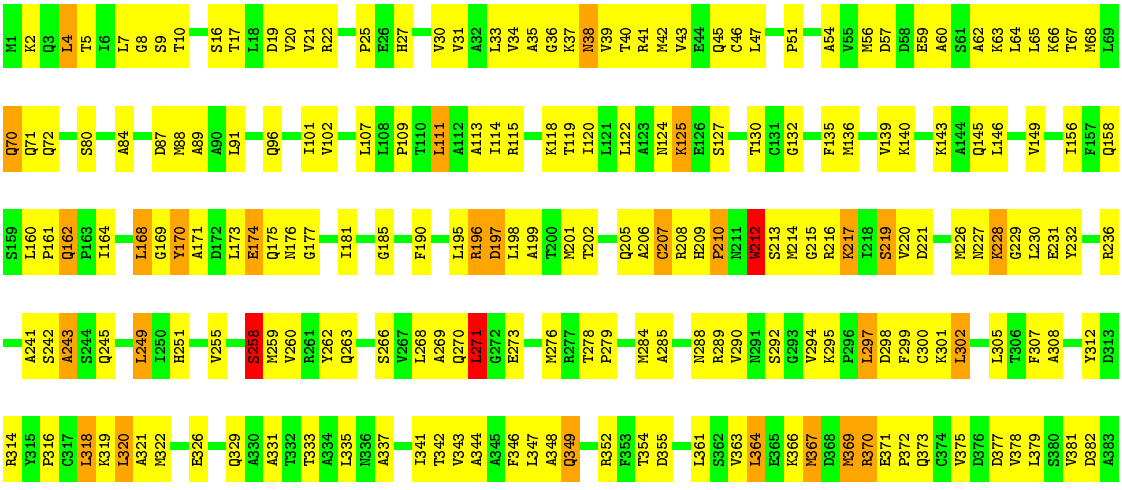
Chain A:

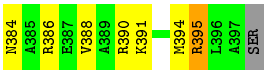


- Molecule 1: 1-deoxy-D-xylulose 5-phosphate reductoisomerase

Chain B:






N384
A385
R386
E387
V388
A389
R390
K391
M394
R395
L396
A397
SER

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	90.75Å 52.30Å 107.59Å 90.00° 92.11° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.50)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.255 , 0.330	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6215	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.49	0/3071	0.78	3/4163 (0.1%)
1	B	0.52	0/3071	0.79	1/4163 (0.0%)
All	All	0.50	0/6142	0.79	4/8326 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	271	LEU	CA-CB-CG	5.67	128.34	115.30
1	B	271	LEU	CA-CB-CG	5.51	127.98	115.30
1	A	4	LEU	CA-CB-CG	5.51	127.97	115.30
1	A	249	LEU	CA-CB-CG	5.46	127.86	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3023	0	3050	213	0
1	B	3023	0	3050	218	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	11	0	7	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	11	0	7	0	0
4	A	83	0	0	7	0
4	B	62	0	0	7	1
All	All	6215	0	6114	426	1

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 35.

All (426) 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:B:132:GLY:H	1:B:329:GLN:HE21	1.04	1.00
1:A:162:GLN:HG3	1:B:162:GLN:HG3	1.52	0.92
1:A:132:GLY:H	1:A:329:GLN:HE21	1.16	0.91
1:B:262:TYR:CE1	1:B:268:LEU:HD12	2.05	0.91
1:B:395:ARG:HB3	1:B:395:ARG:NH1	1.88	0.89
1:B:375:VAL:O	1:B:379:LEU:HG	1.77	0.84
1:B:220:VAL:HG21	1:B:347:LEU:HD21	1.62	0.82
1:A:375:VAL:O	1:A:379:LEU:HG	1.79	0.82
1:A:395:ARG:HB3	1:A:395:ARG:NH1	1.94	0.81
1:A:220:VAL:HG21	1:A:347:LEU:HD21	1.63	0.81
1:A:369:MET:HE3	1:A:369:MET:H	1.47	0.80
1:A:262:TYR:CE1	1:A:268:LEU:HD12	2.15	0.80
1:A:132:GLY:H	1:A:329:GLN:NE2	1.80	0.80
1:B:130:THR:HB	1:B:378:VAL:CG1	2.12	0.79
1:B:391:LYS:HD3	1:B:394:MET:CE	2.13	0.79
1:B:228:LYS:HE3	1:B:228:LYS:HA	1.64	0.78
1:A:39:VAL:HG11	1:A:64:LEU:HD22	1.66	0.78
1:A:38:ASN:ND2	1:A:41:ARG:HB3	1.99	0.78
1:A:7:LEU:C	1:A:101:ILE:HG13	2.05	0.77
1:A:391:LYS:HD3	1:A:394:MET:CE	2.15	0.77
1:B:39:VAL:HG13	1:B:65:LEU:HB2	1.66	0.76
1:B:115:ARG:HG3	1:B:115:ARG:HH11	1.51	0.76
1:B:132:GLY:H	1:B:329:GLN:NE2	1.81	0.76
1:A:363:VAL:HG13	1:A:388:VAL:HB	1.66	0.76
1:B:38:ASN:ND2	1:B:41:ARG:HB3	1.99	0.76
1:A:391:LYS:HD3	1:A:394:MET:HE1	1.67	0.75
1:A:118:LYS:O	1:A:120:ILE:HG13	1.87	0.75
1:B:384:ASN:O	1:B:388:VAL:HG23	1.87	0.74
1:A:249:LEU:HD21	1:A:307:PHE:HB3	1.67	0.74
1:A:369:MET:H	1:A:369:MET:CE	2.00	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ILE:HG23	1:A:171:ALA:HB3	1.68	0.74
1:B:39:VAL:HG11	1:B:64:LEU:HD22	1.70	0.73
1:B:208:ARG:HG2	1:B:215:GLY:N	2.04	0.73
1:B:395:ARG:HH11	1:B:395:ARG:HB3	1.51	0.73
1:B:363:VAL:HG13	1:B:388:VAL:HB	1.71	0.72
