Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:51 PM GMT

PDB ID	:	4AR2
Title	:	Dodecahedron formed of penton base protein from adenovirus Ad3
Authors	:	Burmeister, W.P.; Szolajska, E.; Zochowska, M.; Nerlo, B.; Andreev, I.; Schoehn, G.; Andrieu, J.-P.; Fender, P.; Naskalska, A.; Zubieta, C.; Cusack, S.; Chroboczek, J.
Deposited on	:	2012-04-20
Resolution	:	3.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

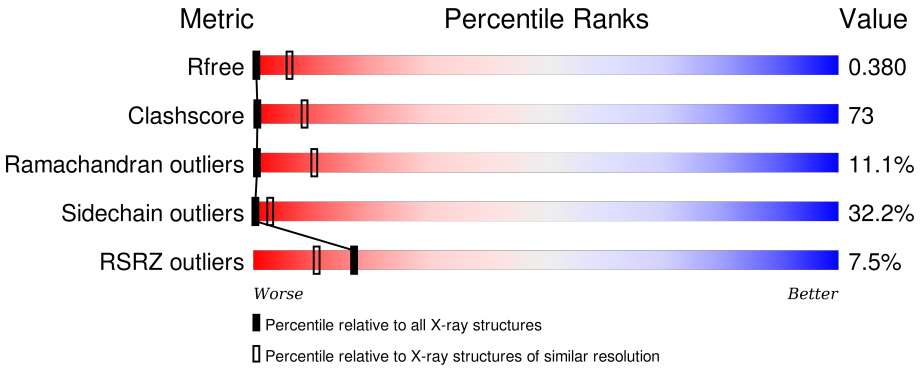
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	509	5% 19% 40% 27% • 11%
2	P	21	48% 29% 19% 52%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3757 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 L2 PROTEIN III (PENTON BASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3673	2324	629	706	14			

- Molecule 2 is a protein called FIBER PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	10	Total	C	N	O	S	0	0	0
			83	53	11	18	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	21	CYS	-	EXPRESSION TAG	UNP P03275

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

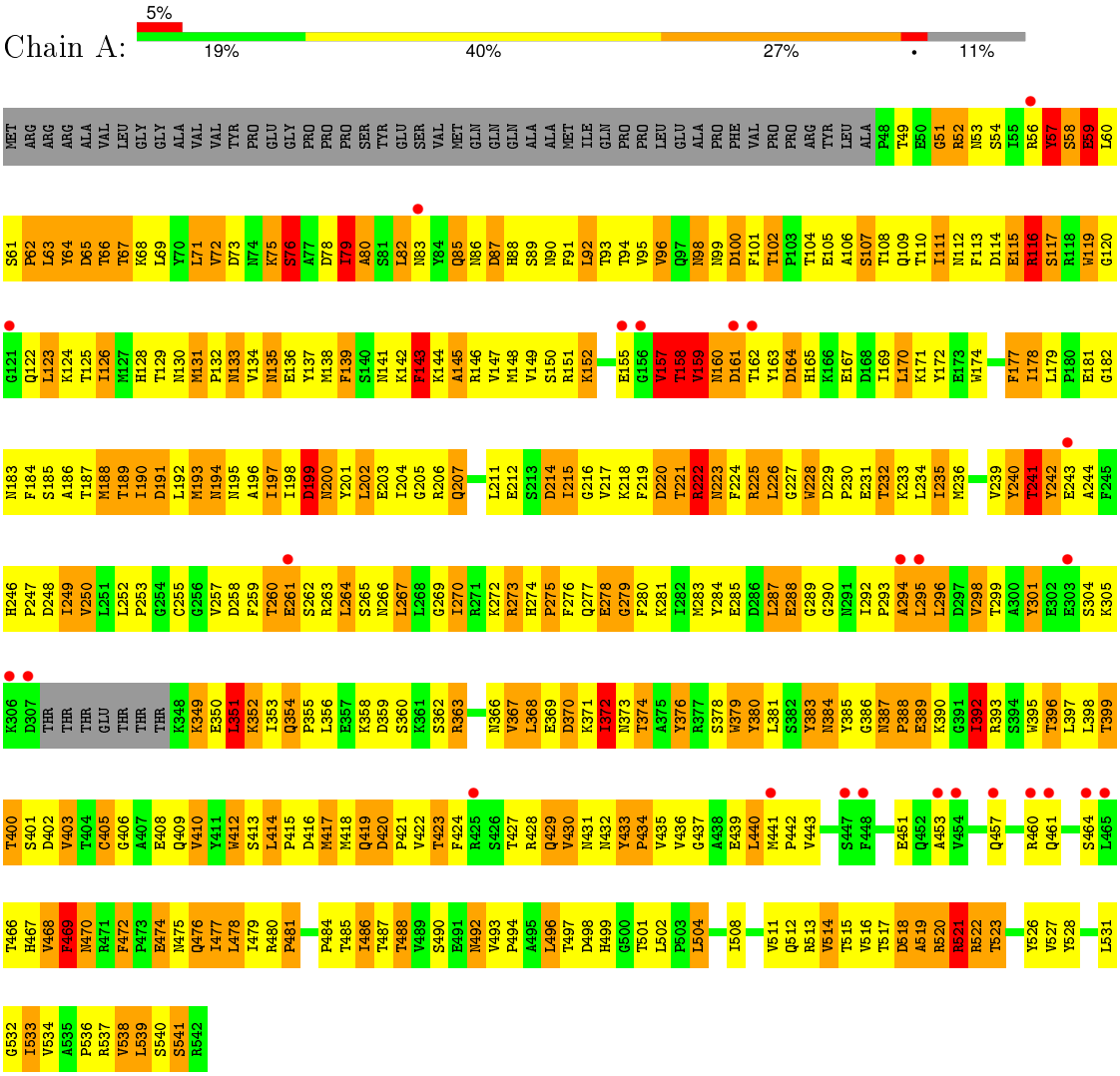
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

3 Residue-property plots (i)

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

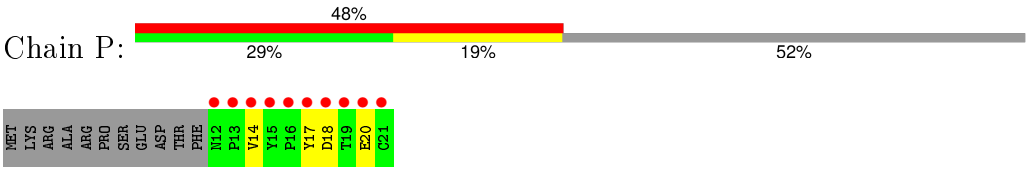
- Molecule 1: L2 PROTEIN III (PENTON BASE)

Chain A:



