Full wwPDB X-ray Structure Validation Report ⓘ

Feb 10, 2024 – 07:13 PM EST

PDB ID	:	2PKG
Title	:	Structure of a complex between the A subunit of protein phosphatase 2A and the small t antigen of SV40
Authors	:	Jeffrey, P.D.; Shi, Y.
Deposited on	:	2007-04-17
Resolution	:	3.30 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:

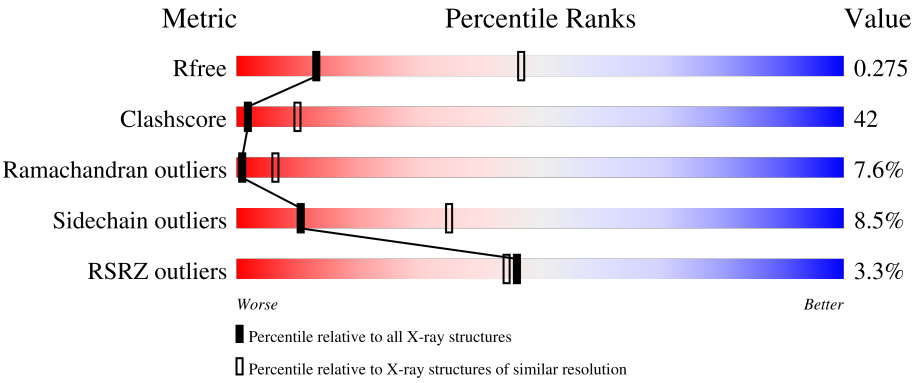
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	580	6% 34% 56% 10%
1	B	580	% 40% 49% 10%
2	C	88	43% 41% 7% 9%
2	D	88	% 47% 34% 10% 9%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10358 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 Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	579	Total	C	N	O	S	0	0	0
			4515	2871	761	856	27			
1	B	579	Total	C	N	O	S	0	0	0
			4515	2871	761	856	27			

- Molecule 2 is a protein called Small T antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	80	Total	C	N	O	S	0	0	0
			662	427	111	110	14			
2	D	80	Total	C	N	O	S	0	0	0
			662	427	111	110	14			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	2	Total	Zn	0	0
			2	2		
3	D	2	Total	Zn	0	0
			2	2		

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: Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform

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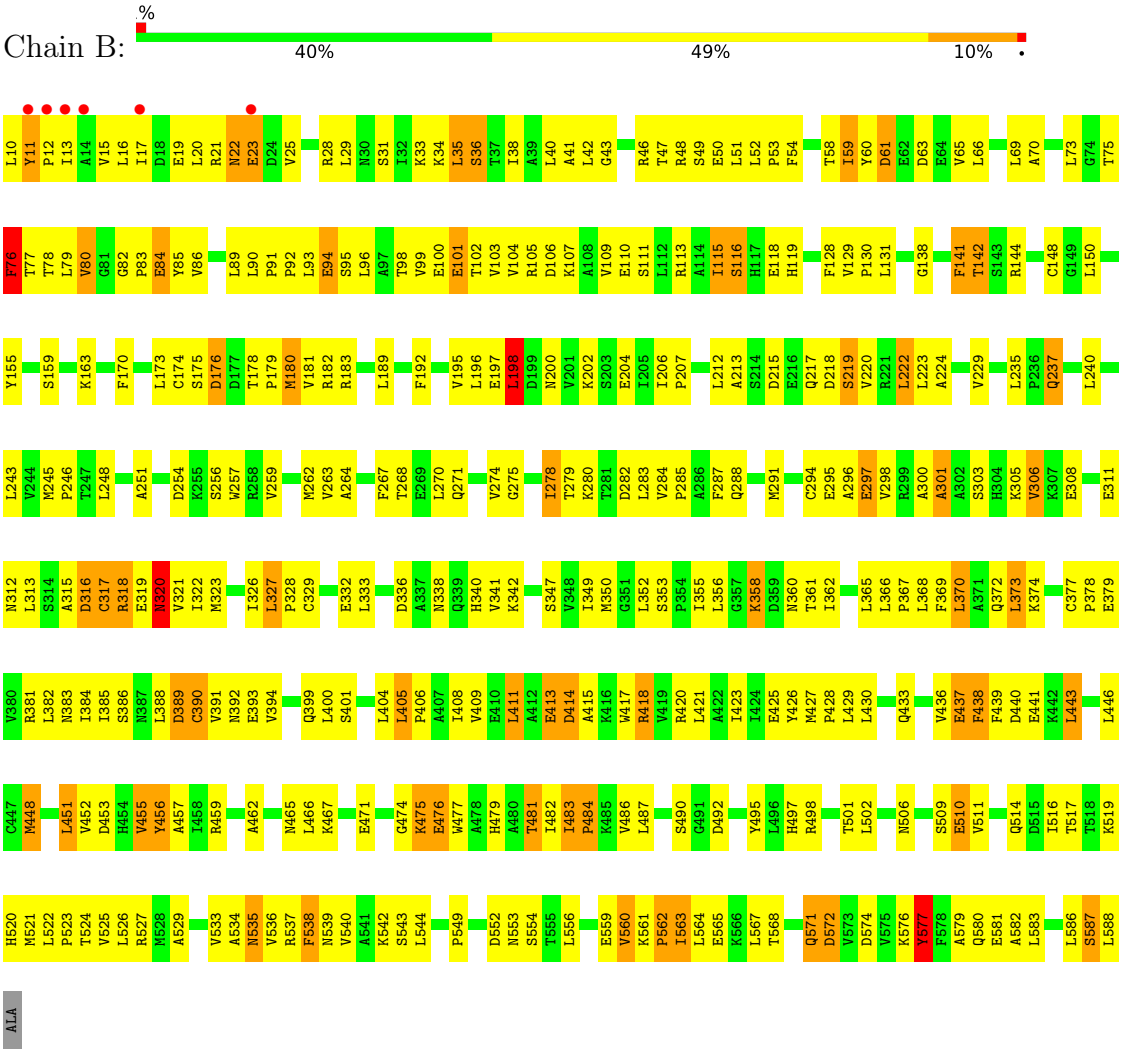
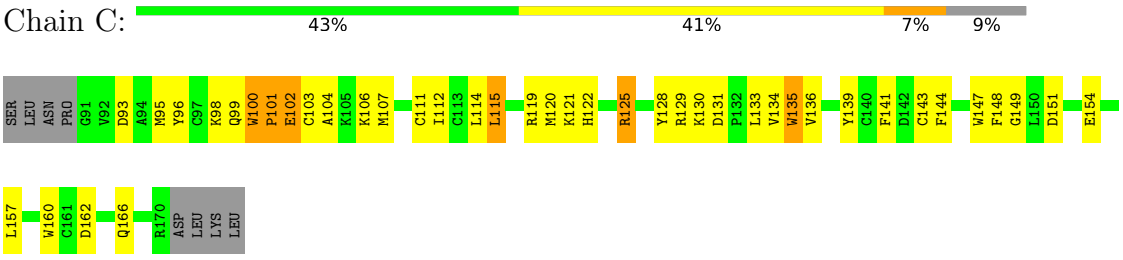
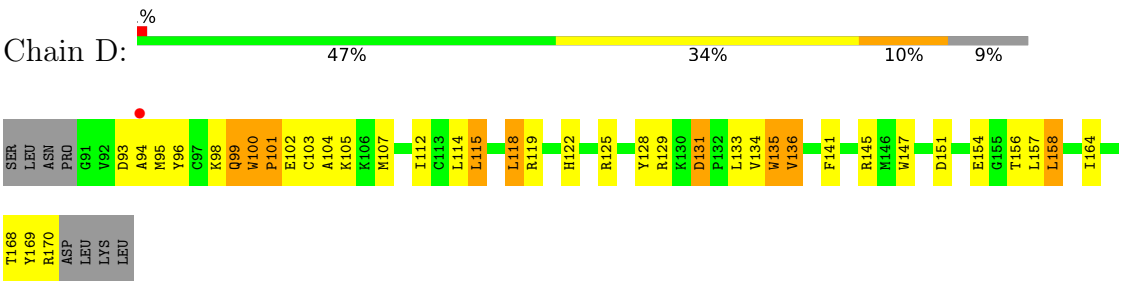


• Molecule 2: Small T antigen



• Molecule 2: Small T antigen



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	137.70Å 147.79Å 209.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.40 – 3.30 60.40 – 3.30	Depositor EDS
% Data completeness (in resolution range)	94.9 (60.40-3.30) 95.0 (60.40-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.82 (at 3.33Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.247 , 0.312 0.222 , 0.275	Depositor DCC
R_{free} test set	1561 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	88.0	Xtriage
Anisotropy	0.589	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 85.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10358	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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, 0.333 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: ZN

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	0.44	0/4589	0.69	0/6231
1	B	0.52	1/4589 (0.0%)	0.72	0/6231
2	C	0.56	0/679	0.71	0/915
2	D	0.52	0/679	0.69	0/915
All	All	0.49	1/10536 (0.0%)	0.70	0/14292

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	174	CYS	CB-SG	-5.23	1.73	1.81

There are no bond angle outliers.