1:A:190:PHE:CZ	1:A:206:ALA:HB2	2.24	0.72
1:B:249:LEU:HD21	1:B:307:PHE:HB3	1.71	0.72
1:A:384:ASN:O	1:A:388:VAL:HG23	1.89	0.72
1:A:251:HIS:HE1	1:A:255:VAL:H	1.38	0.71
1:B:146:LEU:O	1:B:168:LEU:HD12	1.89	0.71
1:A:132:GLY:N	1:A:329:GLN:HE21	1.87	0.71
1:A:130:THR:HB	1:A:378:VAL:CG1	2.21	0.71
1:B:226:MET:HE2	1:B:230:LEU:HG	1.73	0.71
1:A:185:GLY:HA3	1:A:228:LYS:HE3	1.71	0.71
1:B:251:HIS:HE1	1:B:255:VAL:H	1.36	0.71
1:A:226:MET:HE1	1:A:335:LEU:HD11	1.73	0.70
1:A:208:ARG:HG2	1:A:215:GLY:N	2.07	0.70
1:A:298:ASP:O	1:A:302:LEU:HD13	1.92	0.69
1:A:146:LEU:O	1:A:168:LEU:HD12	1.91	0.69
1:B:41:ARG:O	1:B:45:GLN:HG3	1.92	0.69
1:B:228:LYS:CE	1:B:228:LYS:HA	2.22	0.69
1:B:320:LEU:HD13	1:B:335:LEU:HD21	1.74	0.69
1:A:208:ARG:HB2	1:A:208:ARG:HH11	1.58	0.69
1:B:259:MET:HG2	1:B:269:ALA:HB2	1.73	0.69
1:B:236:ARG:NH2	1:B:326:GLU:OE2	2.26	0.68
1:A:196:ARG:HA	1:A:196:ARG:CZ	2.23	0.68
1:B:217:LYS:HB3	1:B:217:LYS:NZ	2.08	0.67
1:B:190:PHE:CZ	1:B:206:ALA:HB2	2.29	0.67
1:A:320:LEU:HD13	1:A:335:LEU:HD21	1.75	0.67
1:B:132:GLY:N	1:B:329:GLN:HE21	1.87	0.67
1:B:164:ILE:HA	1:B:171:ALA:CB	2.25	0.67
1:A:39:VAL:HG13	1:A:65:LEU:HB2	1.76	0.67
1:A:249:LEU:CD2	1:A:307:PHE:HB3	2.24	0.67
1:A:221:ASP:HB3	1:A:227:ASN:HB2	1.77	0.67
1:B:64:LEU:HD23	1:B:64:LEU:O	1.95	0.66
1:B:62:ALA:O	1:B:66:LYS:HB2	1.95	0.66
1:B:118:LYS:O	1:B:120:ILE:HG13	1.95	0.66
1:B:16:SER:O	1:B:20:VAL:HG23	1.94	0.66
1:A:62:ALA:O	1:A:66:LYS:HB2	1.95	0.66
1:B:391:LYS:HD3	1:B:394:MET:HE3	1.76	0.66
1:A:16:SER:O	1:A:20:VAL:HG23	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:ASP:O	1:B:302:LEU:HD13	1.95	0.65
1:B:377:ASP:O	1:B:381:VAL:HG23	1.97	0.65
1:B:115:ARG:NH1	1:B:115:ARG:HG3	2.09	0.64
1:B:130:THR:HG22	1:B:333:THR:HA	1.80	0.64
1:A:114:ILE:HA	1:A:120:ILE:HD11	1.80	0.63
1:A:251:HIS:CE1	1:A:255:VAL:H	2.16	0.63
1:B:391:LYS:HD3	1:B:394:MET:HE1	1.79	0.63
1:A:156:ILE:O	1:A:160:LEU:HG	1.98	0.63
1:B:208:ARG:HB2	1:B:208:ARG:HH11	1.62	0.63
1:A:395:ARG:HH11	1:A:395:ARG:HB3	1.61	0.63
1:A:174:GLU:HB3	1:A:245:GLN:HE22	1.64	0.63
1:B:366:LYS:O	1:B:367:MET:HB2	1.98	0.63
1:B:30:VAL:HG12	1:B:51:PRO:HB3	1.80	0.62
1:B:251:HIS:CE1	1:B:255:VAL:H	2.17	0.62
1:A:236:ARG:HH21	1:A:243:ALA:HB2	1.64	0.62
1:B:114:ILE:HA	1:B:120:ILE:HD11	1.81	0.62
1:B:216:ARG:HB3	1:B:216:ARG:NH1	2.15	0.62
1:A:7:LEU:O	1:A:101:ILE:HG13	1.99	0.61
1:A:226:MET:HE1	1:A:335:LEU:CD1	2.31	0.60
1:A:89:ALA:HB1	1:A:113:ALA:HB2	1.82	0.60
1:B:130:THR:HB	1:B:378:VAL:HG11	1.83	0.60
1:A:115:ARG:NH1	1:A:115:ARG:HG3	2.17	0.60
1:B:68:MET:O	1:B:71:GLN:HB2	2.02	0.60
1:A:164:ILE:HA	1:A:171:ALA:CB	2.32	0.59
1:A:217:LYS:NZ	1:A:217:LYS:HB3	2.17	0.59
1:A:386:ARG:HG2	1:A:386:ARG:HH11	1.67	0.59
1:B:170:TYR:CD2	1:B:170:TYR:N	2.70	0.59
1:A:2:LYS:HD2	1:A:96:GLN:NE2	2.16	0.59
1:A:64:LEU:O	1:A:64:LEU:HD23	2.02	0.59
1:B:107:LEU:O	1:B:111:LEU:HB2	2.02	0.59