- Molecule 2: FIBER PROTEIN

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	346.04Å 348.55Å 372.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	258.20 – 3.80 29.41 – 3.80	Depositor EDS
% Data completeness (in resolution range)	56.8 (258.20-3.80) 55.7 (29.41-3.80)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 3.75Å)	Xtriage
Refinement program	REFMAC 5.6.0114	Depositor
R, R_{free}	0.280 , 0.278 0.383 , 0.380	Depositor DCC
R_{free} test set	5040 reflections (2.06%)	DCC
Wilson B-factor (Å^2)	101.2	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.065 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Outliers	1 of 249444 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.73	EDS
Total number of atoms	3757	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.67	2/3758 (0.1%)	1.06	24/5103 (0.5%)
2	P	0.53	0/86	0.71	0/119
All	All	0.67	2/3844 (0.1%)	1.06	24/5222 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	79	ILE	CA-CB	5.76	1.68	1.54
1	A	80	ALA	N-CA	-5.26	1.35	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	157	VAL	N-CA-C	8.49	133.92	111.00
1	A	279	GLY	N-CA-C	-8.15	92.72	113.10
1	A	469	PHE	N-CA-C	-8.12	89.08	111.00
1	A	155	GLU	N-CA-C	7.64	131.63	111.00
1	A	387	ASN	N-CA-C	7.21	130.46	111.00
1	A	116	ARG	N-CA-C	-6.76	92.75	111.00
1	A	305	LYS	N-CA-C	-6.70	92.92	111.00
1	A	51	GLY	N-CA-C	6.40	129.11	113.10
1	A	433	TYR	N-CA-C	6.21	127.77	111.00
1	A	111	ILE	N-CA-C	-6.05	94.67	111.00
1	A	414	LEU	N-CA-C	-5.99	94.83	111.00
1	A	281	LYS	N-CA-C	-5.97	94.88	111.00
1	A	79	ILE	CG1-CB-CG2	-5.85	98.53	111.40
1	A	115	GLU	N-CA-C	5.75	126.53	111.00
1	A	158	THR	N-CA-C	5.71	126.42	111.00
1	A	240	TYR	N-CA-C	-5.59	95.91	111.00
1	A	80	ALA	N-CA-CB	-5.34	102.62	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	351	LEU	N-CA-C	5.34	125.42	111.00
1	A	116	ARG	CA-CB-CG	5.29	125.04	113.40
1	A	87	ASP	N-CA-C	5.20	125.03	111.00
1	A	159	VAL	N-CA-C	5.17	124.96	111.00
1	A	386	GLY	N-CA-C	5.16	125.99	113.10
1	A	76	SER	N-CA-C	5.13	124.86	111.00
1	A	521	ARG	NE-CZ-NH2	-5.05	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3673	0	3600	538	0
2	P	83	0	68	3	0
3	A	1	0	0	0	0
All	All	3757	0	3668	539	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 73.

