Full wwPDB X-ray Structure Validation Report ⓘ

Dec 2, 2023 – 09:29 pm GMT

PDB ID	:	2VM8
Title	:	Human CRMP-2 crystallised in the presence of Mg
Authors	:	Kursula, P.
Deposited on	:	2008-01-24
Resolution	:	1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

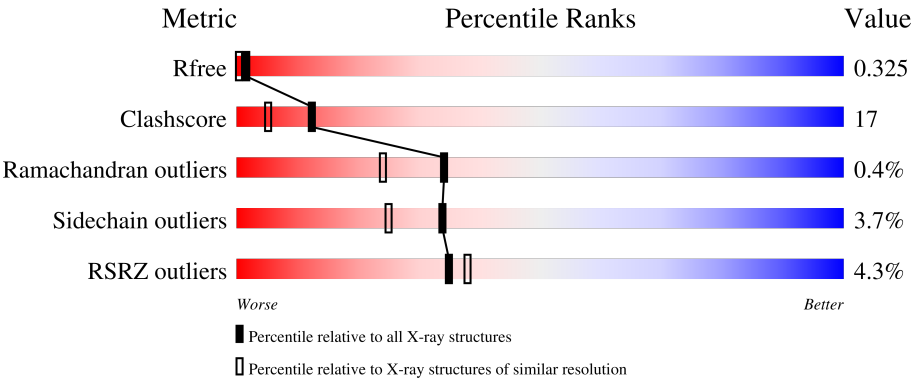
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	501	4% 68% 26% • 5%
1	B	501	4% 64% 29% • 5%
1	C	501	3% 65% 28% • 5%
1	D	501	5% 67% 26% • 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 16539 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 DIHYDROPYRIMIDINASE-RELATED PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	S	0	6	0
			3701	2332	627	723	19			
1	B	476	Total	C	N	O	S	0	2	0
			3680	2318	629	714	19			
1	C	476	Total	C	N	O	S	0	3	0
			3682	2321	627	716	18			
1	D	476	Total	C	N	O	S	0	3	0
			3680	2320	626	714	20			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is water.

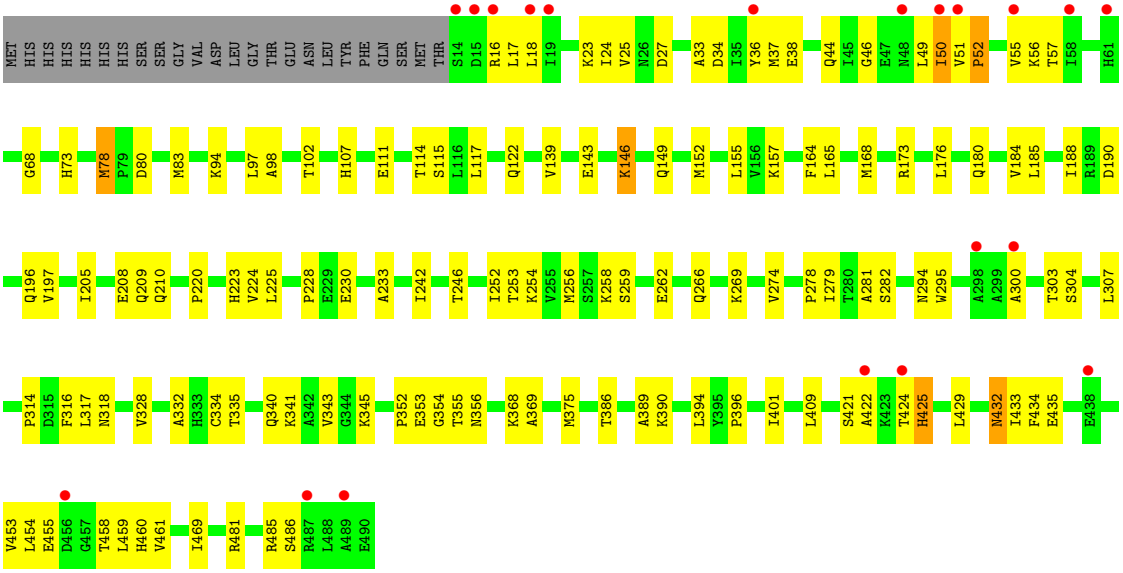
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	426	Total	O	0	0
			426	426		
3	B	398	Total	O	0	1
			398	398		
3	C	485	Total	O	0	0
			485	485		
3	D	484	Total	O	0	0
			484	484		

3 Residue-property plots (i)

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

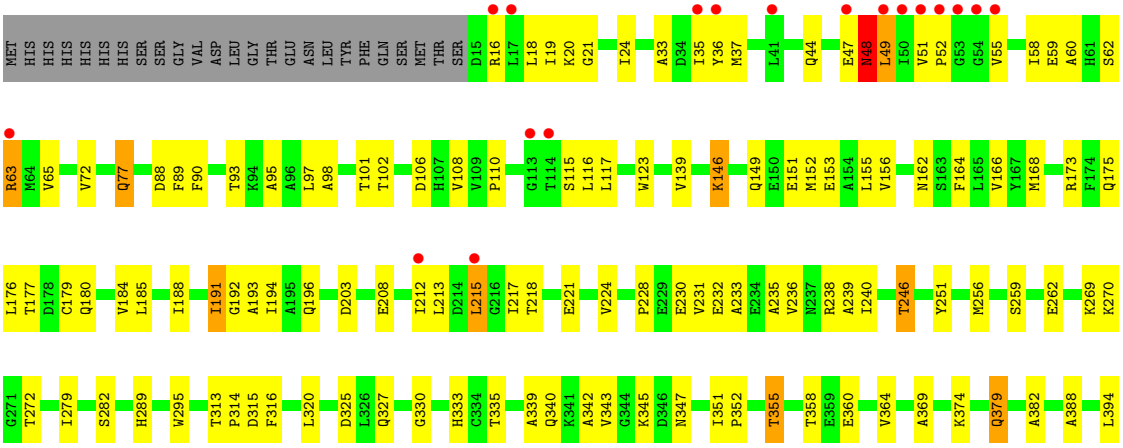
• Molecule 1: DIHYDROPYRIMIDINASE-RELATED PROTEIN 2

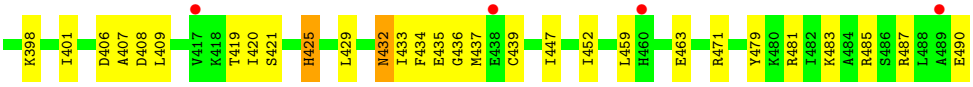
Chain A:



• Molecule 1: DIHYDROPYRIMIDINASE-RELATED PROTEIN 2

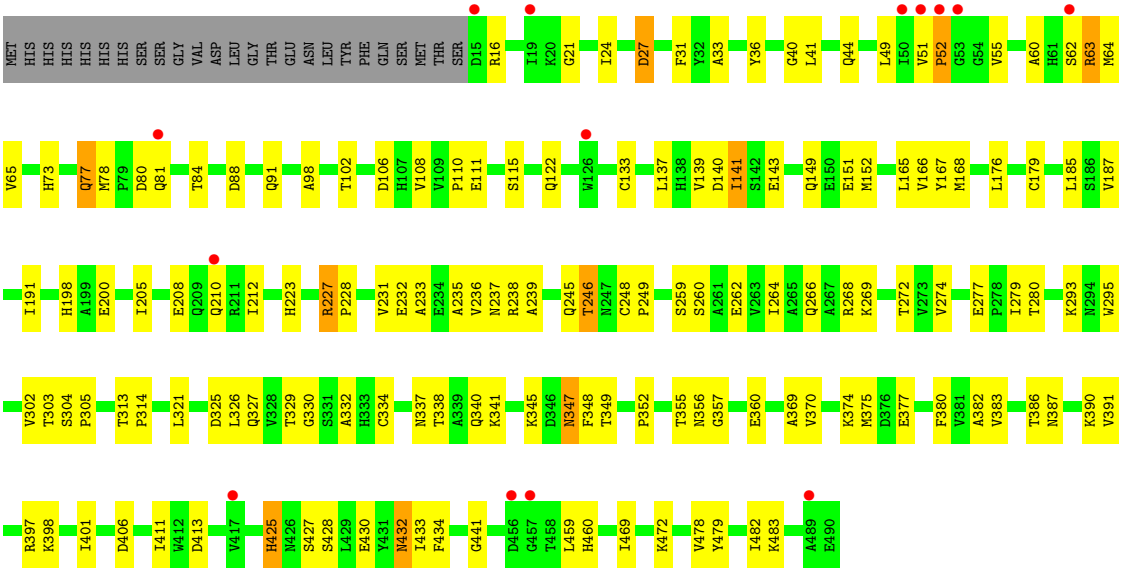
Chain B:





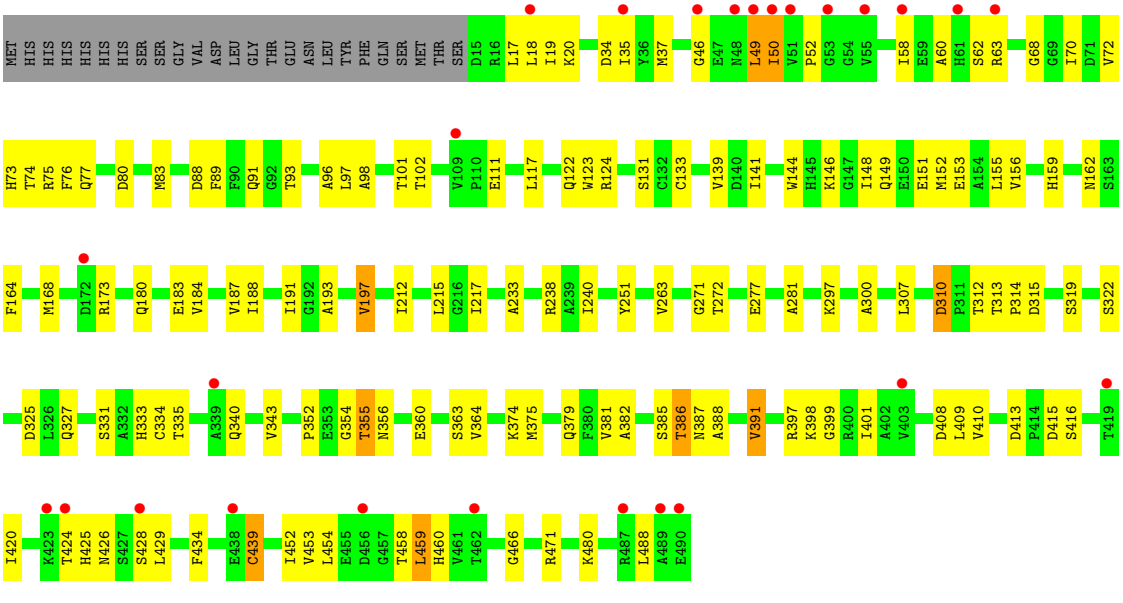
• Molecule 1: DIHYDROPYRIMIDINASE-RELATED PROTEIN 2

Chain C:



• Molecule 1: DIHYDROPYRIMIDINASE-RELATED PROTEIN 2

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	86.51Å 126.24Å 209.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 19.90 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.5 (20.00-1.90) 94.5 (19.90-1.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.22 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.3.0028	Depositor
R, R_{free}	0.256 , 0.325 0.258 , 0.325	Depositor DCC
R_{free} test set	8532 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	14.9	Xtriage
Anisotropy	0.731	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 100.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	16539	wwPDB-VP
Average B, all atoms (Å^2)	22.0	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 30.71 % 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 1.2500e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.68	0/3794	0.76	0/5146
1	B	0.73	0/3761	0.78	0/5100
1	C	0.78	1/3766 (0.0%)	0.82	1/5109 (0.0%)
1	D	0.70	1/3764 (0.0%)	0.77	1/5105 (0.0%)
All	All	0.72	2/15085 (0.0%)	0.78	2/20460 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	334	CYS	CB-SG	-6.09	1.71	1.82
1	D	263	VAL	CB-CG2	5.66	1.64	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	326	LEU	CB-CG-CD1	-5.52	101.61	111.00
1	D	310	ASP	CB-CG-OD1	5.19	122.97	118.30

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	3701	0	3652	120	0
1	B	3680	0	3632	129	0
1	C	3682	0	3636	130	0
1	D	3680	0	3635	119	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	426	0	0	15	0
3	B	398	0	0	9	0
3	C	485	0	0	23	0
3	D	484	0	0	19	0
All	All	16539	0	14555	494	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 17.