1:A:10:THR:HG22	1:A:41:ARG:HG2	1.84	0.59
1:B:19:ASP:OD1	1:B:22:ARG:NH1	2.36	0.59
1:A:70:GLN:HE21	1:A:70:GLN:HA	1.68	0.59
1:A:67:THR:O	1:A:70:GLN:HB3	2.03	0.58
1:B:369:MET:CE	1:B:369:MET:H	2.16	0.58
1:A:170:TYR:N	1:A:170:TYR:CD2	2.71	0.58
1:A:366:LYS:O	1:A:367:MET:HB2	2.03	0.58
1:A:164:ILE:HG23	1:A:171:ALA:CB	2.33	0.58
1:B:33:LEU:HD12	1:B:51:PRO:HG3	1.85	0.58
1:B:135:PHE:O	1:B:139:VAL:HG23	2.04	0.58
1:A:130:THR:HG22	1:A:333:THR:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:VAL:HG21	1:A:305:LEU:HD21	1.85	0.57
1:A:7:LEU:O	1:A:101:ILE:N	2.37	0.57
1:A:208:ARG:CB	1:A:208:ARG:NH1	2.68	0.57
1:B:196:ARG:CZ	1:B:196:ARG:HA	2.34	0.57
1:A:259:MET:HG2	1:A:269:ALA:HB2	1.87	0.57
1:B:208:ARG:NH1	1:B:208:ARG:CB	2.68	0.57
1:B:22:ARG:O	1:B:25:PRO:HD3	2.04	0.57
1:A:229:GLY:O	1:A:232:TYR:HB3	2.03	0.57
1:A:158:GLN:OE1	1:A:289:ARG:NH2	2.31	0.57
1:A:161:PRO:HD3	1:A:262:TYR:OH	2.04	0.57
1:A:115:ARG:HH11	1:A:115:ARG:HG3	1.67	0.57
1:A:216:ARG:NH1	1:A:216:ARG:HB3	2.19	0.57
1:A:341:ILE:O	1:A:344:ALA:HB3	2.05	0.57
1:B:25:PRO:HB3	4:B:1044:HOH:O	2.04	0.56
1:B:164:ILE:HG23	1:B:171:ALA:HB3	1.86	0.56
1:B:208:ARG:HH11	1:B:208:ARG:CB	2.18	0.56
1:A:375:VAL:HG12	1:A:375:VAL:O	2.05	0.56
1:A:391:LYS:HA	1:A:394:MET:HE3	1.86	0.56
1:A:84:ALA:O	1:A:88:MET:HG2	2.06	0.56
1:A:98:MET:HA	1:A:121:LEU:HB2	1.88	0.56
1:B:111:LEU:HD22	1:B:135:PHE:CE1	2.41	0.56
1:A:262:TYR:CZ	1:A:268:LEU:HD12	2.41	0.56
1:A:64:LEU:O	1:A:67:THR:HB	2.05	0.56
1:A:249:LEU:HD23	1:A:308:ALA:O	2.05	0.56
1:A:164:ILE:HA	1:A:171:ALA:HB1	1.88	0.56
1:B:228:LYS:CA	1:B:228:LYS:HE3	2.29	0.56
1:A:295:LYS:NZ	1:A:298:ASP:HB2	2.21	0.56
1:B:146:LEU:HB2	1:B:168:LEU:HD13	1.88	0.56
1:B:299:PHE:HA	1:B:302:LEU:HD22	1.88	0.56
1:B:124:ASN:ND2	1:B:127:SER:H	2.04	0.56
1:A:108:LEU:HG	1:A:375:VAL:HG11	1.87	0.55
1:B:249:LEU:CD2	1:B:307:PHE:HB3	2.33	0.55
1:A:2:LYS:HD2	1:A:96:GLN:HE21	1.70	0.55
1:B:386:ARG:HG2	1:B:386:ARG:HH11	1.71	0.55
1:A:335:LEU:HB2	1:A:364:LEU:HD21	1.88	0.55
1:B:111:LEU:HD23	1:B:375:VAL:CG2	2.37	0.55
1:B:67:THR:O	1:B:70:GLN:HB3	2.07	0.55
1:B:136:MET:O	1:B:140:LYS:HG3	2.06	0.55
1:B:43:VAL:HG12	1:B:47:LEU:CD1	2.37	0.55
1:B:64:LEU:C	1:B:64:LEU:HD23	2.27	0.55
1:B:221:ASP:HB3	1:B:227:ASN:HB2	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ILE:HG22	1:A:164:ILE:O	2.06	0.54
1:A:226:MET:HE2	1:A:230:LEU:HG	1.88	0.54
1:B:130:THR:CG2	1:B:333:THR:HG23	2.37	0.54
1:B:212:TRP:CE3	1:B:212:TRP:HA	2.42	0.54
1:A:391:LYS:HD3	1:A:394:MET:HE3	1.89	0.54
1:A:46:CYS:HA	1:A:51:PRO:HD2	1.90	0.54
1:A:377:ASP:O	1:A:381:VAL:HG23	2.08	0.54
1:A:30:VAL:HG12	1:A:51:PRO:HB3	1.89	0.54
1:A:226:MET:CE	1:A:230:LEU:HG	2.38	0.54
1:A:208:ARG:NH2	1:A:214:MET:SD	2.81	0.54
1:B:209:HIS:O	1:B:213:SER:HB3	2.08	0.53
1:B:158:GLN:OE1	1:B:289:ARG:NH2	2.33	0.53
1:B:215:GLY:O	1:B:219:SER:HB2	2.09	0.53