All (539) 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:304:SER:CB	1:A:351:LEU:HB3	1.65	1.24
1:A:131:MET:H	1:A:492:ASN:ND2	1.46	1.12
1:A:431:ASN:O	1:A:521:ARG:HD3	1.52	1.09
1:A:304:SER:HB3	1:A:351:LEU:HB3	1.12	1.08
1:A:114:ASP:CG	1:A:115:GLU:H	1.49	1.08
1:A:259:PHE:HB2	1:A:280:PHE:HE1	1.16	1.08
1:A:501:THR:HG21	1:A:537:ARG:HH21	1.15	1.07
1:A:235:ILE:HG12	1:A:295:LEU:HA	1.34	1.06
1:A:129:THR:OG1	1:A:442:PRO:HG2	1.54	1.06
1:A:381:LEU:H	1:A:381:LEU:HD12	1.15	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ILE:HD13	1:A:178:ILE:H	1.23	1.02
1:A:105:GLU:O	1:A:108:THR:HG22	1.58	1.01
1:A:351:LEU:O	1:A:352:LYS:HB3	1.59	1.00
1:A:132:PRO:HD2	1:A:526:TYR:CE2	1.97	1.00
1:A:132:PRO:HD2	1:A:526:TYR:HE2	1.27	0.98
1:A:301:TYR:HD2	1:A:352:LYS:HD2	1.28	0.97
1:A:131:MET:N	1:A:492:ASN:HD21	1.64	0.95
1:A:293:PRO:O	1:A:373:ASN:HA	1.67	0.94
1:A:517:THR:HG21	1:A:521:ARG:HG3	1.50	0.94
1:A:235:ILE:CG1	1:A:295:LEU:HA	2.00	0.92
1:A:429:GLN:HA	1:A:429:GLN:HE21	1.33	0.92
1:A:403:VAL:CG2	1:A:488:THR:HB	2.00	0.91
1:A:259:PHE:HB2	1:A:280:PHE:CE1	2.06	0.91
1:A:501:THR:HG21	1:A:537:ARG:NH2	1.83	0.90
1:A:114:ASP:CG	1:A:115:GLU:N	2.26	0.88
1:A:304:SER:CB	1:A:351:LEU:CB	2.52	0.88
1:A:435:VAL:HG23	1:A:521:ARG:HH22	1.39	0.87
1:A:413:SER:HB3	1:A:435:VAL:HA	1.57	0.87
1:A:381:LEU:H	1:A:381:LEU:CD1	1.87	0.87
1:A:131:MET:H	1:A:492:ASN:HD21	0.86	0.86
1:A:263:ARG:HD2	1:A:406:GLY:HA3	1.57	0.86
1:A:226:LEU:HD23	1:A:227:GLY:H	1.41	0.85
1:A:221:THR:O	1:A:222:ARG:HB2	1.75	0.85
1:A:159:VAL:HA	1:A:162:THR:HB	1.58	0.85
1:A:367:VAL:O	1:A:368:LEU:HB2	1.74	0.85
1:A:177:PHE:N	1:A:177:PHE:HD1	1.74	0.84
1:A:392:ILE:N	1:A:392:ILE:HD12	1.93	0.84
1:A:72:VAL:HA	1:A:531:LEU:HD22	1.58	0.84
1:A:196:ALA:HA	1:A:199:ASP:HB2	1.59	0.83
1:A:403:VAL:HG21	1:A:488:THR:HB	1.59	0.82
1:A:177:PHE:N	1:A:177:PHE:CD1	2.47	0.81
1:A:381:LEU:N	1:A:381:LEU:HD12	1.94	0.81
1:A:177:PHE:H	1:A:177:PHE:HD1	1.28	0.81
1:A:89:SER:HB3	1:A:523:THR:HG22	1.62	0.81
1:A:435:VAL:CG2	1:A:521:ARG:HH22	1.93	0.81
1:A:178:ILE:CD1	1:A:178:ILE:H	1.94	0.81
1:A:304:SER:HB2	1:A:351:LEU:HB3	1.60	0.81
1:A:274:HIS:O	1:A:276:PHE:N	2.15	0.79
1:A:409:GLN:HA	1:A:440:LEU:HA	1.64	0.79
1:A:206:ARG:HB2	1:A:207:GLN:NE2	1.98	0.78
1:A:270:ILE:HD11	1:A:379:TRP:CD1	2.18	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ASN:ND2	1:A:219:PHE:O	2.18	0.77
1:A:395:TRP:HD1	1:A:396:THR:HG22	1.50	0.77
1:A:416:ASP:C	1:A:512:GLN:HE22	1.89	0.77
1:A:232:THR:HG21	1:A:236:MET:SD	2.25	0.76
1:A:410:VAL:HG23	1:A:517:THR:O	1.87	0.75
1:A:119:TRP:HB2	1:A:537:ARG:O	1.86	0.75
1:A:63:LEU:HD13	1:A:64:TYR:O	1.87	0.75
1:A:61:SER:O	1:A:63:LEU:N	2.19	0.75
1:A:235:ILE:HD11	1:A:295:LEU:H	1.50	0.75
1:A:431:ASN:O	1:A:521:ARG:CD	2.33	0.75
1:A:383:TYR:HA	1:A:392:ILE:HD13	1.66	0.75
1:A:422:VAL:HG22	1:A:423:THR:HG23	1.69	0.75
1:A:355:PRO:HG3	1:A:371:LYS:HB3	1.68	0.74
1:A:233:LYS:HB2	1:A:372:ILE:HG21	1.67	0.74
1:A:263:ARG:NH1	1:A:405:CYS:O	2.19	0.74
1:A:304:SER:HB2	1:A:351:LEU:CB	2.16	0.74
1:A:301:TYR:CD2	1:A:352:LYS:HD2	2.18	0.74
1:A:142:LYS:O	1:A:143:PHE:HB3	1.86	0.74
1:A:248:ASP:OD2	1:A:380:TYR:HB2	1.87	0.74
1:A:235:ILE:HD13	1:A:235:ILE:N	2.03	0.74
1:A:133:ASN:HB2	1:A:490:SER:CB	2.18	0.74
1:A:278:GLU:OE1	1:A:280:PHE:HB3	1.88	0.74
1:A:235:ILE:CD1	1:A:293:PRO:HB2	2.17	0.73
1:A:518:ASP:O	1:A:521:ARG:N	2.22	0.73
1:A:56:ARG:O	1:A:57:TYR:HB3	1.88	0.73
1:A:414:LEU:CD1	1:A:417:MET:HB3	2.17	0.73
1:A:72:VAL:HA	1:A:531:LEU:CD2	2.18	0.73
1:A:376:TYR:CE2	1:A:477:ILE:HG21	2.23	0.73
1:A:143:PHE:HE2	1:A:219:PHE:CZ	2.05	0.72
1:A:147:VAL:HG22	1:A:148:MET:N	2.03	0.72
1:A:147:VAL:HG11	1:A:200:ASN:HD21	1.54	0.72
1:A:93:THR:HG22	1:A:94:THR:O	1.90	0.72
1:A:199:ASP:HA	1:A:202:LEU:HD21	1.70	0.72
1:A:424:PHE:CD2	1:A:434:PRO:HA	2.25	0.72
1:A:413:SER:HA	1:A:436:VAL:HG23	1.72	0.72
1:A:71:LEU:HB3	1:A:532:GLY:O	1.89	0.72
1:A:147:VAL:HG22	1:A:148:MET:H	1.53	0.71
1:A:279:GLY:O	1:A:395:TRP:HZ2	1.73	0.71
1:A:226:LEU:CD2	1:A:241:THR:HG23	2.20	0.71
1:A:517:THR:CG2	1:A:521:ARG:HG3	2.19	0.71
1:A:139:PHE:N	1:A:139:PHE:HD1	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:ASP:HB2	1:A:372:ILE:HD11	1.71	0.71
1:A:133:ASN:HB2	1:A:490:SER:HB3	1.72	0.71
1:A:63:LEU:HD22	1:A:64:TYR:H	1.56	0.71
1:A:508:ILE:HG23	1:A:512:GLN:HE21	1.56	0.71
1:A:159:VAL:CA	1:A:162:THR:HB	2.19	0.71
1:A:187:THR:O	1:A:190:ILE:N	2.24	0.71
1:A:475:ASN:HB3	1:A:478:LEU:HD23	1.73	0.69
1:A:161:ASP:OD2	1:A:164:ASP:HB3	1.91	0.69
1:A:91:PHE:CE1	1:A:514:VAL:HG13	2.27	0.69
1:A:171:LYS:HA	1:A:171:LYS:NZ	2.08	0.69
1:A:134:VAL:HG22	1:A:182:GLY:O	1.92	0.69
1:A:293:PRO:O	1:A:294:ALA:HB2	1.92	0.69
1:A:232:THR:OG1	1:A:234:LEU:HB2	1.92	0.68
1:A:139:PHE:N	1:A:139:PHE:CD1	2.61	0.68
1:A:223:ASN:O	1:A:226:LEU:HD22	1.94	0.68
1:A:102:THR:HG23	1:A:105:GLU:CD	2.14	0.68
1:A:98:ASN:ND2	1:A:100:ASP:H	1.92	0.68
1:A:225:ARG:O	1:A:228:TRP:HB2	1.94	0.68
1:A:220:ASP:O	1:A:248:ASP:HB3	1.93	0.68
1:A:198:ILE:O	1:A:202:LEU:HG	1.94	0.68
1:A:132:PRO:CD	1:A:526:TYR:CE2	2.76	0.67
1:A:119:TRP:HA	1:A:539:LEU:HD12	1.77	0.67
1:A:159:VAL:H	1:A:162:THR:HB	1.59	0.67
1:A:206:ARG:HB2	1:A:207:GLN:HE21	1.58	0.67
1:A:119:TRP:N	1:A:119:TRP:CD1	2.63	0.67
1:A:171:LYS:HZ3	1:A:171:LYS:HA	1.58	0.67
1:A:380:TYR:HB3	1:A:381:LEU:HD12	1.77	0.66
1:A:202:LEU:HD12	1:A:203:GLU:N	2.10	0.66
1:A:75:LYS:O	1:A:79:ILE:HD12	1.93	0.66
1:A:177:PHE:HE2	1:A:197:ILE:HA	1.60	0.66
1:A:58:SER:O	1:A:59:GLU:C	2.33	0.66
1:A:215:ILE:HG22	1:A:216:GLY:N	2.10	0.66
1:A:83:ASN:HD21	1:A:92:LEU:HD12	1.60	0.66
1:A:517:THR:HG23	1:A:521:ARG:HA	1.78	0.66
1:A:288:GLU:O	1:A:290:GLY:N	2.26	0.66
1:A:294:ALA:HA	1:A:374:THR:HG22	1.76	0.66
1:A:131:MET:HA	1:A:526:TYR:HD2	1.61	0.66
1:A:117:SER:HA	1:A:541:SER:HA	1.79	0.65
1:A:369:GLU:O	1:A:371:LYS:N	2.23	0.65
1:A:259:PHE:O	1:A:262:SER:N	2.29	0.65
1:A:187:THR:HA	1:A:190:ILE:HD13	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:LEU:HD12	1:A:123:LEU:C	2.17	0.65