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	4515	0	4623	410	0
1	B	4515	0	4623	394	0
2	C	662	0	649	48	0
2	D	662	0	649	42	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10358	0	10544	886	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 42.

All (886) 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:278:ILE:HD12	1:B:278:ILE:H	1.10	1.10
1:B:94:GLU:HB2	1:B:131:LEU:HD11	1.32	1.05
1:B:222:LEU:HD22	1:B:223:LEU:HD23	1.40	1.00
1:A:496:LEU:HA	1:A:499:MET:HE3	1.42	1.00
1:A:353:SER:HB3	1:A:394:VAL:HG21	1.39	0.99
1:B:428:PRO:HD3	1:B:465:ASN:HD21	1.26	0.99
1:A:58:THR:HG22	1:A:59:ILE:H	1.29	0.98
1:A:487:LEU:HD11	1:A:520:HIS:O	1.66	0.96
1:B:350:MET:HE3	1:B:384:ILE:HG23	1.47	0.94
1:B:77:THR:HG21	1:B:118:GLU:HG3	1.48	0.93
1:B:338:ASN:HD21	1:B:340:HIS:HB2	1.34	0.92
1:A:206:ILE:HG21	1:A:243:LEU:HD22	1.50	0.91
1:B:347:SER:HB3	1:B:383:ASN:HD22	1.35	0.91
1:B:338:ASN:HD22	1:B:341:VAL:H	1.16	0.90
1:B:303:SER:O	1:B:306:VAL:HG23	1.68	0.90
1:A:47:THR:O	1:A:51:LEU:HB3	1.71	0.89
1:A:278:ILE:HD12	1:A:278:ILE:H	1.35	0.89
1:A:561:LYS:HD2	1:A:588:LEU:HD22	1.56	0.87
1:A:334:VAL:HG21	1:A:368:LEU:HD22	1.55	0.87
1:B:392:ASN:HB2	1:B:400:LEU:HD22	1.56	0.86
1:A:120:SER:H	1:A:123:ASP:HB2	1.39	0.86
1:B:58:THR:HG22	1:B:59:ILE:H	1.41	0.86
1:A:362:ILE:HA	1:A:366:LEU:HD13	1.58	0.84
1:B:561:LYS:O	1:B:565:GLU:HG2	1.78	0.84
1:A:25:VAL:HG22	1:A:28:ARG:HH22	1.42	0.83
1:A:561:LYS:O	1:A:565:GLU:HG2	1.77	0.83
1:B:428:PRO:HD3	1:B:465:ASN:ND2	1.94	0.82
1:B:47:THR:O	1:B:51:LEU:HB3	1.80	0.82
1:B:278:ILE:HD12	1:B:278:ILE:N	1.93	0.81
1:B:373:LEU:HD22	1:B:384:ILE:HG21	1.61	0.81
1:B:222:LEU:HD22	1:B:223:LEU:CD2	2.11	0.81
1:A:425:GLU:OE2	1:B:418:ARG:NH1	2.14	0.81
1:B:537:ARG:O	1:B:540:VAL:HG12	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:MET:HE3	1:A:180:MET:H	1.47	0.79
1:B:113:ARG:O	1:B:116:SER:HB3	1.82	0.79
1:A:102:THR:HG22	1:A:105:ARG:NH2	1.96	0.79
1:B:20:LEU:O	1:B:28:ARG:HD3	1.83	0.79
1:A:392:ASN:ND2	1:A:433:GLN:HE21	1.81	0.78
1:B:178:THR:HG22	1:B:180:MET:HG2	1.64	0.78
1:A:282:ASP:O	1:A:285:PRO:HD2	1.84	0.78
1:B:12:PRO:HA	1:B:15:VAL:HB	1.65	0.78
1:B:63:ASP:HA	1:B:66:LEU:HD12	1.65	0.77
1:A:444:ASN:HD22	1:A:444:ASN:C	1.87	0.77
1:A:109:VAL:O	1:A:113:ARG:HG3	1.85	0.77
1:A:537:ARG:O	1:A:540:VAL:HG12	1.85	0.77
1:A:270:LEU:O	1:A:274:VAL:HG23	1.84	0.76
1:A:127:HIS:C	1:A:130:PRO:HD2	2.05	0.76
2:D:112:ILE:O	2:D:112:ILE:HG22	1.84	0.76
1:B:178:THR:HG22	1:B:180:MET:HE3	1.66	0.76
1:B:347:SER:HB3	1:B:383:ASN:ND2	2.00	0.76
1:A:358:LYS:O	1:A:362:ILE:HG13	1.87	0.75
1:B:25:VAL:HG22	1:B:28:ARG:NH2	2.02	0.75
1:A:496:LEU:HA	1:A:499:MET:CE	2.16	0.75
1:B:94:GLU:CB	1:B:131:LEU:HD11	2.14	0.75
1:A:268:THR:HG23	1:A:305:LYS:HD2	1.68	0.75
1:B:561:LYS:HB3	1:B:562:PRO:HD3	1.68	0.75
1:A:45:GLU:O	1:A:49:SER:HB3	1.87	0.75
1:A:392:ASN:ND2	1:A:433:GLN:NE2	2.35	0.75
1:B:537:ARG:HA	1:B:540:VAL:HG12	1.69	0.74
1:B:25:VAL:HG22	1:B:28:ARG:HH22	1.52	0.74
2:D:114:LEU:HD12	2:D:114:LEU:N	2.03	0.74
1:A:504:CYS:O	1:A:508:LEU:HD23	1.88	0.74
1:A:125:GLU:HG2	1:A:162:VAL:HG21	1.70	0.74
1:A:373:LEU:HD22	1:A:384:ILE:HG21	1.69	0.74
1:A:107:LYS:HD3	1:A:110:GLU:OE1	1.88	0.73
1:A:155:TYR:HB3	1:A:156:PRO:HD3	1.69	0.73
1:A:452:VAL:HG13	1:A:497:HIS:CE1	2.24	0.73
1:B:452:VAL:HG12	1:B:452:VAL:O	1.86	0.73
1:B:526:LEU:HD22	1:B:563:ILE:HG21	1.70	0.73
1:A:20:LEU:O	1:A:28:ARG:HD3	1.87	0.73
1:A:206:ILE:HB	1:A:207:PRO:HD3	1.70	0.73
1:A:490:SER:HB3	1:A:501:THR:HG21	1.70	0.73
1:B:318:ARG:O	1:B:321:VAL:HG22	1.88	0.73
2:C:112:ILE:HG22	2:C:112:ILE:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ILE:HG13	1:A:243:LEU:HD13	1.70	0.73
1:A:420:ARG:HG3	1:A:420:ARG:HH11	1.54	0.73
1:A:47:THR:HG23	1:A:51:LEU:HD23	1.69	0.73
1:A:206:ILE:HD12	1:A:243:LEU:HB3	1.71	0.72
1:A:467:LYS:O	1:A:471:GLU:HG3	1.89	0.72
1:B:506:ASN:HD21	1:B:543:SER:HB3	1.54	0.72
1:A:183:ARG:HG2	1:A:220:VAL:HG22	1.71	0.72