1:A:9:SER:CB	1:A:33:LEU:HD22	2.39	0.53
1:A:297:LEU:HD22	1:A:302:LEU:HD11	1.91	0.53
1:B:207:CYS:N	1:B:209:HIS:NE2	2.49	0.53
1:B:216:ARG:HG3	4:B:1050:HOH:O	2.08	0.53
1:B:375:VAL:O	1:B:375:VAL:HG12	2.08	0.53
1:A:365:GLU:O	1:A:367:MET:N	2.42	0.53
1:A:218:ILE:HA	1:A:221:ASP:HB2	1.91	0.53
1:A:226:MET:CE	1:A:335:LEU:HD11	2.39	0.53
1:B:391:LYS:O	1:B:394:MET:HB2	2.09	0.52
1:A:208:ARG:CB	1:A:208:ARG:HH11	2.23	0.52
1:B:124:ASN:HD21	1:B:127:SER:CB	2.21	0.52
1:B:59:GLU:O	1:B:60:ALA:C	2.48	0.52
1:B:331:ALA:HB1	1:B:364:LEU:HD11	1.89	0.52
1:B:34:VAL:HG12	1:B:101:ILE:HD11	1.90	0.52
1:B:7:LEU:C	1:B:101:ILE:HG13	2.30	0.52
1:B:278:THR:HB	1:B:279:PRO:CD	2.39	0.52
1:A:64:LEU:O	1:A:68:MET:HG3	2.10	0.52
1:B:10:THR:HG22	1:B:41:ARG:HG2	1.91	0.52
1:B:64:LEU:O	1:B:68:MET:HG3	2.10	0.51
1:A:195:LEU:HD21	1:A:314:ARG:HB2	1.92	0.51
1:A:140:LYS:HE3	4:A:1061:HOH:O	2.10	0.51
1:B:226:MET:CE	1:B:230:LEU:HG	2.39	0.51
1:B:259:MET:HG2	1:B:269:ALA:CB	2.40	0.51
1:B:273:GLU:OE2	1:B:297:LEU:HD23	2.10	0.51
1:B:298:ASP:OD1	1:B:300:CYS:HB2	2.09	0.51
1:B:164:ILE:HG12	1:B:171:ALA:HB1	1.92	0.51
1:A:382:ASP:O	1:A:386:ARG:HG3	2.10	0.51
1:B:236:ARG:HH21	1:B:243:ALA:HB2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:TRP:HA	1:A:212:TRP:CE3	2.45	0.51
1:B:164:ILE:HA	1:B:171:ALA:HB1	1.92	0.51
1:A:372:PRO:HB3	1:A:377:ASP:HB3	1.92	0.51
1:B:2:LYS:HD2	1:B:96:GLN:NE2	2.26	0.51
1:A:33:LEU:HD12	1:A:51:PRO:HG3	1.92	0.51
1:A:9:SER:HB2	1:A:33:LEU:HD22	1.93	0.51
1:B:174:GLU:HG3	1:B:175:GLN:N	2.26	0.51
1:A:367:MET:O	1:A:369:MET:HE2	2.11	0.50
1:A:262:TYR:CE1	1:A:268:LEU:CD1	2.92	0.50
1:A:337:ALA:HB2	1:A:382:ASP:OD1	2.10	0.50
1:B:270:GLN:C	1:B:271:LEU:HD23	2.31	0.50
1:B:395:ARG:CZ	1:B:395:ARG:HB3	2.40	0.50
1:A:64:LEU:HD23	1:A:64:LEU:C	2.32	0.50
1:B:212:TRP:HE3	1:B:212:TRP:HA	1.75	0.50
1:B:278:THR:HG21	4:B:1031:HOH:O	2.11	0.50
1:A:160:LEU:HD23	1:A:260:VAL:HG11	1.94	0.50
1:B:56:MET:SD	1:B:65:LEU:HD22	2.52	0.50
1:A:236:ARG:HD3	1:A:241:ALA:O	2.11	0.50
1:B:391:LYS:HA	1:B:394:MET:HE3	1.93	0.50
1:A:305:LEU:HB2	1:B:305:LEU:HB2	1.93	0.50
1:B:9:SER:HB2	1:B:33:LEU:HD22	1.94	0.50
1:A:270:GLN:NE2	1:B:266:SER:OG	2.38	0.50
1:B:102:VAL:HG22	4:B:1055:HOH:O	2.11	0.49
1:B:367:MET:O	1:B:369:MET:HG3	2.11	0.49
1:A:329:GLN:HA	1:A:329:GLN:OE1	2.12	0.49
1:A:395:ARG:CZ	1:A:395:ARG:HB3	2.43	0.49
1:A:369:MET:HE3	1:A:369:MET:N	2.22	0.49
1:B:216:ARG:HH11	1:B:216:ARG:CB	2.26	0.49
1:B:208:ARG:NH1	1:B:208:ARG:HB3	2.28	0.49
1:A:17:THR:O	1:A:21:VAL:HG23	2.13	0.49
1:B:30:VAL:CG1	1:B:51:PRO:HB3	2.42	0.49
1:B:208:ARG:NH2	1:B:214:MET:CG	2.76	0.49
1:B:228:LYS:HE2	1:B:231:GLU:OE2	2.12	0.49
1:B:9:SER:CB	1:B:33:LEU:HD22	2.42	0.49
1:A:129:VAL:HG11	1:A:230:LEU:HD22	1.93	0.49
1:A:236:ARG:NH1	4:A:1064:HOH:O	2.45	0.49
1:B:41:ARG:HG3	1:B:41:ARG:O	2.12	0.49
1:B:216:ARG:NH1	1:B:216:ARG:CB	2.76	0.49