1:A:159:VAL:N	1:A:162:THR:HB	2.11	0.65
1:A:82:LEU:HB2	1:A:92:LEU:HD13	1.78	0.65
1:A:161:ASP:O	1:A:165:HIS:N	2.29	0.65
1:A:244:ALA:CB	1:A:484:PRO:HA	2.27	0.65
1:A:470:ASN:HB2	1:A:480:ARG:HB2	1.79	0.64
1:A:263:ARG:O	1:A:265:SER:N	2.31	0.64
1:A:158:THR:OG1	1:A:159:VAL:N	2.29	0.64
1:A:234:LEU:HD21	1:A:294:ALA:HB3	1.78	0.64
1:A:224:PHE:O	1:A:225:ARG:CB	2.45	0.64
1:A:292:ILE:HB	1:A:374:THR:HG23	1.78	0.64
1:A:131:MET:N	1:A:492:ASN:ND2	2.30	0.64
1:A:188:MET:O	1:A:192:LEU:HD23	1.97	0.64
1:A:226:LEU:HD21	1:A:241:THR:HG23	1.78	0.64
1:A:235:ILE:HD11	1:A:295:LEU:N	2.13	0.64
1:A:351:LEU:O	1:A:352:LYS:CB	2.39	0.64
1:A:397:LEU:HD22	1:A:398:LEU:H	1.62	0.63
1:A:416:ASP:HB2	1:A:512:GLN:OE1	1.98	0.63
1:A:179:LEU:HD22	1:A:192:LEU:HB3	1.80	0.63
1:A:98:ASN:HD22	1:A:99:ASN:N	1.97	0.63
1:A:125:THR:CG2	1:A:499:HIS:CE1	2.81	0.63
1:A:397:LEU:HD22	1:A:398:LEU:N	2.12	0.63
1:A:90:ASN:HB2	1:A:515:THR:OG1	1.99	0.62
1:A:115:GLU:O	1:A:116:ARG:HG2	1.99	0.62
1:A:147:VAL:HG11	1:A:200:ASN:ND2	2.13	0.62
1:A:115:GLU:C	1:A:117:SER:N	2.49	0.62
1:A:379:TRP:CZ2	1:A:383:TYR:HD2	2.18	0.62
1:A:125:THR:HG21	1:A:499:HIS:CE1	2.35	0.62
1:A:418:MET:HG3	1:A:436:VAL:HG13	1.82	0.62
1:A:440:LEU:HD12	1:A:440:LEU:H	1.63	0.62
1:A:517:THR:HG21	1:A:521:ARG:CG	2.27	0.61
1:A:83:ASN:ND2	1:A:92:LEU:CD1	2.63	0.61
1:A:83:ASN:ND2	1:A:92:LEU:HD12	2.15	0.61
1:A:239:VAL:HG13	1:A:476:GLN:HE22	1.65	0.61
1:A:187:THR:CG2	1:A:484:PRO:HD3	2.31	0.61
1:A:82:LEU:CD1	1:A:92:LEU:HD13	2.30	0.61
1:A:129:THR:HG22	1:A:527:VAL:HA	1.82	0.61
1:A:132:PRO:CD	1:A:526:TYR:HE2	2.08	0.61
1:A:379:TRP:HH2	1:A:396:THR:HG1	1.45	0.61
1:A:232:THR:HG23	1:A:234:LEU:H	1.66	0.61
1:A:466:THR:HG22	1:A:467:HIS:N	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:LYS:C	1:A:354:GLN:N	2.52	0.61
1:A:246:HIS:CE1	1:A:398:LEU:HD11	2.36	0.61
1:A:128:HIS:HB3	1:A:528:TYR:HD2	1.66	0.61
1:A:111:ILE:HG22	1:A:508:ILE:HB	1.83	0.60
1:A:287:LEU:HD12	1:A:379:TRP:HA	1.83	0.60
1:A:287:LEU:H	1:A:287:LEU:HD22	1.67	0.60
1:A:187:THR:HG23	1:A:484:PRO:HD3	1.83	0.60
1:A:82:LEU:CB	1:A:92:LEU:HD13	2.31	0.60
1:A:224:PHE:O	1:A:225:ARG:HB3	2.00	0.60
1:A:226:LEU:HG	1:A:241:THR:HG23	1.84	0.60
1:A:111:ILE:CG2	1:A:508:ILE:HB	2.32	0.60
1:A:177:PHE:CE2	1:A:197:ILE:HA	2.37	0.60
1:A:360:SER:C	1:A:362:SER:H	2.05	0.60
1:A:65:ASP:O	1:A:66:THR:HB	2.02	0.59
1:A:246:HIS:NE2	1:A:398:LEU:HD11	2.17	0.59
1:A:83:ASN:HD21	1:A:92:LEU:CD1	2.15	0.59
1:A:92:LEU:HD12	1:A:92:LEU:N	2.17	0.59
1:A:479:ILE:O	1:A:480:ARG:C	2.40	0.59
1:A:421:PRO:HG2	1:A:424:PHE:CD1	2.38	0.59
1:A:508:ILE:HG23	1:A:512:GLN:NE2	2.18	0.59
1:A:65:ASP:O	1:A:66:THR:CB	2.50	0.59
1:A:388:PRO:HB2	1:A:389:GLU:HG3	1.85	0.59
1:A:223:ASN:HB3	1:A:226:LEU:HD13	1.84	0.59
1:A:157:VAL:HB	1:A:158:THR:HG22	1.85	0.59
1:A:125:THR:CG2	1:A:499:HIS:HE1	2.15	0.59
1:A:399:THR:OG1	1:A:400:THR:N	2.34	0.59
1:A:277:GLN:O	1:A:278:GLU:HG2	2.02	0.59
1:A:107:SER:HB2	1:A:511:VAL:CG2	2.33	0.58
1:A:119:TRP:HB3	1:A:538:VAL:HA	1.85	0.58
1:A:193:MET:C	1:A:195:ASN:H	2.05	0.58
1:A:418:MET:CE	1:A:502:LEU:HB2	2.34	0.58
1:A:469:PHE:O	1:A:470:ASN:CB	2.51	0.58
1:A:417:MET:CE	1:A:534:VAL:HG11	2.33	0.58
1:A:392:ILE:H	1:A:392:ILE:HD12	1.67	0.58
1:A:122:GLN:HB2	1:A:501:THR:HG22	1.85	0.58
1:A:383:TYR:C	1:A:383:TYR:CD1	2.76	0.58
1:A:274:HIS:N	1:A:275:PRO:CD	2.67	0.58
1:A:267:LEU:HD12	1:A:267:LEU:O	2.03	0.58
1:A:478:LEU:N	1:A:478:LEU:HD22	2.19	0.57
1:A:395:TRP:CD1	1:A:396:THR:HG22	2.35	0.57
1:A:187:THR:O	1:A:188:MET:C	2.42	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ALA:HA	1:A:257:VAL:HA	1.87	0.57
1:A:108:THR:HG23	1:A:109:GLN:N	2.20	0.57
1:A:150:SER:HB3	1:A:171:LYS:CB	2.35	0.57
1:A:187:THR:O	1:A:189:THR:N	2.38	0.57
1:A:288:GLU:C	1:A:387:ASN:HD21	2.08	0.57
1:A:79:ILE:O	1:A:80:ALA:C	2.40	0.56
1:A:248:ASP:OD1	1:A:249:ILE:N	2.39	0.56
1:A:89:SER:CB	1:A:523:THR:HG22	2.35	0.56
1:A:184:PHE:HB3	1:A:188:MET:HB3	1.86	0.56
1:A:293:PRO:O	1:A:294:ALA:CB	2.52	0.56
1:A:133:ASN:HB3	1:A:183:ASN:HB2	1.87	0.56
1:A:417:MET:HB2	1:A:512:GLN:NE2	2.19	0.56
1:A:267:LEU:C	1:A:267:LEU:HD12	2.26	0.56
1:A:369:GLU:C	1:A:371:LYS:H	2.09	0.56
1:A:136:GLU:HA	1:A:141:ASN:HB3	1.87	0.56
1:A:226:LEU:HD23	1:A:227:GLY:N	2.18	0.55
1:A:150:SER:HB3	1:A:171:LYS:HB3	1.87	0.55
1:A:226:LEU:HG	1:A:241:THR:CG2	2.37	0.55
1:A:418:MET:C	1:A:420:ASP:H	2.10	0.55
1:A:234:LEU:CD2	1:A:294:ALA:HB3	2.36	0.55
1:A:111:ILE:CG2	1:A:111:ILE:O	2.55	0.55
1:A:92:LEU:HD12	1:A:92:LEU:H	1.71	0.55
1:A:427:THR:HG21	1:A:432:ASN:HB3	1.88	0.55
1:A:202:LEU:HB2	1:A:206:ARG:HH21	1.72	0.55
1:A:133:ASN:H	1:A:183:ASN:HB3	1.72	0.55
1:A:288:GLU:C	1:A:290:GLY:H	2.08	0.55
1:A:233:LYS:O	1:A:372:ILE:HG22	2.05	0.54
1:A:58:SER:O	1:A:60:LEU:N	2.40	0.54
1:A:272:LYS:HD2	1:A:280:PHE:HB2	1.89	0.54
1:A:379:TRP:HH2	1:A:396:THR:OG1	1.90	0.54
1:A:226:LEU:CD2	1:A:226:LEU:H	2.21	0.54
1:A:98:ASN:HD22	1:A:98:ASN:C	2.11	0.54
1:A:383:TYR:CA	1:A:392:ILE:HD13	2.37	0.54
1:A:197:ILE:HD12	1:A:217:VAL:O	2.08	0.54
1:A:143:PHE:CD1	1:A:143:PHE:O	2.60	0.54
1:A:147:VAL:CG2	1:A:148:MET:H	2.19	0.54
1:A:82:LEU:HB2	1:A:92:LEU:CD1	2.38	0.54
1:A:215:ILE:CG2	1:A:216:GLY:N	2.72	0.53
1:A:376:TYR:CD2	1:A:477:ILE:HG13	2.43	0.53
1:A:147:VAL:CG2	1:A:148:MET:N	2.70	0.53
1:A:230:PRO:O	1:A:233:LYS:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ARG:HD2	1:A:406:GLY:CA	2.34	0.53
1:A:178:ILE:N	1:A:178:ILE:CD1	2.65	0.53
1:A:177:PHE:HD2	1:A:196:ALA:O	1.92	0.53
1:A:467:HIS:HE1	2:P:20:GLU:HB3	1.73	0.53
1:A:414:LEU:HD13	1:A:417:MET:HB3	1.90	0.53
1:A:304:SER:O	1:A:351:LEU:HD13	2.09	0.53
1:A:383:TYR:C	1:A:383:TYR:HD1	2.11	0.53
1:A:387:ASN:O	1:A:388:PRO:C	2.46	0.53
1:A:218:LYS:O	1:A:250:VAL:HG23	2.08	0.53
1:A:132:PRO:HD2	1:A:526:TYR:CD2	2.44	0.52
1:A:226:LEU:CG	1:A:241:THR:HG23	2.38	0.52
1:A:417:MET:HG2	1:A:418:MET:SD	2.50	0.52
1:A:223:ASN:O	1:A:224:PHE:C	2.47	0.52
1:A:367:VAL:O	1:A:368:LEU:CB	2.52	0.52