1:B:459:ARG:O	1:B:462:ALA:HB3	1.89	0.72
1:B:78:THR:O	1:B:80:VAL:N	2.19	0.72
1:B:197:GLU:HG2	1:B:200:ASN:HD22	1.54	0.72
1:B:284:VAL:O	1:B:288:GLN:HG3	1.90	0.72
1:B:313:LEU:HD13	1:B:321:VAL:HG21	1.71	0.72
2:D:114:LEU:HB3	2:D:118:LEU:HD12	1.72	0.72
1:A:262:MET:HE3	1:A:266:LYS:HG3	1.71	0.71
1:B:38:ILE:H	1:B:38:ILE:HD12	1.56	0.71
1:B:365:LEU:HA	1:B:368:LEU:HD12	1.72	0.71
1:A:262:MET:CE	1:A:266:LYS:HG3	2.21	0.70
1:B:77:THR:CG2	1:B:118:GLU:HG3	2.21	0.70
1:B:155:TYR:CE1	1:B:163:LYS:HB3	2.26	0.70
1:B:526:LEU:HD22	1:B:563:ILE:CG2	2.21	0.70
1:A:517:THR:HG23	1:A:521:MET:HE2	1.73	0.70
1:B:358:LYS:O	1:B:362:ILE:HG13	1.91	0.70
1:A:77:THR:HG22	1:A:86:VAL:HG23	1.75	0.69
1:A:353:SER:H	1:A:354:PRO:HD2	1.57	0.69
1:A:25:VAL:HG13	1:A:28:ARG:NH2	2.08	0.69
1:A:517:THR:HA	1:A:521:MET:HE2	1.75	0.69
1:A:350:MET:HG3	1:A:387:ASN:HB2	1.74	0.69
1:A:452:VAL:HG12	1:A:452:VAL:O	1.93	0.69
1:B:11:TYR:HB3	1:B:12:PRO:HD3	1.74	0.69
1:B:94:GLU:HB2	1:B:131:LEU:CD1	2.19	0.69
1:B:517:THR:HG23	1:B:521:MET:CE	2.23	0.68
1:A:48:ARG:HB3	1:A:80:VAL:HG23	1.75	0.68
1:B:109:VAL:HG13	1:B:150:LEU:HD21	1.74	0.68
1:A:401:SER:HA	1:A:405:LEU:HB2	1.76	0.68
2:D:114:LEU:O	2:D:118:LEU:HB2	1.93	0.68
1:A:34:LYS:NZ	1:A:37:THR:HG21	2.10	0.67
1:A:350:MET:CE	1:A:384:ILE:HG23	2.24	0.67
1:A:381:ARG:O	1:A:385:ILE:HG13	1.94	0.67
1:B:70:ALA:HB2	1:B:96:LEU:HD13	1.75	0.67
1:A:388:LEU:O	1:A:390:CYS:N	2.28	0.67
1:A:264:ALA:O	1:A:267:PHE:HB2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:PHE:CE2	1:A:247:THR:HG21	2.29	0.67
1:A:534:ALA:CA	1:A:537:ARG:HH21	2.08	0.67
1:B:373:LEU:HD22	1:B:384:ILE:CG2	2.25	0.67
1:B:58:THR:HG22	1:B:59:ILE:N	2.10	0.67
1:A:204:GLU:C	1:A:207:PRO:HD2	2.14	0.67
1:B:517:THR:HG23	1:B:521:MET:HE1	1.76	0.66
1:A:378:PRO:O	1:A:382:LEU:HB2	1.96	0.66
1:A:390:CYS:O	1:A:392:ASN:N	2.29	0.66
1:B:452:VAL:HG13	1:B:497:HIS:NE2	2.11	0.66
1:B:506:ASN:HD21	1:B:543:SER:CB	2.09	0.66
1:A:15:VAL:O	1:A:19:GLU:HG3	1.95	0.65
1:A:197:GLU:HG2	1:A:200:ASN:ND2	2.11	0.65
1:A:12:PRO:HA	1:A:15:VAL:HB	1.78	0.65
1:B:179:PRO:HD2	1:B:180:MET:HE3	1.78	0.65
1:B:278:ILE:H	1:B:278:ILE:CD1	1.86	0.65
1:B:338:ASN:ND2	1:B:340:HIS:HB2	2.10	0.65
1:A:483:ILE:HB	1:A:484:PRO:HD3	1.78	0.65
1:B:222:LEU:C	1:B:222:LEU:HD23	2.17	0.65
1:B:378:PRO:O	1:B:382:LEU:HB2	1.96	0.65
1:B:35:LEU:HA	1:B:38:ILE:HD13	1.78	0.65
1:B:267:PHE:CE2	1:B:287:PHE:HB2	2.32	0.65
1:A:93:LEU:O	1:A:95:SER:N	2.30	0.65
1:B:333:LEU:O	1:B:336:ASP:HB2	1.97	0.65
1:A:89:LEU:O	1:A:92:PRO:HD2	1.97	0.65
2:D:154:GLU:O	2:D:158:LEU:HD12	1.96	0.65
1:B:192:PHE:O	1:B:195:VAL:HG22	1.97	0.65
2:D:114:LEU:HD12	2:D:114:LEU:H	1.61	0.65
1:A:444:ASN:HD22	1:A:445:SER:N	1.95	0.64
1:B:229:VAL:HG22	1:B:270:LEU:HD23	1.79	0.64
2:D:101:PRO:HG2	2:D:102:GLU:OE1	1.96	0.64
1:A:268:THR:HG21	1:A:308:GLU:OE1	1.97	0.64
1:A:436:VAL:HG13	1:A:437:GLU:N	2.12	0.64
1:B:38:ILE:O	1:B:42:LEU:HD23	1.96	0.64
1:A:35:LEU:HG	1:A:35:LEU:O	1.96	0.64
1:B:347:SER:CB	1:B:383:ASN:HD22	2.07	0.64
1:B:535:ASN:O	1:B:539:ASN:HB2	1.97	0.64
1:B:362:ILE:HA	1:B:366:LEU:HD13	1.77	0.64
1:B:481:THR:HG22	1:B:482:ILE:HD13	1.78	0.64
2:C:100:TRP:O	2:C:101:PRO:C	2.35	0.64
1:B:338:ASN:ND2	1:B:341:VAL:H	1.91	0.64
1:A:467:LYS:HB2	1:A:507:VAL:CG1	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:LEU:HD22	1:B:46:ARG:HD2	1.79	0.64
1:B:316:ASP:O	1:B:318:ARG:N	2.31	0.64
1:A:405:LEU:HB3	1:A:406:PRO:HD3	1.78	0.64
1:B:451:LEU:HD21	1:B:466:LEU:HD11	1.80	0.64
1:A:314:SER:HB2	1:A:317:CYS:SG	2.38	0.63
1:A:462:ALA:O	1:A:465:ASN:HB3	1.98	0.63
1:B:514:GLN:HE22	1:B:552:ASP:HB3	1.63	0.63
1:A:526:LEU:HD22	1:A:563:ILE:CG2	2.29	0.63
1:B:206:ILE:HG21	1:B:243:LEU:HD22	1.80	0.63
1:B:401:SER:HA	1:B:405:LEU:HB2	1.79	0.63
1:B:356:LEU:HD12	1:B:365:LEU:HD11	1.80	0.63
1:B:222:LEU:CD2	1:B:223:LEU:HD23	2.24	0.63
1:B:274:VAL:HG12	1:B:278:ILE:HB	1.81	0.63
1:A:98:THR:O	1:A:98:THR:HG22	1.99	0.63