1:A:162:GLN:CG	1:B:162:GLN:HG3	2.34	0.49
1:A:329:GLN:HB2	1:A:371:GLU:OE2	2.13	0.49
1:A:34:VAL:HG12	1:A:101:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:PRO:HD2	4:A:1009:HOH:O	2.13	0.49
1:A:130:THR:HB	1:A:378:VAL:HG11	1.92	0.48
1:A:130:THR:HB	1:A:378:VAL:HG13	1.92	0.48
1:A:172:ASP:OD2	1:A:175:GLN:HB2	2.13	0.48
1:B:329:GLN:HA	1:B:329:GLN:OE1	2.12	0.48
1:B:329:GLN:HB2	1:B:371:GLU:OE2	2.13	0.48
1:B:295:LYS:NZ	1:B:298:ASP:HB2	2.29	0.48
1:A:131:CYS:HB3	1:A:135:PHE:CD1	2.48	0.48
1:A:318:LEU:O	1:A:322:MET:HG3	2.13	0.48
1:B:156:ILE:HD13	1:B:181:ILE:CG2	2.44	0.48
1:B:156:ILE:O	1:B:160:LEU:HG	2.14	0.48
1:B:342:THR:O	1:B:343:VAL:C	2.52	0.48
1:A:292:SER:OG	1:A:294:VAL:HG23	2.13	0.48
1:A:319:LYS:HD2	1:A:319:LYS:HA	1.64	0.48
1:A:146:LEU:O	1:A:147:LEU:HD23	2.12	0.48
1:B:89:ALA:HB1	1:B:113:ALA:HB2	1.96	0.48
1:B:382:ASP:O	1:B:386:ARG:HG3	2.14	0.47
1:B:202:THR:OG1	1:B:205:GLN:HG3	2.13	0.47
1:B:226:MET:HE1	1:B:321:ALA:HB2	1.96	0.47
1:A:135:PHE:O	1:A:139:VAL:HG23	2.14	0.47
1:B:17:THR:HG23	1:B:284:MET:SD	2.54	0.47
1:B:161:PRO:HD3	1:B:262:TYR:OH	2.15	0.47
1:B:206:ALA:HA	1:B:209:HIS:NE2	2.29	0.47
1:B:226:MET:HE1	1:B:335:LEU:HD11	1.95	0.47
1:B:300:CYS:O	1:B:302:LEU:N	2.48	0.47
1:A:64:LEU:HD21	1:A:68:MET:SD	2.55	0.47
1:A:208:ARG:NH1	1:A:208:ARG:HB2	2.23	0.47
1:A:208:ARG:CZ	1:A:214:MET:HG3	2.44	0.47
1:A:278:THR:HB	1:A:279:PRO:CD	2.45	0.47
1:A:207:CYS:H	1:A:209:HIS:CD2	2.33	0.47
1:A:63:LYS:HB3	1:A:63:LYS:HE2	1.68	0.47
1:B:341:ILE:O	1:B:344:ALA:HB3	2.15	0.47
1:B:255:VAL:HG21	1:B:305:LEU:HD21	1.95	0.47
1:A:208:ARG:NH2	1:A:214:MET:CG	2.78	0.47
1:B:348:ALA:O	1:B:349:GLN:HB2	2.15	0.46
1:B:2:LYS:HD2	1:B:96:GLN:HE21	1.79	0.46
1:A:125:LYS:NZ	1:A:125:LYS:HB3	2.30	0.46
1:B:335:LEU:HB2	1:B:364:LEU:HD21	1.97	0.46
1:B:297:LEU:HD22	1:B:302:LEU:HD11	1.98	0.46
1:A:166:HIS:HB3	4:A:1075:HOH:O	2.16	0.46
1:B:262:TYR:CZ	1:B:268:LEU:HD12	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:MET:HE2	1:B:230:LEU:CG	2.44	0.46
1:B:312:TYR:HD2	1:B:319:LYS:HB2	1.79	0.46
1:B:249:LEU:HD23	1:B:308:ALA:O	2.16	0.46
1:B:136:MET:CE	1:B:169:GLY:HA3	2.45	0.46
1:A:270:GLN:C	1:A:271:LEU:HD23	2.36	0.46
1:B:84:ALA:O	1:B:88:MET:HG2	2.16	0.46
1:B:260:VAL:HG12	1:B:262:TYR:CE1	2.50	0.46
1:B:111:LEU:HD23	1:B:375:VAL:HG21	1.97	0.46
1:A:38:ASN:HD21	1:A:41:ARG:HB3	1.79	0.46
1:A:55:VAL:HG22	1:A:79:LEU:HB2	1.98	0.46
1:B:318:LEU:O	1:B:322:MET:HG3	2.15	0.46
1:A:226:MET:CE	1:A:335:LEU:CD1	2.94	0.46
1:A:88:MET:HA	1:A:91:LEU:HD13	1.96	0.46
1:A:212:TRP:HE3	1:A:212:TRP:HA	1.80	0.46
1:B:130:THR:HB	1:B:378:VAL:HG13	1.92	0.46
1:A:372:PRO:HA	1:A:377:ASP:HB3	1.97	0.46
1:A:4:LEU:HD11	1:A:284:MET:CE	2.46	0.45
1:B:217:LYS:HZ3	1:B:217:LYS:HB3	1.79	0.45
1:A:236:ARG:NH2	1:A:243:ALA:HB2	2.30	0.45
1:B:143:LYS:HE3	1:B:170:TYR:HE1	1.82	0.45
1:A:212:TRP:CG	1:A:274:PRO:HB3	2.51	0.45