1:A:136:GLU:HA	1:A:141:ASN:CB	2.40	0.52
1:A:418:MET:HG3	1:A:436:VAL:CG1	2.39	0.52
1:A:67:THR:O	1:A:536:PRO:HD2	2.10	0.52
1:A:293:PRO:O	1:A:373:ASN:CA	2.50	0.52
1:A:171:LYS:HZ2	1:A:172:TYR:H	1.58	0.52
1:A:107:SER:HB2	1:A:511:VAL:HG22	1.91	0.52
1:A:292:ILE:HG12	1:A:376:TYR:O	2.10	0.52
1:A:119:TRP:CB	1:A:537:ARG:O	2.57	0.52
1:A:246:HIS:ND1	1:A:247:PRO:O	2.43	0.52
1:A:144:LYS:HB2	1:A:258:ASP:HB3	1.91	0.52
1:A:113:PHE:CE1	1:A:536:PRO:CB	2.93	0.52
1:A:352:LYS:O	1:A:354:GLN:N	2.43	0.52
1:A:486:ILE:O	1:A:486:ILE:HG22	2.09	0.52
1:A:356:LEU:HD11	1:A:358:LYS:O	2.10	0.51
1:A:75:LYS:O	1:A:79:ILE:CD1	2.58	0.51
1:A:259:PHE:O	1:A:261:GLU:N	2.43	0.51
1:A:133:ASN:HB2	1:A:490:SER:OG	2.11	0.51
1:A:198:ILE:C	1:A:200:ASN:H	2.12	0.51
1:A:78:ASP:OD1	1:A:94:THR:HG23	2.09	0.51
1:A:216:GLY:HA2	1:A:252:LEU:HB2	1.90	0.51
1:A:223:ASN:HD22	1:A:223:ASN:C	2.12	0.51
1:A:417:MET:HE3	1:A:534:VAL:HG11	1.93	0.51
1:A:90:ASN:CB	1:A:515:THR:OG1	2.58	0.51
1:A:433:TYR:O	1:A:434:PRO:C	2.49	0.51
1:A:61:SER:O	1:A:62:PRO:C	2.49	0.51
1:A:353:ILE:O	1:A:355:PRO:HD3	2.11	0.51
1:A:475:ASN:O	1:A:477:ILE:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:GLY:HA3	1:A:53:ASN:ND2	2.25	0.51
1:A:441:MET:C	1:A:443:VAL:H	2.14	0.51
1:A:263:ARG:C	1:A:265:SER:N	2.64	0.50
1:A:250:VAL:HG13	1:A:378:SER:HB2	1.93	0.50
1:A:288:GLU:O	1:A:387:ASN:ND2	2.44	0.50
1:A:135:ASN:OD1	1:A:137:TYR:N	2.43	0.50
1:A:280:PHE:CD1	1:A:280:PHE:O	2.65	0.50
1:A:224:PHE:CG	1:A:292:ILE:HD12	2.47	0.50
1:A:143:PHE:HE2	1:A:219:PHE:HZ	1.52	0.50
1:A:78:ASP:O	1:A:79:ILE:O	2.29	0.50
1:A:143:PHE:CE2	1:A:219:PHE:HZ	2.29	0.50
1:A:189:THR:O	1:A:192:LEU:HB2	2.12	0.50
1:A:126:ILE:HD11	1:A:496:LEU:HD13	1.93	0.50
1:A:294:ALA:O	1:A:295:LEU:CB	2.60	0.50
1:A:114:ASP:H	1:A:119:TRP:HZ2	1.59	0.50
1:A:383:TYR:CE1	1:A:393:ARG:HG3	2.47	0.50
1:A:429:GLN:HA	1:A:429:GLN:NE2	2.14	0.50
1:A:203:GLU:C	1:A:204:ILE:HD12	2.32	0.50
1:A:258:ASP:C	1:A:258:ASP:OD1	2.49	0.50
1:A:383:TYR:HA	1:A:392:ILE:CD1	2.40	0.50
1:A:83:ASN:OD1	1:A:85:GLN:OE1	2.30	0.49
1:A:143:PHE:CE2	1:A:219:PHE:CZ	2.95	0.49
1:A:185:SER:O	1:A:186:ALA:C	2.50	0.49
1:A:414:LEU:HG	1:A:436:VAL:HG21	1.93	0.49
1:A:304:SER:HB2	1:A:351:LEU:HB2	1.94	0.49
1:A:235:ILE:HD12	1:A:293:PRO:HB2	1.91	0.49
1:A:132:PRO:CD	1:A:526:TYR:CD2	2.96	0.49
1:A:294:ALA:HA	1:A:374:THR:CG2	2.43	0.49
1:A:352:LYS:O	1:A:353:ILE:C	2.51	0.49
1:A:219:PHE:CD2	1:A:249:ILE:HG22	2.48	0.49
1:A:134:VAL:HG23	1:A:134:VAL:O	2.13	0.49
1:A:82:LEU:HD13	1:A:92:LEU:HD13	1.95	0.49
1:A:235:ILE:HD13	1:A:235:ILE:H	1.77	0.49
1:A:239:VAL:HG13	1:A:476:GLN:NE2	2.27	0.49
1:A:295:LEU:HD23	1:A:296:LEU:O	2.13	0.49
1:A:517:THR:CG2	1:A:521:ARG:CG	2.88	0.49
1:A:234:LEU:HD11	1:A:355:PRO:HB3	1.94	0.48
1:A:292:ILE:HB	1:A:374:THR:CG2	2.43	0.48
1:A:534:VAL:O	1:A:534:VAL:HG13	2.13	0.48
1:A:244:ALA:HB1	1:A:484:PRO:HA	1.95	0.48
1:A:359:ASP:CG	1:A:360:SER:N	2.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:PHE:HA	1:A:105:GLU:OE2	2.13	0.48
1:A:135:ASN:ND2	1:A:138:MET:H	2.10	0.48
1:A:201:TYR:CD2	1:A:202:LEU:N	2.82	0.48
1:A:106:ALA:O	1:A:109:GLN:HG2	2.13	0.48
1:A:226:LEU:H	1:A:226:LEU:HD22	1.78	0.48
1:A:226:LEU:CD2	1:A:226:LEU:N	2.77	0.48
1:A:472:PHE:CD1	1:A:478:LEU:HB3	2.47	0.48
1:A:270:ILE:HD11	1:A:379:TRP:CG	2.47	0.48
1:A:363:ARG:HB2	1:A:475:ASN:HD21	1.77	0.48
1:A:540:SER:O	1:A:541:SER:CB	2.62	0.48
1:A:53:ASN:ND2	1:A:53:ASN:H	2.12	0.48
1:A:396:THR:OG1	1:A:397:LEU:N	2.45	0.48
1:A:160:ASN:H	1:A:160:ASN:ND2	2.12	0.48
1:A:253:PRO:HA	1:A:284:TYR:CG	2.49	0.48
1:A:60:LEU:O	1:A:61:SER:C	2.52	0.48
1:A:301:TYR:HE2	1:A:352:LYS:HZ2	1.59	0.48
1:A:236:MET:HA	1:A:296:LEU:CD2	2.44	0.47
1:A:367:VAL:O	1:A:373:ASN:O	2.32	0.47
1:A:135:ASN:ND2	1:A:138:MET:N	2.62	0.47
1:A:467:HIS:CE1	2:P:20:GLU:HB3	2.49	0.47
1:A:108:THR:HG23	1:A:109:GLN:H	1.79	0.47
1:A:88:HIS:CD2	1:A:528:TYR:O	2.67	0.47
1:A:352:LYS:C	1:A:354:GLN:H	2.15	0.47
1:A:417:MET:HE1	1:A:534:VAL:HG11	1.97	0.47
1:A:469:PHE:O	1:A:470:ASN:HB3	2.14	0.47
1:A:119:TRP:HA	1:A:539:LEU:CD1	2.44	0.47
1:A:69:LEU:HA	1:A:69:LEU:HD23	1.55	0.47
1:A:96:VAL:HG21	1:A:106:ALA:HB1	1.97	0.47
1:A:457:GLN:NE2	1:A:480:ARG:HG2	2.30	0.47
1:A:301:TYR:HA	1:A:351:LEU:O	2.15	0.47
1:A:477:ILE:HG22	1:A:478:LEU:HD22	1.97	0.47
1:A:116:ARG:O	1:A:117:SER:HB3	2.15	0.47
1:A:392:ILE:CD1	1:A:392:ILE:N	2.64	0.47
1:A:56:ARG:O	1:A:57:TYR:CB	2.59	0.47
1:A:76:SER:HA	1:A:79:ILE:CD1	2.45	0.47
1:A:435:VAL:HG12	1:A:437:GLY:N	2.29	0.47
1:A:67:THR:OG1	1:A:68:LYS:N	2.47	0.47
1:A:122:GLN:CB	1:A:501:THR:HG22	2.45	0.47
1:A:511:VAL:O	1:A:511:VAL:HG23	2.15	0.47
1:A:69:LEU:HD22	1:A:95:VAL:HG22	1.96	0.46
1:A:252:LEU:HD22	1:A:253:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:GLY:HA2	1:A:504:LEU:HG	1.96	0.46
1:A:234:LEU:CD1	1:A:355:PRO:HB3	2.45	0.46
1:A:264:LEU:O	1:A:267:LEU:HB3	2.15	0.46
1:A:267:LEU:C	1:A:269:GLY:H	2.19	0.46
1:A:417:MET:CA	1:A:512:GLN:HE22	2.28	0.46
1:A:258:ASP:OD1	1:A:259:PHE:N	2.48	0.46
1:A:89:SER:HA	1:A:516:VAL:HG12	1.97	0.46
1:A:252:LEU:HG	1:A:376:TYR:HE1	1.81	0.46
1:A:508:ILE:CG2	1:A:512:GLN:HE21	2.26	0.46
1:A:440:LEU:N	1:A:440:LEU:HD12	2.29	0.46
1:A:135:ASN:HD21	1:A:138:MET:N	2.14	0.46
1:A:114:ASP:OD1	1:A:115:GLU:N	2.49	0.46
1:A:138:MET:HB3	1:A:263:ARG:HH22	1.80	0.46
1:A:91:PHE:C	1:A:92:LEU:HG	2.35	0.46
1:A:417:MET:N	1:A:512:GLN:HE22	2.14	0.46
1:A:119:TRP:HD1	1:A:119:TRP:N	2.12	0.46
1:A:466:THR:HG22	1:A:468:VAL:N	2.31	0.46
1:A:478:LEU:H	1:A:478:LEU:HD22	1.80	0.45
1:A:414:LEU:HD11	1:A:418:MET:HG2	1.98	0.45
1:A:195:ASN:O	1:A:198:ILE:N	2.49	0.45
1:A:57:TYR:O	1:A:58:SER:C	2.54	0.45
1:A:215:ILE:HG22	1:A:216:GLY:H	1.80	0.45
1:A:233:LYS:HB2	1:A:372:ILE:CG2	2.40	0.45
1:A:235:ILE:CD1	1:A:235:ILE:N	2.68	0.45
1:A:273:ARG:NH2	1:A:397:LEU:HD23	2.31	0.45
1:A:196:ALA:HA	1:A:199:ASP:CB	2.37	0.45
1:A:161:ASP:O	1:A:165:HIS:HB2	2.16	0.45
1:A:418:MET:HE3	1:A:502:LEU:HB2	1.97	0.45