All (494) 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:37:MET:HE3	1:B:407:ALA:HB1	1.21	1.16
1:A:242:ILE:O	1:A:246:THR:HG22	1.45	1.13
1:D:401:ILE:HD12	1:D:409:LEU:HD23	1.18	1.08
1:A:168[B]:MET:CE	1:A:197[B]:VAL:CG2	2.33	1.06
1:A:168[B]:MET:CE	1:A:197[B]:VAL:HG21	1.86	1.05
1:D:168[B]:MET:HE2	1:D:197:VAL:HG11	1.42	1.01
1:D:401:ILE:HD12	1:D:409:LEU:CD2	1.91	1.00
1:D:168[B]:MET:CE	1:D:197:VAL:HG11	1.92	1.00
1:D:333:HIS:CG	3:D:2356:HOH:O	2.16	0.98
1:A:168[B]:MET:HE2	1:A:197[B]:VAL:HG21	1.42	0.98
1:A:281:ALA:HB1	1:A:307:LEU:HD11	1.42	0.98
1:A:149:GLN:HA	1:A:152:MET:HE2	1.52	0.92
1:C:51:VAL:HG13	1:C:55:VAL:HG21	1.51	0.92
1:C:77:GLN:HG2	1:C:88:ASP:HA	1.54	0.89
1:A:168[B]:MET:HE2	1:A:197[B]:VAL:CG2	2.00	0.89
1:D:401:ILE:CD1	1:D:409:LEU:HD23	2.04	0.87
1:D:168[B]:MET:HE2	1:D:197:VAL:CG1	2.05	0.86
1:C:223:HIS:O	1:C:227:ARG:HG3	1.76	0.84
1:D:168[B]:MET:CE	1:D:197:VAL:CG1	2.54	0.84
1:D:18:LEU:HD12	1:D:35:ILE:O	1.78	0.84
1:B:432:ASN:ND2	1:B:434:PHE:H	1.74	0.83
1:D:356:ASN:HA	3:D:2356:HOH:O	1.79	0.83
1:D:144:TRP:HZ3	1:D:152:MET:HE3	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:GLN:HG2	3:C:2142:HOH:O	1.78	0.82
1:C:432:ASN:ND2	1:C:434:PHE:H	1.76	0.82
1:B:37:MET:HE1	1:B:447:ILE:HG21	1.63	0.81
1:D:148:ILE:HG22	1:D:152:MET:HE3	1.63	0.80
1:A:432:ASN:HD22	1:A:434:PHE:H	1.28	0.79
1:D:281:ALA:HB1	1:D:307:LEU:HD11	1.63	0.79
1:B:432:ASN:HD22	1:B:434:PHE:H	1.28	0.78
1:C:432:ASN:C	1:C:432:ASN:HD22	1.85	0.78
1:D:148:ILE:CG2	1:D:152:MET:HE3	2.13	0.78
1:C:149:GLN:HA	1:C:152:MET:CE	2.13	0.77
1:B:355:THR:CG2	1:B:433:ILE:HD13	2.15	0.77
1:A:168[A]:MET:SD	1:A:197[A]:VAL:HG11	2.25	0.77
1:C:44[B]:GLN:HG2	1:C:49:LEU:HD22	1.67	0.77
1:B:355:THR:HG23	1:B:433:ILE:HD13	1.67	0.76
1:B:437:MET:SD	3:B:2305:HOH:O	2.43	0.76
1:D:156:VAL:HG21	1:D:191:ILE:HD12	1.68	0.74
1:D:240:ILE:HG23	1:D:272:THR:HG21	1.68	0.74
1:A:295:TRP:CZ2	1:A:345:LYS:HA	2.22	0.74
1:C:432:ASN:HD22	1:C:434:PHE:H	1.35	0.74
1:D:46:GLY:CA	1:D:49:LEU:HD11	2.18	0.73
1:D:141:ILE:HD13	1:D:152:MET:HE1	1.70	0.73
1:B:168[A]:MET:HE3	1:B:238:ARG:NH1	2.04	0.72
1:B:401:ILE:HD12	1:B:409:LEU:HD23	1.70	0.72
1:D:387:ASN:O	1:D:391:VAL:HG13	1.89	0.72
1:D:458:THR:HG22	1:D:460:HIS:CE1	2.24	0.72
1:D:80:ASP:HA	3:D:2083:HOH:O	1.89	0.72
1:B:24:ILE:HD12	1:B:33:ALA:HB3	1.72	0.72
1:D:168[A]:MET:HE2	1:D:238:ARG:NH2	2.05	0.72
1:D:271:GLY:HA2	3:D:2299:HOH:O	1.89	0.71
1:B:153:GLU:HA	1:B:191:ILE:HD11	1.72	0.71
1:A:168[B]:MET:CE	1:A:197[B]:VAL:HG22	2.19	0.71
1:B:168[B]:MET:HE2	1:B:239:ALA:HB2	1.73	0.71
1:A:341:LYS:HA	1:A:352:PRO:HD2	1.72	0.70
1:A:386:THR:HG22	1:A:390:LYS:HE3	1.73	0.70
1:B:37:MET:CE	1:B:447:ILE:HG21	2.21	0.70
1:B:180:GLN:O	1:B:184:VAL:HG23	1.91	0.70
1:B:95:ALA:O	1:B:98:ALA:HB3	1.93	0.69
1:C:143:GLU:OE1	3:C:2157:HOH:O	2.10	0.69
1:D:50:ILE:HD13	1:D:50:ILE:O	1.92	0.69
1:A:164:PHE:HB2	1:A:188:ILE:HD11	1.75	0.68
1:C:149:GLN:HA	1:C:152:MET:HE3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:GLU:O	1:C:236:VAL:HG23	1.93	0.68
1:B:432:ASN:HD22	1:B:433:ILE:N	1.93	0.67
1:B:175:GLN:NE2	1:B:203:ASP:OD1	2.27	0.67
1:A:269:LYS:NZ	1:B:262:GLU:OE1	2.28	0.67
1:D:148:ILE:HG22	1:D:152:MET:CE	2.24	0.67
1:B:394:LEU:HD21	1:B:471:ARG:HG2	1.77	0.67
1:C:249:PRO:HG3	1:C:482:ILE:HD13	1.77	0.67
1:C:329:THR:HG23	1:C:383:VAL:O	1.95	0.67
1:A:454:LEU:HD13	1:A:459:LEU:HD13	1.76	0.66
1:A:168[B]:MET:HE3	1:A:197[B]:VAL:CG2	2.23	0.66
1:A:168[B]:MET:HE3	1:A:197[B]:VAL:HG22	1.77	0.66
1:A:266:GLN:NE2	3:A:2258:HOH:O	2.28	0.66
1:C:51:VAL:CG1	1:C:55:VAL:HG21	2.25	0.66
1:C:185:LEU:HB3	1:C:246:THR:HG21	1.77	0.66
1:C:280:THR:HG22	1:C:434:PHE:CZ	2.30	0.66
1:D:413:ASP:OD2	1:D:416:SER:OG	2.13	0.66
1:C:149:GLN:HA	1:C:152:MET:HE2	1.76	0.66
1:A:51:VAL:HG13	1:A:52:PRO:HD2	1.78	0.65
1:C:21:GLY:O	1:C:62:SER:HA	1.96	0.65
1:D:144:TRP:CZ3	1:D:152:MET:HE3	2.31	0.65
1:A:432:ASN:ND2	1:A:434:PHE:H	1.95	0.65
1:A:168[A]:MET:SD	1:A:197[A]:VAL:CG1	2.85	0.65
1:D:399:GLY:O	3:D:2390:HOH:O	2.14	0.64
1:C:81:GLN:O	3:C:2078:HOH:O	2.15	0.64
1:C:355[A]:THR:HG23	1:C:356:ASN:O	1.98	0.64
1:C:432:ASN:HD22	1:C:433:ILE:N	1.95	0.64
1:D:413:ASP:CG	1:D:416:SER:OG	2.36	0.64
1:A:180:GLN:O	1:A:184:VAL:HG23	1.97	0.64
1:D:168[A]:MET:CE	1:D:238:ARG:CZ	2.76	0.63
1:A:149:GLN:HA	1:A:152:MET:CE	2.25	0.62
1:C:27:ASP:HB2	1:C:382:ALA:HB2	1.80	0.62
1:C:168:MET:HE3	1:C:238:ARG:NH1	2.14	0.62
1:C:341:LYS:HA	1:C:352:PRO:HD2	1.80	0.62
1:D:315:ASP:OD2	1:D:374:LYS:NZ	2.30	0.62
1:C:386:THR:HG22	1:C:390:LYS:HE3	1.82	0.62
1:D:333:HIS:HA	3:D:2356:HOH:O	2.00	0.62
1:C:249:PRO:HB3	1:C:478:VAL:CG1	2.29	0.62
1:C:77:GLN:HG2	1:C:88:ASP:CA	2.27	0.61
1:B:117:LEU:HD13	1:B:151:GLU:OE1	2.01	0.61
1:A:281:ALA:CB	1:A:307:LEU:HD11	2.26	0.61
1:A:355:THR:OG1	1:A:433:ILE:HG21	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:454:LEU:HD13	1:D:459:LEU:CD1	2.30	0.61
1:D:319:SER:OG	1:D:374:LYS:HE2	2.01	0.60
1:D:34:ASP:HB2	1:D:49:LEU:HD22	1.84	0.60
1:D:141:ILE:HD13	1:D:152:MET:CE	2.30	0.60
1:D:188:ILE:HG23	1:D:193:ALA:HB3	1.83	0.60
1:B:490:GLU:OE2	3:B:2395:HOH:O	2.16	0.60
1:B:179:CYS:SG	3:B:2167:HOH:O	2.42	0.60
1:B:360:GLU:O	1:B:364:VAL:HG23	2.01	0.60
1:C:227:ARG:HH12	1:C:304:SER:HB3	1.67	0.60
1:A:111:GLU:HB3	1:A:114:THR:HG21	1.83	0.59
1:A:262:GLU:OE2	1:B:269:LYS:NZ	2.35	0.59
1:B:188:ILE:HG23	1:B:193:ALA:HB3	1.83	0.59
1:C:369:ALA:O	1:C:374:LYS:HB2	2.02	0.59
1:D:117:LEU:HD12	1:D:151:GLU:OE1	2.01	0.59
1:B:168[B]:MET:HE1	1:B:235:ALA:O	2.02	0.59
1:A:355:THR:HG23	1:A:356:ASN:O	2.03	0.59