1:A:353:SER:C	1:A:355:ILE:H	2.01	0.63
1:B:38:ILE:HD12	1:B:38:ILE:N	2.14	0.63
1:A:503:PHE:O	1:A:506:ASN:HB2	1.99	0.62
1:B:436:VAL:HG13	1:B:437:GLU:H	1.64	0.62
1:B:82:GLY:O	1:B:84:GLU:N	2.33	0.62
1:A:58:THR:HG22	1:A:59:ILE:N	2.10	0.62
1:B:426:TYR:CE2	1:B:430:LEU:HD12	2.35	0.62
2:D:114:LEU:H	2:D:114:LEU:CD1	2.13	0.62
1:A:107:LYS:O	1:A:110:GLU:HB3	1.99	0.62
1:A:229:VAL:HG22	1:A:270:LEU:HD23	1.82	0.62
1:B:284:VAL:HB	1:B:285:PRO:HD3	1.81	0.62
1:B:483:ILE:HB	1:B:484:PRO:HD3	1.82	0.62
1:B:311:GLU:HG3	1:B:355:ILE:HD11	1.82	0.62
2:D:119:ARG:O	2:D:122:HIS:HB3	2.00	0.62
1:B:373:LEU:HD12	1:B:411:LEU:HD21	1.81	0.62
1:B:223:LEU:HD23	1:B:223:LEU:N	2.14	0.61
1:B:405:LEU:HB3	1:B:406:PRO:HD3	1.81	0.61
1:A:93:LEU:C	1:A:95:SER:H	2.01	0.61
1:A:372:GLN:HB2	1:A:384:ILE:HG13	1.81	0.61
1:A:564:LEU:O	1:A:567:LEU:HB2	1.99	0.61
1:B:48:ARG:HB3	1:B:80:VAL:CG2	2.30	0.61
1:B:197:GLU:HG2	1:B:200:ASN:ND2	2.14	0.61
1:B:77:THR:HG22	1:B:86:VAL:HG23	1.82	0.61
2:C:111:CYS:C	2:C:112:ILE:HG13	2.21	0.61
1:B:16:LEU:HD12	1:B:19:GLU:HB2	1.83	0.61
2:C:98:LYS:O	2:C:103:CYS:SG	2.59	0.61
2:C:102:GLU:CB	2:C:107:MET:HB2	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:TYR:HB3	1:B:12:PRO:CD	2.30	0.61
1:B:390:CYS:O	1:B:393:GLU:HB2	2.01	0.61
2:C:115:LEU:HD13	2:C:141:PHE:HB2	1.81	0.61
1:A:378:PRO:HG3	1:A:381:ARG:NH2	2.15	0.61
1:B:417:TRP:CZ3	1:B:418:ARG:HG2	2.35	0.61
1:B:271:GLN:NE2	1:B:312:ASN:HB2	2.16	0.61
1:A:325:GLN:O	1:A:328:PRO:HD2	2.00	0.60
1:B:206:ILE:HB	1:B:207:PRO:HD3	1.83	0.60
1:B:381:ARG:O	1:B:385:ILE:HG13	2.00	0.60
1:B:34:LYS:C	1:B:36:SER:H	2.04	0.60
1:B:183:ARG:HG2	1:B:220:VAL:HG22	1.83	0.60
1:A:444:ASN:C	1:A:444:ASN:ND2	2.54	0.60
1:B:522:LEU:HB3	1:B:523:PRO:HD3	1.84	0.60
1:A:77:THR:HG21	1:A:118:GLU:HG3	1.84	0.60
1:A:420:ARG:HG3	1:A:420:ARG:NH1	2.16	0.60
1:B:392:ASN:O	1:B:392:ASN:CG	2.39	0.60
1:A:93:LEU:C	1:A:95:SER:N	2.54	0.60
1:A:105:ARG:O	1:A:109:VAL:HG23	2.01	0.60
1:A:506:ASN:HD21	1:A:543:SER:HA	1.66	0.60
1:B:109:VAL:O	1:B:113:ARG:HG3	2.01	0.60
1:B:349:ILE:HG23	1:B:350:MET:N	2.16	0.60
1:A:534:ALA:HA	1:A:537:ARG:HE	1.65	0.60
1:B:481:THR:HG22	1:B:482:ILE:CD1	2.32	0.60
1:A:431:ALA:O	1:A:432:GLY:C	2.38	0.60
1:A:34:LYS:HZ2	1:A:37:THR:HG21	1.67	0.59
1:B:350:MET:HE2	1:B:384:ILE:HD12	1.84	0.59
1:B:427:MET:HE3	1:B:430:LEU:HB3	1.84	0.59
2:D:122:HIS:CE1	2:D:133:LEU:HD12	2.38	0.59
1:B:338:ASN:HD22	1:B:341:VAL:N	1.94	0.59
2:D:98:LYS:O	2:D:103:CYS:SG	2.61	0.59
1:A:181:VAL:O	1:A:184:ALA:HB3	2.02	0.59
1:A:204:GLU:O	1:A:207:PRO:HD2	2.02	0.59
1:A:245:MET:O	1:A:249:ARG:HB2	2.03	0.59
1:B:495:TYR:CD2	1:B:533:VAL:HG11	2.37	0.59
2:C:115:LEU:HD12	2:C:115:LEU:O	2.02	0.59
1:A:75:THR:O	1:A:76:PHE:HD1	1.85	0.59
1:A:93:LEU:O	1:A:96:LEU:N	2.36	0.59
1:A:353:SER:C	1:A:355:ILE:N	2.56	0.59
1:A:427:MET:CE	1:A:430:LEU:HD13	2.32	0.59
1:A:517:THR:HG23	1:A:521:MET:CE	2.33	0.59
1:B:105:ARG:O	1:B:109:VAL:HG23	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:LEU:HD23	1:A:499:MET:HE3	1.85	0.59
1:B:572:ASP:OD1	1:B:574:ASP:HB2	2.03	0.59
1:A:527:ARG:HG2	1:A:527:ARG:HH11	1.68	0.58
1:B:52:LEU:HB2	1:B:53:PRO:HD3	1.85	0.58
1:A:96:LEU:O	1:A:99:VAL:HG23	2.03	0.58
1:B:327:LEU:HB3	1:B:328:PRO:HD3	1.85	0.58
1:A:563:ILE:HG23	1:A:563:ILE:O	2.02	0.58
1:A:52:LEU:HD13	1:A:88:CYS:O	2.03	0.58
1:A:528:MET:C	1:A:530:GLY:H	2.06	0.58
1:B:486:VAL:O	1:B:501:THR:HG23	2.04	0.58
1:A:427:MET:HE3	1:A:427:MET:HA	1.85	0.58
1:A:537:ARG:HA	1:A:540:VAL:HG12	1.86	0.58
1:A:358:LYS:HG3	1:A:395:ILE:HA	1.86	0.58
1:A:156:PRO:HG3	1:A:195:VAL:HB	1.84	0.58
1:A:158:VAL:HG21	1:A:162:VAL:CG1	2.34	0.58
1:A:436:VAL:HG13	1:A:437:GLU:H	1.67	0.58
2:C:115:LEU:HD12	2:C:115:LEU:C	2.24	0.58
1:A:94:GLU:HB2	1:A:131:LEU:HD12	1.86	0.57
1:A:179:PRO:HD2	1:A:180:MET:HE3	1.84	0.57
1:A:180:MET:HE1	2:C:147:TRP:HA	1.85	0.57
1:B:94:GLU:OE1	1:B:131:LEU:HD12	2.03	0.57
1:B:538:PHE:CD1	1:B:538:PHE:C	2.77	0.57