1:A:259:PHE:O	1:A:260:THR:C	2.54	0.45
1:A:202:LEU:HD12	1:A:203:GLU:H	1.77	0.45
1:A:193:MET:C	1:A:195:ASN:N	2.68	0.45
1:A:134:VAL:HG21	1:A:184:PHE:CE2	2.52	0.45
1:A:148:MET:HE2	1:A:172:TYR:HE1	1.82	0.45
1:A:387:ASN:HA	1:A:388:PRO:HD2	1.61	0.45
1:A:137:TYR:HE1	1:A:522:ARG:CZ	2.30	0.45
1:A:269:GLY:C	1:A:399:THR:HG23	2.37	0.45
1:A:98:ASN:HD22	1:A:100:ASP:H	1.64	0.45
1:A:131:MET:HA	1:A:526:TYR:CD2	2.47	0.45
1:A:405:CYS:O	1:A:405:CYS:SG	2.75	0.45
1:A:63:LEU:HD13	1:A:64:TYR:N	2.32	0.45
1:A:252:LEU:CG	1:A:376:TYR:HE1	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ASN:OD1	1:A:136:GLU:N	2.50	0.45
1:A:413:SER:HB2	1:A:433:TYR:O	2.16	0.45
1:A:392:ILE:HA	1:A:395:TRP:HB3	1.98	0.45
1:A:83:ASN:ND2	1:A:92:LEU:HD11	2.32	0.45
1:A:370:ASP:HB2	1:A:372:ILE:CD1	2.42	0.44
1:A:248:ASP:OD2	1:A:378:SER:OG	2.35	0.44
1:A:466:THR:HB	1:A:468:VAL:HG22	1.99	0.44
1:A:224:PHE:CB	1:A:292:ILE:HD12	2.48	0.44
1:A:236:MET:HA	1:A:296:LEU:HD22	1.99	0.44
1:A:433:TYR:O	1:A:434:PRO:O	2.35	0.44
1:A:464:SER:C	1:A:466:THR:H	2.19	0.44
1:A:363:ARG:HD3	1:A:475:ASN:CG	2.38	0.44
1:A:263:ARG:O	1:A:264:LEU:C	2.55	0.44
1:A:248:ASP:OD2	1:A:380:TYR:CB	2.63	0.44
1:A:466:THR:CG2	1:A:467:HIS:N	2.80	0.44
1:A:277:GLN:O	1:A:278:GLU:CG	2.65	0.44
1:A:170:LEU:HD13	1:A:170:LEU:N	2.32	0.44
1:A:252:LEU:HD21	1:A:376:TYR:CE1	2.52	0.44
1:A:136:GLU:HG3	1:A:137:TYR:N	2.33	0.44
1:A:493:VAL:HG22	1:A:494:PRO:N	2.32	0.44
1:A:227:GLY:C	1:A:235:ILE:HG22	2.38	0.44
1:A:133:ASN:CB	1:A:490:SER:OG	2.66	0.44
1:A:276:PHE:C	1:A:277:GLN:HG3	2.38	0.44
1:A:125:THR:CG2	1:A:412:TRP:CZ3	3.01	0.44
1:A:201:TYR:O	1:A:205:GLY:N	2.40	0.44
1:A:107:SER:HB2	1:A:511:VAL:HG21	2.00	0.44
1:A:496:LEU:HD23	1:A:496:LEU:N	2.32	0.44
1:A:435:VAL:CG2	1:A:521:ARG:NH2	2.73	0.44
1:A:498:ASP:OD1	1:A:498:ASP:C	2.56	0.44
1:A:137:TYR:CE1	1:A:522:ARG:CZ	3.01	0.44
1:A:474:GLU:CD	1:A:474:GLU:N	2.72	0.44
1:A:89:SER:HA	1:A:516:VAL:CG1	2.48	0.43
1:A:90:ASN:ND2	1:A:513:ARG:HH21	2.15	0.43
1:A:111:ILE:HG22	1:A:111:ILE:O	2.18	0.43
1:A:414:LEU:HD12	1:A:414:LEU:C	2.39	0.43
1:A:219:PHE:CD2	1:A:249:ILE:CG2	3.02	0.43
1:A:239:VAL:HG22	1:A:476:GLN:NE2	2.33	0.43
1:A:159:VAL:H	1:A:162:THR:CB	2.30	0.43
2:P:17:TYR:O	2:P:18:ASP:HB2	2.18	0.43
1:A:520:ARG:HG3	1:A:522:ARG:NE	2.33	0.43
1:A:85:GLN:O	1:A:86:ASN:ND2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:GLY:O	1:A:52:ARG:HD3	2.18	0.43
1:A:475:ASN:O	1:A:476:GLN:C	2.56	0.43
1:A:198:ILE:O	1:A:200:ASN:N	2.51	0.43
1:A:146:ARG:HB3	1:A:174:TRP:CE3	2.53	0.43
1:A:152:LYS:C	1:A:169:ILE:HG22	2.39	0.43
1:A:353:ILE:HG13	1:A:353:ILE:H	1.60	0.43
1:A:138:MET:HB3	1:A:263:ARG:NH2	2.34	0.43
1:A:246:HIS:CE1	1:A:398:LEU:CD1	3.02	0.43
1:A:198:ILE:C	1:A:200:ASN:N	2.72	0.43
1:A:72:VAL:HG12	1:A:73:ASP:H	1.84	0.43
1:A:69:LEU:HD22	1:A:95:VAL:CG2	2.49	0.43
1:A:124:LYS:HB2	1:A:533:ILE:CD1	2.48	0.43
1:A:298:VAL:HG22	1:A:299:THR:N	2.33	0.43
1:A:376:TYR:CD2	1:A:477:ILE:CG1	3.02	0.42
1:A:133:ASN:HB3	1:A:183:ASN:CB	2.49	0.42
1:A:474:GLU:OE1	1:A:474:GLU:N	2.52	0.42
1:A:132:PRO:HA	1:A:183:ASN:HB3	2.00	0.42
1:A:518:ASP:O	1:A:521:ARG:HA	2.20	0.42
1:A:102:THR:O	1:A:105:GLU:HG2	2.19	0.42
1:A:403:VAL:HG22	1:A:488:THR:HB	1.94	0.42
1:A:125:THR:HG21	1:A:412:TRP:CZ3	2.55	0.42
1:A:249:ILE:HD12	1:A:257:VAL:HG11	2.01	0.42
1:A:214:ASP:HA	1:A:252:LEU:CD1	2.49	0.42
1:A:64:TYR:O	1:A:65:ASP:CB	2.67	0.42
1:A:124:LYS:HB2	1:A:533:ILE:HD13	2.01	0.42
1:A:111:ILE:HG22	1:A:508:ILE:CB	2.47	0.42
1:A:143:PHE:C	1:A:143:PHE:CD1	2.89	0.42
1:A:203:GLU:HB3	1:A:204:ILE:HD12	2.01	0.42
1:A:235:ILE:H	1:A:235:ILE:CD1	2.32	0.42
1:A:263:ARG:O	1:A:266:ASN:N	2.51	0.42
1:A:113:PHE:HE1	1:A:536:PRO:CB	2.31	0.42
1:A:115:GLU:HB3	1:A:116:ARG:H	1.10	0.42
1:A:164:ASP:HA	1:A:167:GLU:HG2	2.00	0.42
1:A:235:ILE:HD11	1:A:293:PRO:HB2	1.98	0.42
1:A:355:PRO:O	1:A:356:LEU:C	2.56	0.42
1:A:416:ASP:O	1:A:512:GLN:NE2	2.46	0.42
1:A:435:VAL:HG12	1:A:437:GLY:H	1.84	0.42
1:A:126:ILE:HG13	1:A:496:LEU:HD22	2.02	0.42
1:A:371:LYS:C	1:A:372:ILE:HG13	2.39	0.41
1:A:218:LYS:HE2	1:A:220:ASP:HB2	2.01	0.41
1:A:388:PRO:HB2	1:A:389:GLU:H	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:GLU:H	1:A:389:GLU:HG3	1.66	0.41
1:A:486:ILE:O	1:A:486:ILE:CG2	2.69	0.41
1:A:418:MET:C	1:A:420:ASP:N	2.73	0.41
1:A:427:THR:OG1	1:A:428:ARG:N	2.53	0.41
1:A:133:ASN:H	1:A:183:ASN:CB	2.31	0.41
1:A:111:ILE:HA	1:A:111:ILE:HD12	1.85	0.41
1:A:273:ARG:HH21	1:A:397:LEU:HD23	1.86	0.41
1:A:257:VAL:HG13	1:A:257:VAL:O	2.20	0.41
1:A:190:ILE:HG22	1:A:191:ASP:N	2.35	0.41
1:A:151:ARG:C	1:A:152:LYS:HG3	2.40	0.41
1:A:134:VAL:HG23	1:A:181:GLU:HA	2.01	0.41
1:A:350:GLU:CD	1:A:350:GLU:H	2.23	0.41
1:A:349:LYS:C	1:A:351:LEU:HG	2.41	0.41
1:A:479:ILE:O	1:A:481:PRO:N	2.54	0.41
1:A:360:SER:C	1:A:362:SER:N	2.72	0.41
1:A:475:ASN:O	1:A:478:LEU:N	2.54	0.41
1:A:131:MET:CE	1:A:138:MET:HG2	2.50	0.41
1:A:273:ARG:C	1:A:275:PRO:CD	2.89	0.41
1:A:169:ILE:HA	1:A:169:ILE:HD12	1.91	0.41
1:A:295:LEU:HD23	1:A:296:LEU:N	2.35	0.41
1:A:240:TYR:CE2	1:A:295:LEU:HD12	2.56	0.41
1:A:519:ALA:C	1:A:521:ARG:H	2.23	0.41
1:A:232:THR:O	1:A:233:LYS:HB2	2.20	0.41
1:A:220:ASP:N	1:A:248:ASP:O	2.48	0.41
1:A:150:SER:HB3	1:A:171:LYS:HB2	2.01	0.41
1:A:252:LEU:HG	1:A:376:TYR:CE1	2.55	0.41
1:A:283:MET:O	1:A:284:TYR:C	2.58	0.41
1:A:263:ARG:C	1:A:265:SER:H	2.24	0.40
1:A:414:LEU:HD11	1:A:417:MET:HB3	1.97	0.40
1:A:442:PRO:HD2	1:A:443:VAL:HG23	2.04	0.40
1:A:194:ASN:HD21	1:A:219:PHE:N	2.18	0.40
1:A:223:ASN:HD21	1:A:385:TYR:HE2	1.68	0.40
1:A:380:TYR:CE1	1:A:384:ASN:ND2	2.89	0.40
1:A:419:GLN:O	1:A:420:ASP:HB2	2.21	0.40
1:A:57:TYR:CE1	1:A:58:SER:HB3	2.57	0.40
1:A:379:TRP:CZ2	1:A:383:TYR:CD2	3.05	0.40
1:A:427:THR:HG21	1:A:432:ASN:HD22	1.87	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	451/509 (89%)	320 (71%)	81 (18%)	50 (11%)	0 10
2	P	8/21 (38%)	5 (62%)	2 (25%)	1 (12%)	0 8
All	All	459/530 (87%)	325 (71%)	83 (18%)	51 (11%)	0 10