1:B:343:VAL:O	1:B:346:PHE:HB3	2.17	0.45
1:A:156:ILE:HD13	1:A:181:ILE:CG2	2.45	0.45
1:A:174:GLU:HB3	1:A:245:GLN:NE2	2.29	0.45
1:B:208:ARG:CZ	1:B:214:MET:HG3	2.46	0.45
1:A:217:LYS:HD2	1:A:343:VAL:CG1	2.46	0.45
1:B:119:THR:HA	1:B:145:GLN:HB3	1.98	0.45
1:A:37:LYS:O	1:A:39:VAL:N	2.49	0.45
1:B:8:GLY:N	1:B:101:ILE:HG13	2.32	0.45
1:A:216:ARG:CB	1:A:216:ARG:HH11	2.30	0.45
1:B:199:ALA:HA	1:B:354:THR:HG22	1.99	0.45
1:A:41:ARG:O	1:A:45:GLN:HG3	2.17	0.45
1:B:39:VAL:O	1:B:43:VAL:HG23	2.17	0.45
1:A:299:PHE:O	1:B:307:PHE:HB2	2.17	0.45
1:A:98:MET:HE1	1:A:121:LEU:HB3	1.98	0.45
1:A:220:VAL:CG2	1:A:347:LEU:HD21	2.40	0.44
1:A:156:ILE:HG13	1:A:258:SER:HB3	1.99	0.44
1:B:185:GLY:HA3	1:B:228:LYS:HD2	1.99	0.44
1:B:38:ASN:HD21	1:B:41:ARG:HB3	1.79	0.44
1:B:35:ALA:HB3	1:B:42:MET:HE2	1.99	0.44
1:A:59:GLU:O	1:A:60:ALA:C	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:MET:SD	1:A:65:LEU:HD22	2.58	0.44
1:B:46:CYS:SG	1:B:54:ALA:HB2	2.57	0.44
1:A:36:GLY:HA2	1:A:57:ASP:OD2	2.17	0.44
1:A:161:PRO:CG	1:A:164:ILE:HD12	2.47	0.44
1:B:285:ALA:HB2	1:B:290:VAL:HG13	2.00	0.44
1:B:292:SER:OG	1:B:294:VAL:HG23	2.17	0.44
1:B:208:ARG:NH2	1:B:214:MET:SD	2.91	0.44
1:B:27:HIS:HB3	4:B:1043:HOH:O	2.18	0.44
1:A:158:GLN:HG2	1:A:282:HIS:NE2	2.33	0.44
1:B:7:LEU:O	1:B:101:ILE:N	2.51	0.44
1:B:164:ILE:O	1:B:164:ILE:HG22	2.17	0.44
1:A:299:PHE:HA	1:A:302:LEU:HD22	2.00	0.44
1:A:64:LEU:CD2	1:A:68:MET:SD	3.06	0.43
1:A:295:LYS:HZ1	1:A:298:ASP:HB2	1.81	0.43
1:A:111:LEU:HD12	1:A:111:LEU:O	2.17	0.43
1:B:7:LEU:HD13	1:B:109:PRO:HB2	2.00	0.43
1:B:276:MET:HB2	4:B:1051:HOH:O	2.18	0.43
1:A:160:LEU:HB3	1:A:161:PRO:HD2	1.99	0.43
1:A:369:MET:HE1	4:A:1084:HOH:O	2.18	0.43
1:A:37:LYS:O	1:A:39:VAL:HG23	2.18	0.43
1:B:9:SER:O	1:B:45:GLN:NE2	2.50	0.43
1:A:236:ARG:NH2	1:A:326:GLU:OE2	2.51	0.43
1:A:209:HIS:O	1:A:213:SER:HB3	2.18	0.43
1:A:140:LYS:NZ	4:A:1061:HOH:O	2.51	0.43
1:A:33:LEU:HD23	1:A:33:LEU:HA	1.91	0.43
1:A:30:VAL:CG1	1:A:51:PRO:HB3	2.49	0.43
1:A:209:HIS:HA	1:A:210:PRO:HD2	1.66	0.43
1:B:217:LYS:HZ2	1:B:217:LYS:HB3	1.82	0.43
1:A:216:ARG:CB	1:A:216:ARG:NH1	2.81	0.43
1:B:242:SER:O	1:B:245:GLN:N	2.50	0.43
1:B:319:LYS:HA	1:B:319:LYS:HD2	1.78	0.43
1:A:111:LEU:O	1:A:115:ARG:HG2	2.19	0.43
1:B:195:LEU:HA	1:B:195:LEU:HD23	1.81	0.43
1:B:156:ILE:HG13	1:B:258:SER:HB3	2.01	0.42
1:B:331:ALA:O	1:B:335:LEU:HB2	2.19	0.42
1:B:31:VAL:CG1	1:B:91:LEU:HD23	2.49	0.42
1:A:276:MET:HB2	4:A:1033:HOH:O	2.18	0.42
1:B:174:GLU:HB3	1:B:245:GLN:HE22	1.83	0.42
1:B:314:ARG:O	1:B:316:PRO:HD3	2.19	0.42
1:A:124:ASN:ND2	1:A:127:SER:H	2.17	0.42
1:A:286:TRP:CG	1:A:287:PRO:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:MET:HG2	1:A:269:ALA:CB	2.48	0.42
1:A:358:ALA:O	1:A:361:LEU:HB3	2.19	0.42
1:A:190:PHE:CD2	1:A:201:MET:HE3	2.55	0.42
1:A:392:GLU:HA	1:A:392:GLU:OE1	2.19	0.42
1:B:17:THR:O	1:B:21:VAL:HG23	2.19	0.42