1:A:273:ALA:O	1:A:274:VAL:O	2.21	0.57
1:A:564:LEU:HA	1:A:567:LEU:HD12	1.86	0.57
1:A:25:VAL:HA	1:A:28:ARG:NH1	2.19	0.57
1:A:366:LEU:O	1:A:370:LEU:HB2	2.05	0.57
1:A:496:LEU:O	1:A:499:MET:HB2	2.03	0.57
1:A:572:ASP:OD1	1:A:574:ASP:HB2	2.05	0.57
1:A:20:LEU:C	1:A:22:ASN:N	2.55	0.57
1:B:456:TYR:O	1:B:457:ALA:C	2.42	0.57
2:D:100:TRP:CE3	2:D:157:LEU:HD22	2.39	0.57
1:B:420:ARG:HH11	1:B:420:ARG:HG3	1.70	0.57
2:D:93:ASP:C	2:D:95:MET:H	2.07	0.57
1:B:475:LYS:NZ	2:C:154:GLU:OE1	2.36	0.57
1:A:365:LEU:HD23	1:A:368:LEU:HD12	1.87	0.57
1:B:178:THR:CG2	1:B:180:MET:HG2	2.35	0.57
1:A:522:LEU:HB3	1:A:523:PRO:HD3	1.87	0.57
1:A:11:TYR:CD2	1:A:12:PRO:HD3	2.39	0.56
1:A:11:TYR:HB3	1:A:12:PRO:HD3	1.85	0.56
1:B:99:VAL:HG12	1:B:101:GLU:H	1.70	0.56
1:B:377:CYS:SG	1:B:379:GLU:HB2	2.45	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:101:PRO:HG2	2:C:102:GLU:OE1	2.05	0.56
1:A:77:THR:HG22	1:A:86:VAL:CG2	2.35	0.56
1:A:303:SER:O	1:A:306:VAL:HG23	2.04	0.56
1:B:93:LEU:O	1:B:95:SER:N	2.37	0.56
1:B:280:LYS:HA	1:B:284:VAL:CG2	2.36	0.56
1:A:421:LEU:HD12	1:A:421:LEU:O	2.06	0.56
1:A:538:PHE:O	1:A:542:LYS:HG3	2.06	0.56
1:B:556:LEU:HD23	1:B:556:LEU:O	2.06	0.56
1:A:268:THR:CG2	1:A:305:LYS:HD2	2.36	0.56
1:A:411:LEU:HB3	1:A:423:ILE:HG13	1.88	0.56
1:B:436:VAL:HG13	1:B:437:GLU:N	2.20	0.56
1:A:201:VAL:O	1:A:206:ILE:HG12	2.04	0.56
1:B:490:SER:HB3	1:B:501:THR:HG21	1.87	0.56
1:A:350:MET:HE1	1:A:384:ILE:HG23	1.85	0.56
1:B:287:PHE:O	1:B:291:MET:HG3	2.06	0.56
1:B:392:ASN:ND2	1:B:433:GLN:NE2	2.53	0.56
2:C:100:TRP:CG	2:C:101:PRO:N	2.73	0.56
2:D:100:TRP:O	2:D:101:PRO:C	2.44	0.56
1:B:15:VAL:O	1:B:19:GLU:HG3	2.06	0.56
1:B:313:LEU:HD13	1:B:321:VAL:CG2	2.35	0.56
1:B:452:VAL:O	1:B:452:VAL:CG1	2.54	0.55
1:A:16:LEU:O	1:A:20:LEU:HG	2.07	0.55
1:A:561:LYS:HB3	1:A:562:PRO:HD3	1.87	0.55
1:B:20:LEU:C	1:B:22:ASN:N	2.57	0.55
1:B:311:GLU:HA	1:B:355:ILE:HD11	1.87	0.55
2:C:122:HIS:CE1	2:C:133:LEU:HD12	2.41	0.55
1:A:38:ILE:O	1:A:42:LEU:HD23	2.06	0.55
1:B:388:LEU:HD13	1:B:408:ILE:HD11	1.88	0.55
1:A:39:ALA:HB3	1:A:79:LEU:HD23	1.88	0.55
1:B:98:THR:HG22	1:B:98:THR:O	2.06	0.55
1:A:326:ILE:HD12	1:A:326:ILE:N	2.21	0.55
1:A:587:SER:O	1:A:588:LEU:HD23	2.07	0.55
1:B:20:LEU:C	1:B:22:ASN:H	2.09	0.55
1:A:259:VAL:O	1:A:263:VAL:HG23	2.07	0.55
1:B:75:THR:O	1:B:76:PHE:HD1	1.89	0.55
2:C:135:TRP:HB2	2:C:147:TRP:HB2	1.89	0.55
2:D:114:LEU:N	2:D:114:LEU:CD1	2.68	0.55
1:A:10:LEU:HD22	1:A:46:ARG:HD2	1.88	0.55
1:A:197:GLU:HG2	1:A:200:ASN:HD22	1.69	0.55
1:A:34:LYS:O	1:A:38:ILE:HD13	2.07	0.55
1:A:171:ARG:NH2	1:A:204:GLU:HG2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:LYS:HE3	1:A:588:LEU:HB3	1.88	0.55
1:A:326:ILE:HD12	1:A:326:ILE:H	1.71	0.55
1:B:275:GLY:HA3	1:B:278:ILE:HD13	1.89	0.54
1:B:509:SER:OG	1:B:510:GLU:N	2.40	0.54
1:A:327:LEU:HB3	1:A:328:PRO:HD3	1.89	0.54
1:A:534:ALA:HA	1:A:537:ARG:HH21	1.73	0.54
1:A:392:ASN:HD22	1:A:433:GLN:HE21	1.52	0.54
1:A:517:THR:HA	1:A:521:MET:CE	2.38	0.54
2:C:93:ASP:C	2:C:95:MET:H	2.09	0.54
1:A:20:LEU:C	1:A:22:ASN:H	2.10	0.54
1:A:373:LEU:CD2	1:A:384:ILE:HG21	2.37	0.54
1:A:390:CYS:O	1:A:393:GLU:N	2.32	0.54
1:B:356:LEU:HB3	1:B:360:ASN:HB3	1.87	0.54
1:B:129:VAL:HB	1:B:130:PRO:HD3	1.90	0.54
1:B:183:ARG:HD3	1:B:219:SER:HB2	1.90	0.54
2:C:119:ARG:O	2:C:122:HIS:HB3	2.07	0.54
1:A:60:TYR:O	1:A:61:ASP:O	2.25	0.54
1:A:448:MET:HA	1:A:451:LEU:HD23	1.89	0.54
1:B:78:THR:C	1:B:80:VAL:H	2.07	0.54
1:A:450:TRP:HB3	1:A:462:ALA:HB2	1.89	0.54
1:A:453:ASP:OD1	1:A:455:VAL:HG13	2.07	0.54
1:B:411:LEU:HB3	1:B:423:ILE:HG13	1.90	0.54
1:A:98:THR:HG23	1:A:143:SER:OG	2.08	0.54
1:A:198:LEU:HD22	1:A:198:LEU:H	1.73	0.54
1:A:300:ALA:N	1:A:341:VAL:HG22	2.22	0.54
1:B:509:SER:O	1:B:511:VAL:N	2.41	0.54
1:A:126:ALA:O	1:A:130:PRO:HG2	2.08	0.54
1:A:323:MET:SD	1:A:327:LEU:HD22	2.47	0.54
1:A:20:LEU:O	1:A:22:ASN:N	2.41	0.53
1:B:436:VAL:HG22	1:B:440:ASP:OD2	2.07	0.53
1:B:42:LEU:HD22	1:B:42:LEU:H	1.72	0.53