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	THR
1	A	57	TYR
1	A	59	GLU
1	A	66	THR
1	A	79	ILE
1	A	117	SER
1	A	143	PHE
1	A	188	MET
1	A	242	TYR
1	A	260	THR
1	A	275	PRO
1	A	278	GLU
1	A	351	LEU
1	A	352	LYS
1	A	368	LEU
1	A	370	ASP
1	A	388	PRO
1	A	392	ILE
1	A	415	PRO
1	A	434	PRO
1	A	470	ASN
1	A	519	ALA
1	A	541	SER
1	A	58	SER
1	A	222	ARG

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Mol	Chain	Res	Type
1	A	225	ARG
1	A	264	LEU
1	A	289	GLY
1	A	294	ALA
1	A	405	CYS
1	A	430	VAL
1	A	476	GLN
1	A	152	LYS
1	A	199	ASP
1	A	241	THR
1	A	423	THR
1	A	453	ALA
1	A	521	ARG
1	A	62	PRO
1	A	295	LEU
1	A	420	ASP
1	A	87	ASP
1	A	145	ALA
1	A	379	TRP
1	A	419	GLN
1	A	190	ILE
1	A	372	ILE
1	A	481	PRO
1	A	367	VAL
2	P	14	VAL
1	A	159	VAL