1:B:80:SER:O	1:B:84:ALA:HB2	2.20	0.42
1:B:372:PRO:HA	1:B:377:ASP:HB3	2.00	0.42
1:A:31:VAL:CG1	1:A:91:LEU:HD23	2.50	0.42
1:A:212:TRP:CA	1:A:212:TRP:CE3	3.02	0.42
1:B:160:LEU:HD23	1:B:260:VAL:HG11	2.01	0.42
1:A:375:VAL:CG1	1:A:375:VAL:O	2.66	0.42
1:A:198:LEU:HA	1:A:201:MET:HG2	2.01	0.42
1:A:312:TYR:HD2	1:A:319:LYS:HB2	1.84	0.42
1:B:4:LEU:N	1:B:4:LEU:HD23	2.35	0.42
1:B:162:GLN:HE21	1:B:162:GLN:HB3	1.61	0.42
1:B:236:ARG:NH2	1:B:243:ALA:HB2	2.34	0.42
1:B:177:GLY:HA2	1:B:263:GLN:NE2	2.35	0.42
1:A:331:ALA:HB1	1:A:364:LEU:HD11	2.01	0.42
1:B:207:CYS:H	1:B:209:HIS:CD2	2.37	0.42
1:B:278:THR:HB	1:B:279:PRO:HD3	2.02	0.42
1:B:198:LEU:HA	1:B:201:MET:HG2	2.01	0.42
1:A:183:LEU:O	1:A:248:VAL:HA	2.19	0.42
1:A:182:LEU:HD12	1:A:247:GLU:HB2	2.01	0.41
1:B:255:VAL:HG21	1:B:305:LEU:CD2	2.50	0.41
1:B:196:ARG:HG3	1:B:196:ARG:HH11	1.84	0.41
1:B:212:TRP:CE3	1:B:212:TRP:CA	3.03	0.41
1:A:207:CYS:N	1:A:209:HIS:NE2	2.59	0.41
1:B:36:GLY:HA2	1:B:57:ASP:CG	2.40	0.41
1:B:375:VAL:O	1:B:375:VAL:CG1	2.69	0.41
1:A:386:ARG:HG2	1:A:386:ARG:NH1	2.33	0.41
1:A:145:GLN:HE22	1:A:166:HIS:HA	1.85	0.41
1:B:130:THR:HG22	1:B:333:THR:HG23	2.01	0.41
1:A:228:LYS:HD3	1:A:228:LYS:HA	1.92	0.41
1:B:209:HIS:HA	1:B:210:PRO:HD2	1.61	0.41
1:B:37:LYS:O	1:B:39:VAL:N	2.53	0.41
1:B:341:ILE:HD12	1:B:390:ARG:HG3	2.01	0.41
1:A:43:VAL:HG12	1:A:47:LEU:CD1	2.50	0.41
1:A:70:GLN:NE2	1:A:70:GLN:HA	2.34	0.41
1:A:7:LEU:HD13	1:A:109:PRO:HB2	2.03	0.41
1:A:298:ASP:OD1	1:A:300:CYS:HB2	2.20	0.41
1:A:210:PRO:O	1:A:211:ASN:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:ARG:O	1:B:355:ASP:HB2	2.20	0.41
1:B:130:THR:CB	1:B:378:VAL:HG11	2.51	0.41
1:B:276:MET:HE3	4:B:1010:HOH:O	2.21	0.41
1:B:149:VAL:HG12	1:B:149:VAL:O	2.21	0.41
1:B:173:LEU:HD11	1:B:241:ALA:HB2	2.03	0.41
1:B:125:LYS:NZ	1:B:125:LYS:HB3	2.36	0.41
1:B:337:ALA:HB2	1:B:382:ASP:OD1	2.21	0.41
1:B:348:ALA:O	1:B:349:GLN:CB	2.69	0.41
1:A:233:ILE:HD13	1:A:332:THR:HB	2.02	0.41
1:B:229:GLY:O	1:B:232:TYR:HB3	2.20	0.41
1:B:226:MET:HE1	1:B:335:LEU:CD1	2.51	0.41
1:A:331:ALA:O	1:A:335:LEU:HB2	2.21	0.41
1:A:208:ARG:HB3	1:A:208:ARG:NH1	2.36	0.41
1:B:63:LYS:HB3	1:B:63:LYS:HE2	1.66	0.40
1:B:161:PRO:CG	1:B:164:ILE:HD12	2.51	0.40
1:A:164:ILE:CG2	1:A:164:ILE:O	2.70	0.40
1:A:363:VAL:HG13	1:A:388:VAL:CB	2.46	0.40
1:B:33:LEU:CD1	1:B:51:PRO:HG3	2.49	0.40
1:A:236:ARG:NH1	1:A:242:SER:HA	2.37	0.40
1:A:372:PRO:HB3	1:A:377:ASP:CB	2.51	0.40
1:A:251:HIS:CE1	1:A:256:ILE:H	2.39	0.40
1:B:156:ILE:HD13	1:B:181:ILE:HG21	2.04	0.40
1:B:262:TYR:HE1	1:B:268:LEU:HD12	1.75	0.40
1:A:255:VAL:HG21	1:A:305:LEU:CD2	2.49	0.40
1:A:211:ASN:O	1:A:212:TRP:CB	2.70	0.40
1:A:139:VAL:O	1:A:143:LYS:N	2.54	0.40
1:B:173:LEU:HA	1:B:173:LEU:HD23	1.82	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:ARG:NH2	4:B:1045:HOH:O[1_565]	2.14	0.06