1:B:49:SER:OG	1:B:50:GLU:N	2.40	0.53
1:B:582:ALA:O	1:B:586:LEU:HG	2.09	0.53
1:B:369:PHE:O	1:B:373:LEU:HB2	2.08	0.53
2:D:100:TRP:CG	2:D:101:PRO:N	2.75	0.53
1:A:430:LEU:O	1:A:431:ALA:C	2.47	0.53
1:A:141:PHE:CD1	1:A:142:THR:N	2.76	0.53
1:A:245:MET:HB3	1:A:249:ARG:HH21	1.74	0.53
1:A:282:ASP:C	1:A:285:PRO:HD2	2.28	0.53
1:A:330:ILE:O	1:A:333:LEU:N	2.41	0.53
1:A:427:MET:HE1	1:A:430:LEU:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:93:ASP:C	2:D:95:MET:N	2.61	0.53
2:C:111:CYS:O	2:C:112:ILE:HG13	2.08	0.53
1:A:365:LEU:O	1:A:368:LEU:HB2	2.08	0.53
1:B:16:LEU:HG	1:B:20:LEU:HG	1.91	0.53
2:C:134:VAL:CG1	2:C:147:TRP:CZ3	2.91	0.53
1:A:529:ALA:HA	1:A:540:VAL:HG11	1.91	0.53
1:A:141:PHE:CD1	1:A:141:PHE:C	2.82	0.52
1:A:394:VAL:HG12	1:A:395:ILE:N	2.24	0.52
1:B:561:LYS:HD2	1:B:588:LEU:HD22	1.91	0.52
1:B:34:LYS:O	1:B:36:SER:N	2.42	0.52
1:B:141:PHE:HA	1:B:144:ARG:NH1	2.24	0.52
1:A:48:ARG:HB3	1:A:80:VAL:CG2	2.39	0.52
1:A:145:THR:HG22	1:A:146:SER:N	2.24	0.52
1:A:310:CYS:O	1:A:313:LEU:HB2	2.10	0.52
1:B:192:PHE:CZ	1:B:196:LEU:HD21	2.44	0.52
2:C:102:GLU:HB3	2:C:107:MET:HB2	1.91	0.52
1:A:180:MET:CE	2:C:147:TRP:HA	2.40	0.52
1:B:28:ARG:O	1:B:31:SER:HB3	2.09	0.52
1:B:105:ARG:CZ	1:B:142:THR:HG22	2.40	0.52
2:C:122:HIS:NE2	2:C:133:LEU:HD12	2.24	0.52
1:A:492:ASP:O	1:A:498:ARG:HD3	2.09	0.52
1:B:452:VAL:HG13	1:B:497:HIS:CE1	2.45	0.52
1:A:564:LEU:HD22	1:A:583:LEU:HD21	1.92	0.52
2:D:135:TRP:HB2	2:D:147:TRP:HB2	1.92	0.52
1:B:280:LYS:HA	1:B:284:VAL:HG23	1.92	0.52
1:B:437:GLU:N	1:B:437:GLU:OE1	2.42	0.52
1:A:262:MET:HE3	1:A:262:MET:O	2.09	0.52
1:B:235:LEU:HD12	1:B:240:LEU:HD23	1.91	0.52
1:B:537:ARG:CA	1:B:540:VAL:HG12	2.38	0.52
1:B:556:LEU:O	1:B:560:VAL:HB	2.10	0.52
2:C:134:VAL:O	2:C:136:VAL:N	2.43	0.52
1:A:15:VAL:HG12	1:A:19:GLU:OE2	2.09	0.51
1:B:355:ILE:HG22	1:B:356:LEU:N	2.24	0.51
1:B:481:THR:HG22	1:B:482:ILE:N	2.24	0.51
1:A:221:ARG:O	1:A:224:ALA:HB3	2.10	0.51
1:B:111:SER:O	1:B:115:ILE:HG23	2.10	0.51
1:B:155:TYR:CZ	1:B:196:LEU:HD22	2.44	0.51
1:A:274:VAL:HG11	1:A:278:ILE:HB	1.92	0.51
1:B:448:MET:HE2	1:B:451:LEU:HD23	1.92	0.51
1:A:182:ARG:NE	1:A:215:ASP:OD2	2.42	0.51
2:C:114:LEU:HD12	2:C:114:LEU:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ARG:HA	1:A:49:SER:HB3	1.92	0.51
1:A:239:ASP:O	1:A:242:ALA:N	2.43	0.51
1:A:107:LYS:O	1:A:110:GLU:N	2.43	0.51
1:A:317:CYS:O	1:A:320:ASN:HB2	2.11	0.51
1:B:576:LYS:O	1:B:577:TYR:C	2.48	0.51
2:C:125:ARG:NH1	2:C:125:ARG:HG3	2.26	0.51
1:A:372:GLN:O	1:A:374:LYS:N	2.44	0.51
1:A:411:LEU:O	1:A:414:ASP:HB2	2.11	0.51
1:A:522:LEU:N	1:A:523:PRO:CD	2.73	0.51
1:B:10:LEU:HD11	1:B:50:GLU:HB3	1.92	0.50
1:B:75:THR:O	1:B:76:PHE:CD1	2.64	0.50
2:D:134:VAL:O	2:D:136:VAL:N	2.44	0.50
2:D:169:TYR:O	2:D:170:ARG:HB3	2.11	0.50
1:A:217:GLN:HB3	1:A:220:VAL:HG23	1.93	0.50
1:B:141:PHE:CD1	1:B:141:PHE:C	2.85	0.50
1:B:222:LEU:C	1:B:222:LEU:CD2	2.80	0.50
1:A:339:GLN:O	1:A:343:SER:HB2	2.11	0.50
1:A:474:GLY:O	1:A:477:TRP:HB3	2.12	0.50
1:B:372:GLN:HB2	1:B:384:ILE:HG13	1.93	0.50
1:B:529:ALA:O	1:B:537:ARG:HG2	2.11	0.50
1:A:65:VAL:O	1:A:68:ALA:HB3	2.11	0.50
1:A:274:VAL:CG1	1:A:278:ILE:HB	2.41	0.50
1:B:38:ILE:H	1:B:38:ILE:CD1	2.21	0.50
1:B:448:MET:O	1:B:451:LEU:HB2	2.10	0.50
1:A:325:GLN:HB2	1:A:326:ILE:HD12	1.94	0.50
1:A:527:ARG:HG2	1:A:527:ARG:NH1	2.26	0.50
1:B:100:GLU:O	1:B:105:ARG:NH1	2.45	0.50
1:B:267:PHE:HE2	1:B:287:PHE:HB2	1.76	0.50
1:B:535:ASN:HA	1:B:538:PHE:CD2	2.47	0.50
1:B:268:THR:HG23	1:B:305:LYS:HD2	1.93	0.50
2:D:115:LEU:C	2:D:115:LEU:HD12	2.32	0.50
1:B:492:ASP:O	1:B:498:ARG:HD3	2.12	0.50
1:B:159:SER:O	1:B:163:LYS:HG3	2.12	0.50
1:A:56:THR:C	1:A:58:THR:H	2.14	0.50
2:C:122:HIS:HE1	2:C:143:CYS:SG	2.35	0.49
1:A:19:GLU:O	1:A:22:ASN:HB2	2.13	0.49
1:A:28:ARG:HG3	1:A:28:ARG:HH11	1.76	0.49
1:A:72:GLN:C	1:A:74:GLY:H	2.15	0.49
1:B:86:VAL:HG21	1:B:118:GLU:HB2	1.94	0.49
1:B:537:ARG:O	1:B:540:VAL:CG1	2.57	0.49