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	412/457 (90%)	276 (67%)	136 (33%)	0 3
2	P	10/20 (50%)	10 (100%)	0	100 100
All	All	422/477 (88%)	286 (68%)	136 (32%)	0 3

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ARG
1	A	54	SER
1	A	57	TYR
1	A	59	GLU
1	A	63	LEU
1	A	64	TYR
1	A	65	ASP
1	A	67	THR
1	A	71	LEU
1	A	72	VAL
1	A	75	LYS
1	A	76	SER
1	A	82	LEU
1	A	85	GLN
1	A	92	LEU
1	A	96	VAL
1	A	98	ASN
1	A	100	ASP
1	A	102	THR
1	A	104	THR
1	A	107	SER
1	A	110	THR
1	A	112	ASN
1	A	116	ARG
1	A	119	TRP
1	A	123	LEU
1	A	126	ILE
1	A	130	ASN
1	A	131	MET
1	A	133	ASN
1	A	135	ASN
1	A	139	PHE
1	A	143	PHE
1	A	149	VAL
1	A	157	VAL
1	A	158	THR
1	A	160	ASN
1	A	161	ASP
1	A	163	TYR
1	A	164	ASP
1	A	170	LEU
1	A	177	PHE
1	A	178	ILE

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Mol	Chain	Res	Type
1	A	189	THR
1	A	191	ASP
1	A	193	MET
1	A	194	ASN
1	A	197	ILE
1	A	199	ASP
1	A	200	ASN
1	A	202	LEU
1	A	207	GLN
1	A	211	LEU
1	A	212	GLU
1	A	214	ASP
1	A	215	ILE
1	A	220	ASP
1	A	221	THR
1	A	222	ARG
1	A	223	ASN
1	A	226	LEU
1	A	228	TRP
1	A	229	ASP
1	A	231	GLU
1	A	232	THR
1	A	235	ILE
1	A	241	THR
1	A	242	TYR
1	A	243	GLU
1	A	249	ILE
1	A	250	VAL
1	A	255	CYS
1	A	261	GLU
1	A	267	LEU
1	A	270	ILE
1	A	273	ARG
1	A	285	GLU
1	A	287	LEU
1	A	288	GLU
1	A	296	LEU
1	A	298	VAL
1	A	301	TYR
1	A	349	LYS
1	A	351	LEU
1	A	354	GLN

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Mol	Chain	Res	Type
1	A	363	ARG
1	A	366	ASN
1	A	372	ILE
1	A	374	THR
1	A	376	TYR
1	A	380	TYR
1	A	383	TYR
1	A	384	ASN
1	A	389	GLU
1	A	390	LYS
1	A	392	ILE
1	A	396	THR
1	A	399	THR
1	A	400	THR
1	A	401	SER
1	A	402	ASP
1	A	403	VAL
1	A	408	GLU
1	A	410	VAL
1	A	412	TRP
1	A	417	MET
1	A	429	GLN
1	A	430	VAL
1	A	439	GLU
1	A	440	LEU
1	A	451	GLU
1	A	460	ARG
1	A	461	GLN
1	A	468	VAL
1	A	469	PHE
1	A	472	PHE
1	A	474	GLU
1	A	477	ILE
1	A	478	LEU
1	A	485	THR
1	A	486	ILE
1	A	487	THR
1	A	488	THR
1	A	492	ASN
1	A	496	LEU
1	A	497	THR
1	A	504	LEU

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Mol	Chain	Res	Type
1	A	514	VAL
1	A	518	ASP
1	A	520	ARG
1	A	521	ARG
1	A	522	ARG
1	A	523	THR
1	A	533	ILE
1	A	538	VAL
1	A	539	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	83	ASN
1	A	86	ASN
1	A	88	HIS
1	A	90	ASN
1	A	98	ASN
1	A	130	ASN
1	A	141	ASN
1	A	160	ASN
1	A	200	ASN
1	A	207	GLN
1	A	223	ASN
1	A	354	GLN
1	A	366	ASN
1	A	387	ASN
1	A	429	GLN
1	A	432	ASN
1	A	461	GLN
1	A	476	GLN
1	A	492	ASN
1	A	499	HIS
1	A	512	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 1 ligands modelled in this entry, 1 is 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	455/509 (89%)	0.25	25 (5%) 29 19	13, 61, 170, 199	0
2	P	10/21 (47%)	6.20	10 (100%) 0 0	151, 160, 163, 163	10 (100%)
All	All	465/530 (87%)	0.38	35 (7%) 17 11	13, 61, 169, 199	10 (2%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	21	CYS	10.5
2	P	19	THR	10.0
2	P	14	VAL	9.3
1	A	307	ASP	7.6
2	P	13	PRO	6.7
2	P	16	PRO	5.5
2	P	20	GLU	5.5
2	P	12	ASN	4.8
1	A	306	LYS	4.7
1	A	447	SER	4.6
1	A	243	GLU	4.3
2	P	17	TYR	4.3
1	A	465	LEU	4.3
1	A	464	SER	4.1
1	A	454	VAL	4.0
2	P	15	TYR	3.2
1	A	460	ARG	2.9
1	A	161	ASP	2.8
1	A	155	GLU	2.7
1	A	457	GLN	2.7
1	A	295	LEU	2.6
1	A	441	MET	2.6
1	A	461	GLN	2.5
1	A	453	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	121	GLY	2.4
1	A	83	ASN	2.4
1	A	156	GLY	2.3
1	A	425	ARG	2.2
1	A	261	GLU	2.2
2	P	18	ASP	2.2
1	A	56	ARG	2.1
1	A	448	PHE	2.1
1	A	294	ALA	2.1
1	A	303	GLU	2.1
1	A	162	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	CA	A	999	1/1	0.91	0.26	-	72,72,72,72	1

6.5 Other polymers (i)

There are no such residues in this entry.