1:C:80:ASP:OD2	3:C:2075:HOH:O	2.16	0.59
1:A:107:HIS:HE1	1:A:196:GLN:HE22	1.51	0.59
1:D:360:GLU:O	1:D:364:VAL:HG23	2.02	0.59
1:B:432:ASN:HD22	1:B:432:ASN:C	2.06	0.59
1:D:168[B]:MET:HE1	1:D:197:VAL:HG11	1.82	0.59
1:D:335:THR:HB	1:D:429:LEU:HD11	1.85	0.59
1:D:355:THR:O	3:D:2356:HOH:O	2.17	0.59
1:A:168[B]:MET:HE1	1:A:197[B]:VAL:HG21	1.81	0.59
1:C:355[A]:THR:HG21	1:C:433:ILE:HD13	1.84	0.59
1:D:98:ALA:HB2	1:D:459:LEU:HD11	1.84	0.58
1:D:180:GLN:O	1:D:184:VAL:HG23	2.03	0.58
1:A:111:GLU:HG2	3:A:2027:HOH:O	2.03	0.58
1:A:314:PRO:O	1:A:318:ASN:ND2	2.26	0.58
1:C:237:ASN:ND2	3:C:2281:HOH:O	2.36	0.58
1:A:37:MET:SD	1:A:409:LEU:CD1	2.92	0.58
1:A:17:LEU:HD12	1:A:56:LYS:O	2.03	0.58
1:A:224:VAL:O	3:A:2224:HOH:O	2.17	0.58
1:B:401:ILE:HD12	1:B:409:LEU:CD2	2.34	0.58
1:D:325:ASP:C	1:D:327:GLN:NE2	2.57	0.58
1:B:19:ILE:N	1:B:19:ILE:HD12	2.19	0.57
1:A:44:GLN:HB3	1:A:49:LEU:HD22	1.86	0.57
1:A:278:PRO:HD2	1:A:328:VAL:O	2.04	0.57
1:C:295:TRP:CZ2	1:C:345:LYS:HA	2.40	0.57
1:A:18:LEU:HD23	1:A:57:THR:HG23	1.87	0.57
1:B:360:GLU:HG2	1:B:420:ILE:HD13	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:ILE:HG23	1:D:217:ILE:HD12	1.87	0.57
1:B:208:GLU:O	1:B:212:ILE:HG12	2.05	0.57
1:A:458:THR:HG22	1:A:460:HIS:CE1	2.40	0.57
1:D:74:THR:HG21	1:D:76:PHE:CZ	2.40	0.57
1:D:148:ILE:CG2	1:D:152:MET:CE	2.82	0.57
1:B:236:VAL:O	1:B:240:ILE:HG13	2.05	0.57
1:C:233:ALA:HB2	1:C:259:SER:HB3	1.86	0.57
1:A:256:MET:SD	1:A:279:ILE:HD11	2.45	0.56
1:C:110:PRO:HG2	3:C:2153:HOH:O	2.05	0.56
1:A:386:THR:O	1:A:389:ALA:HB3	2.04	0.56
1:A:220:PRO:O	1:A:223:HIS:N	2.37	0.56
1:D:333:HIS:ND1	3:D:2356:HOH:O	2.31	0.56
1:D:97:LEU:HD22	1:D:453:VAL:HG21	1.87	0.56
1:B:168[A]:MET:HE3	1:B:238:ARG:CZ	2.36	0.56
1:A:369:ALA:HB1	1:A:375:MET:HE3	1.86	0.56
1:B:48:ASN:O	1:B:49:LEU:C	2.43	0.56
1:C:347:ASN:ND2	1:C:349:THR:OG1	2.39	0.56
1:C:387:ASN:O	1:C:391:VAL:HG23	2.05	0.56
1:C:73:HIS:CD2	1:C:332:ALA:HA	2.41	0.55
1:B:21:GLY:O	1:B:62:SER:HA	2.07	0.55
1:D:19:ILE:HG13	1:D:37:MET:HE1	1.89	0.55
1:D:168[A]:MET:CE	1:D:238:ARG:NH2	2.69	0.55
1:A:16:ARG:HG2	1:A:36:TYR:OH	2.07	0.55
1:C:198:HIS:NE2	1:C:200:GLU:OE1	2.38	0.55
1:A:269:LYS:HE3	1:B:320:LEU:HD11	1.88	0.55
1:A:205:ILE:O	1:A:209:GLN:HG3	2.07	0.55
1:C:340:GLN:NE2	3:C:2362:HOH:O	2.40	0.55
1:B:232:GLU:O	1:B:236:VAL:HG23	2.07	0.54
1:C:249:PRO:HB3	1:C:478:VAL:HG13	1.88	0.54
1:D:155:LEU:HD23	1:D:159:HIS:CD2	2.42	0.54
1:C:21:GLY:O	1:C:62:SER:N	2.39	0.54
1:B:279:ILE:HA	1:B:330:GLY:O	2.07	0.54
1:B:168[B]:MET:CE	1:B:239:ALA:HB2	2.36	0.54
1:B:36:TYR:CD1	1:B:51:VAL:HG11	2.42	0.54
1:B:58:ILE:HD11	1:B:452:ILE:HD11	1.89	0.54
1:C:348:PHE:HD1	3:C:2269:HOH:O	1.90	0.54
1:A:269:LYS:HD2	3:B:2272:HOH:O	2.07	0.54
1:B:20:LYS:NZ	1:B:59:GLU:OE2	2.40	0.54
1:B:325:ASP:O	1:B:327:GLN:NE2	2.40	0.54
1:A:146:LYS:NZ	3:A:2139:HOH:O	2.35	0.54
1:A:228:PRO:HG3	3:A:2225:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:MET:HE1	1:B:409:LEU:CD1	2.38	0.54
1:D:46:GLY:N	1:D:49:LEU:HD11	2.23	0.53
1:B:419:THR:HG23	1:B:436:GLY:HA2	1.90	0.53
1:D:58:ILE:HD11	1:D:452:ILE:HD11	1.89	0.53
1:C:432:ASN:ND2	1:C:432:ASN:C	2.58	0.53
1:B:240:ILE:HG23	1:B:272:THR:HG21	1.91	0.53
1:A:258:LYS:HG2	1:A:316:PHE:CD2	2.43	0.53
1:D:117:LEU:CD1	1:D:151:GLU:OE1	2.56	0.53
1:C:238:ARG:O	1:C:239:ALA:C	2.45	0.53
1:A:94:LYS:HG3	1:A:461:VAL:HG11	1.90	0.52
1:C:187:VAL:O	1:C:191:ILE:HG23	2.09	0.52
1:C:337:ASN:O	1:C:341:LYS:HG2	2.09	0.52
1:D:124:ARG:NH1	3:D:2144:HOH:O	2.42	0.52
1:D:148:ILE:HG21	1:D:152:MET:HE3	1.88	0.52
1:B:355:THR:HG21	1:B:433:ILE:HD13	1.89	0.52
1:C:51:VAL:HG13	1:C:52:PRO:HD2	1.90	0.52
1:C:262:GLU:O	1:C:266:GLN:HG2	2.09	0.52
1:A:50:ILE:HD13	1:A:51:VAL:N	2.24	0.52
1:A:394:LEU:HD22	1:A:469:ILE:HG21	1.92	0.52
1:A:453:VAL:O	1:A:459:LEU:HD12	2.08	0.52
1:B:289:HIS:ND1	3:B:2246:HOH:O	2.33	0.52
1:A:233:ALA:HB2	1:A:259:SER:HB3	1.90	0.52
1:C:347:ASN:HD22	1:C:349:THR:H	1.56	0.52
1:B:102:THR:OG1	1:B:408:ASP:HB3	2.09	0.52
1:B:333:HIS:ND1	1:B:358:THR:HG22	2.25	0.52
1:A:454:LEU:CD1	1:A:459:LEU:HD13	2.40	0.52
1:C:110:PRO:CG	3:C:2153:HOH:O	2.58	0.52
1:A:24:ILE:HG23	1:A:401:ILE:HD12	1.91	0.52
1:A:37:MET:SD	1:A:409:LEU:HD11	2.50	0.52
1:B:313:THR:N	1:B:314:PRO:CD	2.73	0.52
1:A:111:GLU:HB3	1:A:114:THR:CG2	2.40	0.51
1:B:194:ILE:N	1:B:194:ILE:HD12	2.26	0.51
1:C:355[A]:THR:HG23	1:C:356:ASN:N	2.25	0.51
1:A:269:LYS:CG	3:A:2257:HOH:O	2.58	0.51
1:D:322:SER:O	1:D:379:GLN:NE2	2.41	0.51
1:C:355[A]:THR:HG21	1:C:433:ILE:CD1	2.40	0.51
1:C:165:LEU:HD22	1:C:167:TYR:CE1	2.46	0.51
1:C:269:LYS:NZ	3:C:2306:HOH:O	2.38	0.51
1:B:213:LEU:HD11	1:B:347:ASN:OD1	2.10	0.51
1:A:80:ASP:O	1:A:83:MET:N	2.38	0.51
1:A:355:THR:HG22	3:A:2305:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:PHE:CD1	1:B:463:GLU:HG3	2.45	0.51
1:C:78:MET:CE	3:C:2377:HOH:O	2.59	0.51
1:C:413:ASP:O	1:C:441:GLY:HA2	2.11	0.51
1:C:325:ASP:O	1:C:327:GLN:NE2	2.44	0.51
1:D:46:GLY:HA3	1:D:49:LEU:HD11	1.91	0.50
1:B:185:LEU:HB3	1:B:246:THR:HG21	1.92	0.50
1:B:315:ASP:OD2	1:B:374:LYS:NZ	2.37	0.50
1:D:133:CYS:O	1:D:466:GLY:HA3	2.11	0.50
1:D:352:PRO:HA	3:D:2089:HOH:O	2.10	0.50
1:A:300:ALA:HB1	3:A:2286:HOH:O	2.11	0.50
1:C:21:GLY:O	1:C:62:SER:CA	2.60	0.50
1:C:91:GLN:HG2	3:C:2430:HOH:O	2.12	0.50
1:D:401:ILE:HG23	1:D:409:LEU:HD21	1.94	0.50
1:C:228:PRO:O	1:C:231:VAL:HG22	2.12	0.50
1:A:208:GLU:OE1	1:C:245:GLN:NE2	2.45	0.50
1:D:454:LEU:HD13	1:D:459:LEU:HD12	1.93	0.50
1:C:165:LEU:HD23	1:C:166:VAL:N	2.27	0.50
1:A:37:MET:SD	1:A:409:LEU:HD12	2.52	0.49
1:A:50:ILE:HD13	1:A:50:ILE:C	2.33	0.49