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	395/398 (99%)	344 (87%)	42 (11%)	9 (2%)	8 12
1	B	395/398 (99%)	340 (86%)	46 (12%)	9 (2%)	8 12
All	All	790/796 (99%)	684 (87%)	88 (11%)	18 (2%)	8 12

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	PRO
1	A	367	MET
1	B	210	PRO
1	B	367	MET
1	A	197	ASP
1	A	212	TRP
1	A	258	SER
1	A	366	LYS
1	B	38	ASN
1	B	197	ASP
1	B	258	SER
1	A	38	ASN
1	B	212	TRP
1	A	373	GLN
1	B	301	LYS
1	B	349	GLN
1	B	243	ALA
1	A	372	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	327/328 (100%)	298 (91%)	29 (9%)	12 23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	327/328 (100%)	292 (89%)	35 (11%)	8 15
All	All	654/656 (100%)	590 (90%)	64 (10%)	10 19

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	40	THR
1	A	70	GLN
1	A	87	ASP
1	A	111	LEU
1	A	162	GLN
1	A	168	LEU
1	A	170	TYR
1	A	174	GLU
1	A	176	ASN
1	A	196	ARG
1	A	207	CYS
1	A	212	TRP
1	A	217	LYS
1	A	249	LEU
1	A	258	SER
1	A	271	LEU
1	A	288	ASN
1	A	297	LEU
1	A	302	LEU
1	A	318	LEU
1	A	320	LEU
1	A	361	LEU
1	A	364	LEU
1	A	369	MET
1	A	370	ARG
1	A	377	ASP
1	A	382	ASP
1	A	395	ARG
1	B	4	LEU
1	B	5	THR
1	B	40	THR
1	B	70	GLN
1	B	72	GLN
1	B	87	ASP
1	B	111	LEU

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Mol	Chain	Res	Type
1	B	122	LEU
1	B	125	LYS
1	B	162	GLN
1	B	168	LEU
1	B	170	TYR
1	B	174	GLU
1	B	176	ASN
1	B	196	ARG
1	B	197	ASP
1	B	207	CYS
1	B	212	TRP
1	B	217	LYS
1	B	219	SER
1	B	228	LYS
1	B	249	LEU
1	B	258	SER
1	B	271	LEU
1	B	288	ASN
1	B	297	LEU
1	B	302	LEU
1	B	318	LEU
1	B	320	LEU
1	B	361	LEU
1	B	364	LEU
1	B	369	MET
1	B	370	ARG
1	B	373	GLN
1	B	395	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	45	GLN
1	A	70	GLN
1	A	71	GLN
1	A	72	GLN
1	A	96	GLN
1	A	124	ASN
1	A	145	GLN
1	A	162	GLN
1	A	165	GLN

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Mol	Chain	Res	Type
1	A	175	GLN
1	A	176	ASN
1	A	240	ASN
1	A	245	GLN
1	A	251	HIS
1	A	257	HIS
1	A	263	GLN
1	A	270	GLN
1	A	329	GLN
1	B	3	GLN
1	B	70	GLN
1	B	71	GLN
1	B	72	GLN
1	B	124	ASN
1	B	145	GLN
1	B	162	GLN
1	B	165	GLN
1	B	175	GLN
1	B	240	ASN
1	B	251	HIS
1	B	257	HIS
1	B	263	GLN
1	B	270	GLN
1	B	329	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FOM	A	1001	2	8,10,10	1.92	1 (12%)	8,13,13	2.21	2 (25%)
3	FOM	B	1001	2	8,10,10	1.79	2 (25%)	8,13,13	2.20	2 (25%)

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	FOM	A	1001	2	-	0/6/9/9	0/0/0/0
3	FOM	B	1001	2	-	0/6/9/9	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1001	FOM	PA1-OP2	2.06	1.59	1.54
3	B	1001	FOM	PA1-OP1	4.11	1.59	1.50
3	A	1001	FOM	PA1-OP1	4.49	1.60	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1001	FOM	OP2-PA1-OP1	-3.82	102.64	112.40
3	A	1001	FOM	OP2-PA1-OP1	-3.60	103.19	112.40
3	B	1001	FOM	OP3-PA1-C4	4.49	118.02	106.89
3	A	1001	FOM	OP3-PA1-C4	4.55	118.19	106.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.