1:B:587:SER:O	1:B:588:LEU:HD23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:129:ARG:HG2	2:C:130:LYS:N	2.27	0.49
1:A:104:VAL:HG12	1:A:105:ARG:N	2.26	0.49
1:A:287:PHE:O	1:A:291:MET:HG3	2.12	0.49
1:A:388:LEU:C	1:A:390:CYS:N	2.63	0.49
1:B:10:LEU:HD22	1:B:46:ARG:CD	2.42	0.49
1:B:476:GLU:O	1:B:479:HIS:HB3	2.12	0.49
2:C:122:HIS:CD2	2:C:133:LEU:HD12	2.48	0.49
1:A:16:LEU:HA	1:A:19:GLU:OE2	2.12	0.49
1:A:372:GLN:CB	1:A:384:ILE:HG13	2.42	0.49
1:B:12:PRO:HG3	1:B:38:ILE:HG23	1.94	0.49
1:B:170:PHE:HA	1:B:173:LEU:HD12	1.93	0.49
1:A:58:THR:CG2	1:A:59:ILE:H	2.10	0.49
1:A:274:VAL:HG12	1:A:278:ILE:HD13	1.93	0.49
1:A:534:ALA:N	1:A:537:ARG:HH21	2.10	0.49
1:B:350:MET:CE	1:B:384:ILE:HD12	2.42	0.49
1:B:378:PRO:HG3	1:B:381:ARG:NH2	2.28	0.49
1:B:519:LYS:O	1:B:519:LYS:HG3	2.12	0.49
1:B:29:LEU:C	1:B:31:SER:H	2.15	0.49
1:B:318:ARG:O	1:B:322:ILE:HG13	2.12	0.49
1:B:534:ALA:O	1:B:537:ARG:N	2.46	0.49
1:A:317:CYS:O	1:A:321:VAL:HG22	2.13	0.49
1:A:412:ALA:HB2	1:A:423:ILE:HG21	1.93	0.49
1:B:82:GLY:C	1:B:84:GLU:H	2.16	0.49
1:B:115:ILE:O	1:B:119:HIS:HD2	1.96	0.49
2:D:93:ASP:HB2	2:D:96:TYR:HD1	1.77	0.49
1:B:90:LEU:HB2	1:B:91:PRO:HD3	1.95	0.49
1:A:318:ARG:HD3	1:A:355:ILE:CG1	2.42	0.49
1:A:404:LEU:O	1:A:405:LEU:C	2.51	0.49
1:A:535:ASN:HA	1:A:538:PHE:CD2	2.48	0.49
1:B:361:THR:O	1:B:365:LEU:HB2	2.13	0.49
1:A:43:GLY:N	1:A:46:ARG:HB2	2.27	0.48
1:A:147:ALA:O	1:A:149:GLY:N	2.46	0.48
1:B:392:ASN:CB	1:B:400:LEU:HD22	2.38	0.48
1:B:537:ARG:HA	1:B:540:VAL:CG1	2.43	0.48
2:D:145:ARG:HG2	2:D:156:THR:HG21	1.95	0.48
1:A:91:PRO:N	1:A:92:PRO:HD2	2.28	0.48
1:A:222:LEU:HD23	1:A:222:LEU:C	2.33	0.48
1:A:350:MET:HE1	1:A:384:ILE:HD12	1.93	0.48
1:B:391:VAL:C	1:B:393:GLU:H	2.17	0.48
1:A:77:THR:HG23	1:A:115:ILE:HG22	1.94	0.48
1:A:270:LEU:O	1:A:271:GLN:C	2.50	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:GLU:O	1:A:563:ILE:HG22	2.12	0.48
2:C:100:TRP:CZ3	2:C:104:ALA:HB2	2.48	0.48
1:A:16:LEU:HA	1:A:19:GLU:CD	2.33	0.48
1:A:42:LEU:HD12	1:A:46:ARG:HB3	1.95	0.48
1:A:307:LYS:HG2	1:A:311:GLU:OE1	2.13	0.48
1:B:204:GLU:C	1:B:207:PRO:HD2	2.33	0.48
1:B:365:LEU:O	1:B:368:LEU:HB2	2.13	0.48
1:B:420:ARG:O	1:B:421:LEU:C	2.51	0.48
2:D:129:ARG:HD3	2:D:131:ASP:CB	2.43	0.48
1:A:136:ALA:O	1:A:144:ARG:HG2	2.13	0.48
1:B:326:ILE:O	1:B:329:CYS:N	2.41	0.48
1:B:527:ARG:HG2	1:B:527:ARG:HH11	1.77	0.48
2:D:94:ALA:HB1	2:D:98:LYS:HG3	1.96	0.48
1:A:96:LEU:C	1:A:98:THR:H	2.17	0.48
1:A:116:SER:O	1:A:119:HIS:HB2	2.13	0.48
1:A:194:LYS:HG2	1:A:234:LEU:HD11	1.94	0.48
1:B:556:LEU:HD23	1:B:556:LEU:C	2.33	0.48
1:A:39:ALA:O	1:A:42:LEU:O	2.32	0.48
1:A:262:MET:HE1	1:A:266:LYS:HG3	1.95	0.48
1:A:392:ASN:HD22	1:A:433:GLN:NE2	2.09	0.48
1:A:542:LYS:O	1:A:545:GLN:HB3	2.13	0.48
1:B:29:LEU:HD23	1:B:33:LYS:HG3	1.95	0.48
1:B:517:THR:HG23	1:B:521:MET:HE2	1.95	0.48
1:B:256:SER:HB3	1:B:259:VAL:HG23	1.94	0.48
1:B:437:GLU:N	1:B:437:GLU:CD	2.67	0.48
1:A:89:LEU:C	1:A:92:PRO:HD2	2.35	0.48
1:B:93:LEU:O	1:B:96:LEU:N	2.46	0.48
1:B:349:ILE:CG2	1:B:350:MET:N	2.77	0.48
1:A:78:THR:HG23	1:A:79:LEU:HD12	1.95	0.48
1:B:420:ARG:HG3	1:B:420:ARG:NH1	2.27	0.48
1:B:576:LYS:HA	1:B:579:ALA:HB3	1.96	0.48
1:A:144:ARG:O	1:A:147:ALA:HB3	2.14	0.47
1:A:452:VAL:O	1:A:452:VAL:CG1	2.62	0.47
1:A:558:SER:O	1:A:562:PRO:HG2	2.14	0.47
1:B:90:LEU:HD12	1:B:131:LEU:HD13	1.96	0.47
1:B:448:MET:HE2	1:B:451:LEU:CD2	2.43	0.47
1:B:561:LYS:CE	1:B:588:LEU:HD22	2.44	0.47
1:A:405:LEU:HD23	1:A:434:LEU:HD11	1.96	0.47
1:B:93:LEU:C	1:B:95:SER:N	2.65	0.47
1:B:275:GLY:CA	1:B:278:ILE:HD13	2.43	0.47
1:B:298:VAL:O	1:B:301:ALA:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:564:LEU:HD22	1:B:583:LEU:HD21	1.95	0.47
2:C:100:TRP:CE3	2:C:157:LEU:HD22	2.49	0.47
2:C:106:LYS:HG2	2:C:119:ARG:NH2	2.29	0.47
2:D:112:ILE:O	2:D:112:ILE:CG2	2.57	0.47
1:A:318:ARG:HD3	1:A:355:ILE:HG12	1.96	0.47
1:A:456:TYR:O	1:A:457:ALA:C	2.53	0.47