1:D:18:LEU:HG	1:D:20:LYS:HG3	1.94	0.49
1:A:34:ASP:N	1:A:46:GLY:O	2.38	0.49
1:B:97:LEU:HD23	1:B:101:THR:O	2.11	0.49
1:C:110:PRO:HB2	3:C:2153:HOH:O	2.12	0.49
1:C:272:THR:HG22	1:C:274:VAL:HB	1.95	0.49
1:A:307:LEU:HD22	1:A:307:LEU:H	1.77	0.49
1:A:117:LEU:HD22	3:A:2156:HOH:O	2.12	0.49
1:B:342:ALA:O	1:B:345:LYS:HB3	2.13	0.49
1:C:24:ILE:HG21	1:C:31:PHE:CZ	2.47	0.49
1:B:379:GLN:O	1:B:382:ALA:HB3	2.12	0.49
1:B:153:GLU:CA	1:B:191:ILE:HD11	2.40	0.49
1:B:256:MET:CE	1:B:282:SER:HB3	2.42	0.49
1:D:480:LYS:NZ	3:D:2466:HOH:O	2.21	0.49
1:B:51:VAL:HG21	1:B:55:VAL:HG11	1.94	0.49
1:D:381:VAL:HG12	1:D:386:THR:CG2	2.43	0.49
1:D:102:THR:OG1	1:D:408:ASP:HB3	2.12	0.49
1:D:488:LEU:O	3:D:2479:HOH:O	2.20	0.48
1:A:424:THR:HG22	1:A:424:THR:O	2.13	0.48
1:B:481:ARG:O	1:B:485:ARG:HG3	2.13	0.48
1:D:152:MET:O	1:D:156:VAL:HG23	2.13	0.48
1:D:382:ALA:HA	1:D:386:THR:HG23	1.95	0.48
1:D:58:ILE:HD11	1:D:452:ILE:CD1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:GLN:NE2	1:D:426:ASN:O	2.43	0.48
1:B:168[A]:MET:CE	1:B:235:ALA:HB1	2.44	0.48
1:B:421:SER:HB2	1:B:435:GLU:OE2	2.13	0.48
1:C:302:VAL:HB	3:C:2364:HOH:O	2.14	0.48
3:A:2170:HOH:O	1:C:179:CYS:HB3	2.13	0.48
1:C:327:GLN:NE2	3:C:2355:HOH:O	2.46	0.48
1:C:208:GLU:O	1:C:212:ILE:HG12	2.13	0.48
1:C:478:VAL:O	1:C:482:ILE:HD12	2.14	0.48
1:D:96:ALA:HB1	1:D:101:THR:HB	1.96	0.48
1:C:313:THR:N	1:C:314:PRO:CD	2.77	0.48
1:C:338:THR:OG1	1:C:430:GLU:OE1	2.27	0.48
1:A:16:ARG:HD2	1:A:55:VAL:HG22	1.95	0.47
1:A:256:MET:CE	1:A:307:LEU:HD13	2.44	0.47
1:A:269:LYS:HG3	3:A:2257:HOH:O	2.14	0.47
1:B:168[A]:MET:HE2	1:B:235:ALA:HB1	1.96	0.47
1:B:295:TRP:CH2	1:B:342:ALA:HA	2.49	0.47
1:B:215:LEU:HD13	3:B:2195:HOH:O	2.14	0.47
1:C:472:LYS:NZ	3:C:2462:HOH:O	2.45	0.47
1:D:83:MET:HE1	1:D:343:VAL:HG21	1.96	0.47
1:C:227:ARG:HH12	1:C:304:SER:CB	2.26	0.47
1:C:425:HIS:HD2	1:C:425:HIS:O	1.97	0.47
1:B:72:VAL:CG1	1:B:388:ALA:HB1	2.43	0.47
1:B:117:LEU:HD13	1:B:151:GLU:CG	2.43	0.47
1:C:277:GLU:O	1:C:277:GLU:HG2	2.13	0.47
1:D:102:THR:CB	1:D:408:ASP:HB3	2.44	0.47
1:D:173:ARG:HD2	1:D:173:ARG:C	2.35	0.47
1:A:185:LEU:HB3	1:A:246:THR:HG21	1.97	0.47
1:C:140:ASP:OD2	1:C:167:TYR:OH	2.29	0.47
1:C:268:ARG:HD2	1:C:327:GLN:HE22	1.79	0.47
1:C:304:SER:HA	1:C:305:PRO:C	2.35	0.47
1:D:19:ILE:HG13	1:D:37:MET:CE	2.45	0.47
1:A:165:LEU:C	1:A:165:LEU:HD23	2.34	0.47
1:A:421[B]:SER:OG	1:A:435:GLU:OE2	2.27	0.47
1:B:116:LEU:HB3	1:B:155:LEU:HD11	1.95	0.47
1:B:233:ALA:HB2	1:B:259:SER:HB3	1.95	0.47
1:B:270:LYS:HE2	3:B:2239:HOH:O	2.14	0.47
1:B:355:THR:CG2	1:B:433:ILE:CD1	2.92	0.47
1:C:65:VAL:HG22	1:C:411:ILE:HG12	1.97	0.47
1:D:363:SER:HB3	1:D:439:CYS:SG	2.55	0.47
1:D:146:LYS:H	1:D:146:LYS:HZ3	1.63	0.47
1:A:34:ASP:HB2	1:A:49:LEU:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:ARG:O	1:A:485:ARG:HG3	2.14	0.47
1:C:227:ARG:NH1	1:C:304:SER:OG	2.48	0.47
1:A:307:LEU:HA	3:A:2291:HOH:O	2.15	0.47
1:C:108:VAL:O	1:C:140:ASP:HB2	2.15	0.47
1:D:297:LYS:O	1:D:300:ALA:HB3	2.15	0.47
1:B:16:ARG:HB3	1:B:55:VAL:HG22	1.96	0.46
1:B:168[A]:MET:CE	1:B:238:ARG:CZ	2.93	0.46
1:C:64:MET:O	1:C:411:ILE:HA	2.16	0.46
1:C:40:GLY:O	1:C:41:LEU:HD23	2.15	0.46
1:B:146:LYS:CD	1:B:146:LYS:H	2.28	0.46
1:C:152:MET:HE3	1:C:187:VAL:HG11	1.97	0.46
1:C:227:ARG:NH1	1:C:304:SER:CB	2.79	0.46
1:C:347:ASN:HD22	1:C:347:ASN:C	2.19	0.46
1:D:75:ARG:CZ	3:D:2074:HOH:O	2.62	0.46
1:B:401:ILE:CD1	1:B:409:LEU:HD23	2.44	0.46
1:C:44[A]:GLN:NE2	3:C:2032:HOH:O	2.47	0.46
1:D:381:VAL:HG12	1:D:386:THR:HG22	1.98	0.46
1:B:152:MET:HG2	1:B:164:PHE:CE2	2.51	0.46
1:D:73:HIS:HB2	1:D:277:GLU:OE2	2.16	0.46
1:B:108:VAL:HG22	1:B:123:TRP:HB2	1.97	0.46
1:B:327:GLN:CD	1:B:327:GLN:N	2.68	0.45
1:B:228:PRO:O	1:B:231:VAL:HG22	2.16	0.45
1:C:60:ALA:O	1:C:63:ARG:HB2	2.16	0.45
1:D:17:LEU:HD12	1:D:18:LEU:H	1.81	0.45
1:D:428:SER:HB2	3:D:2415:HOH:O	2.17	0.45
1:B:37:MET:HE1	1:B:409:LEU:HD13	1.97	0.45
1:B:379:GLN:HE21	1:B:379:GLN:HA	1.81	0.45
1:A:196:GLN:C	1:A:197[A]:VAL:HG23	2.36	0.45
1:D:385:SER:O	1:D:388:ALA:HB3	2.16	0.45
1:A:52:PRO:HB2	1:A:55:VAL:HG23	1.99	0.45
1:B:48:ASN:O	1:B:49:LEU:O	2.35	0.45
1:C:370:VAL:HG22	1:C:375:MET:HG3	1.98	0.45
1:C:397:ARG:CZ	1:C:469:ILE:HD12	2.47	0.45
1:A:165:LEU:HB2	1:A:196:GLN:HE21	1.82	0.45
1:D:168[B]:MET:CE	1:D:197:VAL:HG12	2.40	0.45
1:A:432:ASN:HD22	1:A:432:ASN:C	2.19	0.45
1:D:72:VAL:HG21	1:D:251:TYR:OH	2.17	0.45
1:C:321:LEU:HD11	1:C:329:THR:HG22	1.99	0.45
1:C:360:GLU:HG2	1:C:434:PHE:HD2	1.81	0.45
1:C:398:LYS:NZ	1:C:406:ASP:OD2	2.22	0.45
1:C:293:LYS:HD2	3:C:2329:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:LYS:HE3	1:A:25:VAL:HG22	1.99	0.44
1:A:368:LYS:NZ	3:A:2334:HOH:O	2.40	0.44
1:B:355:THR:HG23	1:B:433:ILE:CD1	2.44	0.44
1:C:432:ASN:HD22	1:C:434:PHE:N	2.09	0.44
1:A:303:THR:HA	1:A:353:GLU:HB3	1.98	0.44
1:B:89:PHE:O	1:B:93:THR:HG23	2.17	0.44
1:A:253:THR:O	1:A:254:LYS:C	2.55	0.44
1:A:335:THR:HB	1:A:429:LEU:HD11	1.99	0.44
1:B:213:LEU:HD23	1:B:213:LEU:HA	1.85	0.44
1:A:24:ILE:HD12	1:A:33:ALA:HB3	1.99	0.44
1:B:44:GLN:HB3	1:B:49:LEU:HD22	2.00	0.44
1:B:24:ILE:CD1	1:B:33:ALA:HB3	2.45	0.44
1:B:35:ILE:HD12	1:B:65:VAL:HG11	2.00	0.44
1:B:108:VAL:HG22	1:B:123:TRP:CB	2.48	0.44
1:B:196:GLN:HG2	1:B:251:TYR:CD1	2.52	0.44
1:D:83:MET:CE	1:D:343:VAL:HG21	2.48	0.44
1:D:149:GLN:HG2	1:D:153:GLU:OE2	2.18	0.44
1:C:122:GLN:HA	1:C:122:GLN:OE1	2.18	0.44
1:A:458:THR:CG2	1:A:460:HIS:CE1	3.00	0.44
1:B:340:GLN:O	1:B:343:VAL:HG23	2.18	0.44
1:B:316:PHE:CE2	1:B:320:LEU:HD22	2.53	0.44
1:C:382:ALA:HA	1:C:386:THR:HB	2.00	0.44
1:D:333:HIS:CA	3:D:2356:HOH:O	2.64	0.44
1:A:117:LEU:HD23	1:A:155:LEU:CD2	2.48	0.43
1:A:143:GLU:OE1	3:A:2136:HOH:O	2.20	0.43
1:B:37:MET:CE	1:B:409:LEU:CD1	2.96	0.43
1:B:335:THR:HB	1:B:429:LEU:HD21	2.00	0.43
1:B:479:TYR:HB3	1:B:483:LYS:HE2	2.00	0.43
1:A:34:ASP:CB	1:A:49:LEU:HD12	2.48	0.43
1:C:98:ALA:HB2	1:C:459:LEU:HD21	2.00	0.43
1:D:156:VAL:CG2	1:D:191:ILE:HD12	2.43	0.43
1:D:233:ALA:HB3	3:D:2270:HOH:O	2.18	0.43
1:D:340:GLN:O	1:D:343:VAL:HG23	2.19	0.43
1:A:97:LEU:O	1:A:98:ALA:C	2.57	0.43
1:B:398:LYS:HE2	1:B:406:ASP:OD2	2.19	0.43
1:D:334:CYS:O	1:D:354:GLY:HA3	2.18	0.43
1:D:355:THR:HG22	3:D:2338:HOH:O	2.18	0.43
1:A:107:HIS:CE1	1:A:196:GLN:HE22	2.33	0.43
1:B:230:GLU:H	1:B:230:GLU:CD	2.21	0.43
1:B:351:ILE:O	1:B:352:PRO:C	2.55	0.43
1:C:141:ILE:HD13	1:C:141:ILE:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:ALA:O	1:D:63:ARG:CG	2.66	0.43
1:A:340:GLN:O	1:A:343:VAL:HG23	2.18	0.43
1:C:24:ILE:HD12	1:C:33:ALA:HB3	2.01	0.43
1:C:279:ILE:HA	1:C:330:GLY:O	2.19	0.43
1:D:183:GLU:O	1:D:187:VAL:HG23	2.18	0.43
1:C:152:MET:CE	1:C:187:VAL:HG11	2.48	0.43
1:B:166:VAL:HB	1:B:176:LEU:HD22	2.00	0.43
1:B:192:GLY:HA2	1:B:479:TYR:CZ	2.53	0.43
1:B:339:ALA:HB2	3:B:2282:HOH:O	2.19	0.43
1:C:303:THR:HB	1:C:355[B]:THR:HG23	2.01	0.43
1:D:139:VAL:O	1:D:164:PHE:HA	2.19	0.43
1:D:149:GLN:O	1:D:153:GLU:HG3	2.18	0.43
1:C:349:THR:HA	3:C:2269:HOH:O	2.18	0.43
1:D:144:TRP:HZ3	1:D:152:MET:CE	2.21	0.43
1:A:117:LEU:HD23	1:A:155:LEU:HD21	2.00	0.43
1:C:168:MET:HE1	1:C:235:ALA:HA	1.99	0.43
1:D:212:ILE:HG22	1:D:217:ILE:HB	2.01	0.43
1:A:197[B]:VAL:CG1	1:A:252:ILE:HD13	2.48	0.42
1:D:313:THR:HB	1:D:314:PRO:HD3	2.01	0.42
1:A:78:MET:HB3	1:A:78:MET:HE2	1.70	0.42
1:D:375:MET:HB2	1:D:379:GLN:HB3	2.01	0.42
1:A:274:VAL:HG13	1:A:274:VAL:O	2.18	0.42
1:B:110:PRO:HG2	1:B:116:LEU:CD2	2.49	0.42
1:B:139:VAL:O	1:B:164:PHE:HA	2.19	0.42
1:C:102:THR:O	1:C:133:CYS:HB2	2.20	0.42
1:B:47:GLU:O	1:B:48:ASN:CB	2.68	0.42
1:C:260:SER:O	1:C:264:ILE:HG13	2.20	0.42
1:D:68:GLY:HA2	1:D:410:VAL:HG23	2.01	0.42
1:B:177:THR:HG22	3:B:2055:HOH:O	2.20	0.42
1:D:141:ILE:CD1	1:D:152:MET:CE	2.97	0.42
1:D:335:THR:HB	1:D:429:LEU:CD1	2.48	0.42
1:D:424:THR:HG23	3:D:2407:HOH:O	2.18	0.42
1:A:334:CYS:O	1:A:354:GLY:HA3	2.20	0.42
1:A:225:LEU:HD23	1:A:225:LEU:HA	1.88	0.42
1:C:111:GLU:HG2	3:C:2119:HOH:O	2.18	0.42
1:C:115:SER:HB2	1:C:151:GLU:OE1	2.20	0.42
1:C:210:GLN:HG3	3:C:2255:HOH:O	2.19	0.42
1:C:246:THR:HG23	1:C:248:CYS:CB	2.50	0.42
1:C:460:HIS:HB3	3:C:2217:HOH:O	2.20	0.42
1:D:68:GLY:HA3	1:D:102:THR:OG1	2.19	0.42
1:B:420:ILE:HG21	1:B:434:PHE:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:SER:OG	1:D:333:HIS:HB2	2.20	0.42
1:A:68:GLY:HA3	1:A:102:THR:OG1	2.19	0.41
1:A:230:GLU:N	1:A:230:GLU:OE1	2.50	0.41
1:C:108:VAL:HB	1:C:139:VAL:HA	2.00	0.41
1:C:205:ILE:HD13	1:C:227:ARG:NH2	2.35	0.41
1:C:246:THR:HG23	1:C:248:CYS:HB2	2.02	0.41
1:B:18:LEU:HG	1:B:20:LYS:HG3	2.02	0.41
1:B:110:PRO:HG2	1:B:116:LEU:HD23	2.01	0.41
1:B:221:GLU:O	1:B:224:VAL:HG12	2.19	0.41
1:C:479:TYR:HB3	1:C:483:LYS:HE3	2.02	0.41
1:D:420:ILE:HG21	1:D:434:PHE:HB2	2.02	0.41
1:A:282:SER:HB2	1:A:317:LEU:CD1	2.50	0.41
1:D:70:ILE:HD11	1:D:398:LYS:HB3	2.01	0.41
1:B:77:GLN:OE1	1:B:88:ASP:HB2	2.19	0.41
1:C:110:PRO:HA	3:C:2114:HOH:O	2.20	0.41
1:C:168:MET:HE2	1:C:235:ALA:HB1	2.03	0.41
1:A:254:LYS:NZ	1:A:304:SER:O	2.42	0.41
1:C:377:GLU:O	1:C:380:PHE:HB3	2.21	0.41
1:A:73:HIS:O	1:A:332:ALA:N	2.52	0.41
1:A:111:GLU:O	1:A:114:THR:HG23	2.21	0.41
1:A:146:LYS:CD	1:A:146:LYS:H	2.33	0.41
1:B:60:ALA:O	1:B:63:ARG:HB2	2.20	0.41
1:B:162:ASN:O	1:B:194:ILE:HD12	2.20	0.41
1:B:425:HIS:HD2	1:B:425:HIS:O	2.03	0.41
1:B:168[A]:MET:CE	1:B:238:ARG:NH2	2.84	0.41
1:B:146:LYS:H	1:B:146:LYS:HD2	1.85	0.41
1:B:156:VAL:HG21	1:B:191:ILE:CG2	2.50	0.41
1:C:31:PHE:N	1:C:31:PHE:CD1	2.89	0.41
1:C:106:ASP:HB3	1:C:137:LEU:HD23	2.02	0.41
1:A:210:GLN:HG3	3:A:2078:HOH:O	2.21	0.41
1:A:394:LEU:HD22	1:A:469:ILE:CG2	2.50	0.41
1:B:213:LEU:HD22	1:B:218:THR:HG22	2.03	0.41
1:D:93:THR:HG21	1:D:131:SER:OG	2.20	0.41
1:D:325:ASP:C	1:D:327:GLN:HE22	2.22	0.41
1:A:139:VAL:O	1:A:164:PHE:HA	2.20	0.41
1:A:356:ASN:HD21	1:A:432:ASN:ND2	2.19	0.41
1:A:422:ALA:HA	1:A:425:HIS:CE1	2.56	0.41
1:B:212:ILE:CG2	1:B:217:ILE:HB	2.51	0.41
1:C:347:ASN:ND2	1:C:349:THR:H	2.17	0.41
1:C:459:LEU:HD12	1:C:459:LEU:N	2.36	0.41
1:D:162:ASN:OD1	1:D:471:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ASN:OD1	1:A:294:ASN:C	2.60	0.40
1:B:21:GLY:O	1:B:62:SER:N	2.54	0.40
1:B:72:VAL:HG11	1:B:388:ALA:HB1	2.03	0.40
1:C:233:ALA:CB	1:C:259:SER:HB3	2.51	0.40
1:A:50:ILE:HG23	1:A:50:ILE:O	2.21	0.40
1:A:164:PHE:HB2	1:A:188:ILE:CD1	2.49	0.40
1:B:51:VAL:HB	1:B:52:PRO:HD2	2.03	0.40
1:B:369:ALA:O	1:B:374:LYS:HB2	2.22	0.40
1:D:310:ASP:OD1	1:D:312:THR:OG1	2.27	0.40
1:A:386:THR:CG2	1:A:390:LYS:HE3	2.49	0.40
1:B:36:TYR:CG	1:B:51:VAL:HG11	2.57	0.40
1:B:168[A]:MET:HE1	1:B:235:ALA:HA	2.03	0.40
1:B:437:MET:HG2	1:B:439:CYS:HB2	2.03	0.40
1:C:16:ARG:HG2	1:C:36:TYR:OH	2.20	0.40
1:C:360:GLU:HG2	1:C:434:PHE:CD2	2.56	0.40
1:B:483:LYS:O	1:B:487:ARG:HG3	2.22	0.40
1:C:24:ILE:HD12	1:C:31:PHE:CE2	2.56	0.40
1:D:77:GLN:HE21	1:D:89:PHE:HD2	1.69	0.40
1:D:397:ARG:HG3	3:D:2397:HOH:O	2.21	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	481/501 (96%)	454 (94%)	26 (5%)	1 (0%)	47 38
1	B	476/501 (95%)	445 (94%)	26 (6%)	5 (1%)	14 5
1	C	477/501 (95%)	446 (94%)	29 (6%)	2 (0%)	34 24
1	D	477/501 (95%)	447 (94%)	29 (6%)	1 (0%)	47 38
All	All	1911/2004 (95%)	1792 (94%)	110 (6%)	9 (0%)	34 18

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	48	ASN
1	B	49	LEU
1	B	77	GLN
1	B	173[A]	ARG
1	B	173[B]	ARG
1	C	52	PRO
1	D	52	PRO
1	C	357	GLY
1	A	52	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	406/422 (96%)	391 (96%)	15 (4%)	34	25
1	B	401/422 (95%)	387 (96%)	14 (4%)	36	27
1	C	402/422 (95%)	388 (96%)	14 (4%)	36	27
1	D	402/422 (95%)	386 (96%)	16 (4%)	31	22
All	All	1611/1688 (95%)	1552 (96%)	59 (4%)	34	25

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ASP
1	A	38	GLU
1	A	50	ILE
1	A	78	MET
1	A	115	SER
1	A	122	GLN
1	A	146	LYS
1	A	157	LYS
1	A	173	ARG
1	A	176	LEU
1	A	396	PRO

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Mol	Chain	Res	Type
1	A	425	HIS
1	A	432	ASN
1	A	455	GLU
1	A	486	SER
1	B	48	ASN
1	B	63	ARG
1	B	106	ASP
1	B	115	SER
1	B	146	LYS
1	B	149	GLN
1	B	191	ILE
1	B	215	LEU
1	B	246	THR
1	B	355	THR
1	B	379	GLN
1	B	425	HIS
1	B	432	ASN
1	B	459	LEU
1	C	27	ASP
1	C	63	ARG
1	C	77	GLN
1	C	84	THR
1	C	141	ILE
1	C	176	LEU
1	C	227	ARG
1	C	246	THR
1	C	347	ASN
1	C	401	ILE
1	C	425	HIS
1	C	427	SER
1	C	428	SER
1	C	432	ASN
1	D	49	LEU
1	D	50	ILE
1	D	62	SER
1	D	88	ASP
1	D	111	GLU
1	D	122	GLN
1	D	123	TRP
1	D	197	VAL
1	D	215	LEU
1	D	355	THR

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Mol	Chain	Res	Type
1	D	386	THR
1	D	391	VAL
1	D	415	ASP
1	D	425	HIS
1	D	439	CYS
1	D	459	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	196	GLN
1	A	237	ASN
1	A	245	GLN
1	A	266	GLN
1	A	432	ASN
1	A	460	HIS
1	B	209	GLN
1	B	237	ASN
1	B	245	GLN
1	B	379	GLN
1	B	432	ASN
1	C	81	GLN
1	C	210	GLN
1	C	237	ASN
1	C	245	GLN
1	C	347	ASN
1	C	432	ASN
1	D	29	GLN
1	D	44	GLN
1	D	77	GLN
1	D	159	HIS
1	D	237	ASN
1	D	460	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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

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	477/501 (95%)	0.41	20 (4%)	36	39	8, 22, 41, 57	0
1	B	476/501 (95%)	0.34	22 (4%)	32	35	5, 20, 40, 67	0
1	C	476/501 (95%)	0.33	14 (2%)	51	54	2, 18, 40, 55	0
1	D	476/501 (95%)	0.50	26 (5%)	25	28	8, 21, 40, 63	0
All	All	1905/2004 (95%)	0.40	82 (4%)	35	38	2, 20, 40, 67	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	51	VAL	6.0
1	D	49	LEU	5.9
1	D	489	ALA	5.8
1	A	489	ALA	5.6
1	C	51	VAL	5.1
1	A	48	ASN	5.0
1	B	53	GLY	4.8
1	D	50	ILE	4.6
1	D	53	GLY	4.4
1	D	490	GLU	4.4
1	D	172	ASP	4.3
1	C	50	ILE	4.2
1	B	489	ALA	4.2
1	B	50	ILE	4.1
1	B	55	VAL	3.9
1	B	54	GLY	3.8
1	A	61	HIS	3.5
1	A	16	ARG	3.5
1	A	58	ILE	3.4
1	B	460	HIS	3.4
1	A	51	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	50	ILE	3.3
1	B	36	TYR	3.2
1	C	489	ALA	3.2
1	D	419	THR	3.1
1	B	52	PRO	3.0
1	B	51	VAL	3.0
1	A	36	TYR	3.0
1	A	456	ASP	2.9
1	D	456	ASP	2.9
1	D	18	LEU	2.9
1	A	424	THR	2.8
1	C	456	ASP	2.8
1	B	47	GLU	2.8
1	D	35	ILE	2.8
1	B	49	LEU	2.8
1	C	19	ILE	2.8
1	B	35	ILE	2.7
1	A	14	SER	2.7
1	D	403	VAL	2.7
1	A	438	GLU	2.6
1	C	52	PRO	2.6
1	A	55	VAL	2.6
1	D	462	THR	2.6
1	C	457	GLY	2.6
1	A	15	ASP	2.5
1	D	61	HIS	2.5
1	B	417	VAL	2.5
1	D	55	VAL	2.5
1	D	438	GLU	2.5
1	A	19	ILE	2.5
1	D	109	VAL	2.5
1	C	210	GLN	2.4
1	B	17	LEU	2.4
1	B	212	ILE	2.4
1	C	417	VAL	2.4
1	D	339	ALA	2.4
1	C	81	GLN	2.4
1	D	48	ASN	2.3
1	B	16	ARG	2.3
1	C	53	GLY	2.3
1	B	114	THR	2.3
1	D	58	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	438	GLU	2.2
1	D	46	GLY	2.2
1	B	215	LEU	2.2
1	B	113	GLY	2.2
1	D	63	ARG	2.2
1	C	15	ASP	2.2
1	A	487	ARG	2.2
1	A	298	ALA	2.1
1	A	422	ALA	2.1
1	C	62	SER	2.1
1	D	424	THR	2.1
1	D	487	ARG	2.1
1	A	300	ALA	2.1
1	A	18	LEU	2.1
1	B	41	LEU	2.1
1	D	428	SER	2.0
1	C	126	TRP	2.0
1	D	423	LYS	2.0
1	B	63	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	B	1491	1/1	0.84	0.15	47,47,47,47	0
2	MG	A	1491	1/1	0.89	0.12	44,44,44,44	0
2	MG	C	1491	1/1	0.93	0.10	32,32,32,32	0

6.5 Other polymers (i)

There are no such residues in this entry.