1:B:189:LEU:HD22	1:B:212:LEU:HD12	1.96	0.47
1:B:264:ALA:O	1:B:267:PHE:HB2	2.13	0.47
1:A:120:SER:O	1:A:123:ASP:HB2	2.14	0.47
1:A:180:MET:H	1:A:180:MET:CE	2.20	0.47
1:A:508:LEU:H	1:A:508:LEU:CD2	2.27	0.47
1:B:77:THR:O	1:B:82:GLY:HA2	2.14	0.47
1:A:388:LEU:C	1:A:390:CYS:H	2.18	0.47
1:A:450:TRP:C	1:A:452:VAL:H	2.17	0.47
1:A:586:LEU:O	1:A:587:SER:HB2	2.13	0.47
1:B:36:SER:O	1:B:40:LEU:HD23	2.14	0.47
1:B:222:LEU:HD23	1:B:222:LEU:O	2.14	0.47
1:B:321:VAL:HG23	1:B:322:ILE:N	2.29	0.47
1:A:11:TYR:CB	1:A:12:PRO:HD3	2.45	0.47
1:A:46:ARG:HA	1:A:49:SER:CB	2.45	0.47
1:A:54:PHE:C	1:A:56:THR:H	2.18	0.47
1:A:218:ASP:HA	1:A:221:ARG:NH1	2.30	0.47
1:B:15:VAL:HG12	1:B:19:GLU:OE2	2.15	0.47
1:B:179:PRO:O	1:B:183:ARG:HG3	2.15	0.47
1:B:213:ALA:HA	1:B:224:ALA:CB	2.45	0.47
1:B:453:ASP:OD1	1:B:455:VAL:HG13	2.15	0.47
1:B:581:GLU:O	1:B:581:GLU:HG3	2.15	0.47
2:D:134:VAL:HG12	2:D:136:VAL:H	1.80	0.47
1:A:154:CYS:SG	1:A:155:TYR:N	2.88	0.47
1:B:413:GLU:O	1:B:414:ASP:O	2.33	0.47
1:A:198:LEU:O	1:A:199:ASP:C	2.53	0.47
1:A:350:MET:HE2	1:A:384:ILE:HD13	1.97	0.47
2:C:114:LEU:O	2:C:115:LEU:C	2.52	0.47
1:A:128:PHE:O	1:A:131:LEU:N	2.47	0.47
1:A:283:LEU:O	1:A:286:ALA:HB3	2.15	0.47
1:B:60:TYR:O	1:B:61:ASP:O	2.33	0.47
1:B:82:GLY:C	1:B:84:GLU:N	2.68	0.47
1:B:564:LEU:O	1:B:564:LEU:HD23	2.15	0.47
2:C:112:ILE:O	2:C:112:ILE:CG2	2.61	0.47
1:A:11:TYR:HB3	1:A:12:PRO:CD	2.45	0.46
1:A:235:LEU:HB2	1:A:240:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:ASP:OD1	1:A:532:PRO:HD2	2.15	0.46
1:B:80:VAL:O	1:B:80:VAL:HG22	2.15	0.46
1:B:495:TYR:HB3	1:B:533:VAL:HG21	1.97	0.46
2:C:125:ARG:HG3	2:C:125:ARG:HH11	1.80	0.46
1:A:118:GLU:OE2	1:A:118:GLU:HA	2.15	0.46
1:A:209:PHE:CZ	1:A:247:THR:HG21	2.51	0.46
1:A:257:TRP:HA	1:A:260:ARG:NH1	2.30	0.46
1:A:370:LEU:CD2	1:A:404:LEU:HD12	2.45	0.46
1:A:438:PHE:CD1	1:A:438:PHE:C	2.89	0.46
1:B:176:ASP:HB3	1:B:181:VAL:HB	1.97	0.46
1:B:392:ASN:HD21	1:B:433:GLN:NE2	2.12	0.46
1:B:559:GLU:O	1:B:563:ILE:HG22	2.15	0.46
1:A:225:VAL:O	1:A:226:GLU:C	2.54	0.46
1:A:82:GLY:O	1:A:84:GLU:N	2.48	0.46
1:A:405:LEU:CD2	1:A:434:LEU:HD11	2.46	0.46
1:A:456:TYR:CD1	1:A:456:TYR:C	2.88	0.46
1:B:318:ARG:O	1:B:319:GLU:C	2.53	0.46
1:B:42:LEU:HD22	1:B:42:LEU:N	2.31	0.46
1:B:197:GLU:CD	1:B:197:GLU:H	2.17	0.46
1:B:296:ALA:O	1:B:297:GLU:C	2.54	0.46
1:B:495:TYR:HA	1:B:498:ARG:CZ	2.46	0.46
1:B:537:ARG:C	1:B:540:VAL:HG12	2.35	0.46
1:A:245:MET:CB	1:A:249:ARG:HH21	2.28	0.46
1:A:353:SER:CB	1:A:394:VAL:HG21	2.29	0.46
1:A:358:LYS:HE3	1:A:396:GLY:H	1.80	0.46
1:A:418:ARG:NH1	1:B:425:GLU:OE2	2.49	0.46
1:A:452:VAL:HG13	1:A:497:HIS:HE1	1.79	0.46
1:B:93:LEU:C	1:B:95:SER:H	2.19	0.46
1:B:534:ALA:O	1:B:536:VAL:N	2.49	0.46
1:A:159:SER:OG	1:A:162:VAL:HG23	2.16	0.46
1:A:314:SER:O	1:A:316:ASP:N	2.49	0.46
1:B:84:GLU:HB3	1:B:85:TYR:HD1	1.81	0.46
1:B:218:ASP:OD1	1:B:218:ASP:N	2.49	0.46
1:A:127:HIS:O	1:A:130:PRO:HD2	2.16	0.46
1:A:171:ARG:HH21	1:A:204:GLU:HG2	1.80	0.46
1:A:189:LEU:HD21	1:A:209:PHE:HA	1.98	0.46
1:A:102:THR:O	1:A:103:VAL:C	2.54	0.45
1:A:165:GLU:O	1:A:166:LEU:C	2.52	0.45
1:A:198:LEU:H	1:A:198:LEU:CD2	2.29	0.45
1:A:209:PHE:CD1	1:A:231:ILE:HD12	2.52	0.45
1:A:479:HIS:ND1	1:A:479:HIS:C	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ARG:HB3	1:B:80:VAL:HG23	1.98	0.45
1:A:112:LEU:HD13	1:A:150:LEU:HD11	1.99	0.45
1:A:280:LYS:HA	1:A:284:VAL:CG2	2.46	0.45
1:A:296:ALA:C	1:A:298:VAL:N	2.68	0.45
1:A:427:MET:CE	1:A:427:MET:HA	2.46	0.45
1:B:316:ASP:O	1:B:317:CYS:C	2.55	0.45
1:B:411:LEU:HB3	1:B:423:ILE:CG1	2.47	0.45
1:B:413:GLU:C	1:B:414:ASP:O	2.52	0.45
1:B:430:LEU:HD23	1:B:430:LEU:O	2.15	0.45
2:C:100:TRP:O	2:C:102:GLU:N	2.49	0.45
2:C:114:LEU:HD12	2:C:114:LEU:N	2.31	0.45
1:A:107:LYS:CD	1:A:110:GLU:OE1	2.62	0.45
1:A:340:HIS:O	1:A:341:VAL:C	2.53	0.45
2:D:122:HIS:CD2	2:D:133:LEU:HD12	2.51	0.45
1:A:120:SER:O	1:A:123:ASP:N	2.50	0.45
1:A:151:PHE:CD1	1:A:151:PHE:N	2.84	0.45
1:A:280:LYS:HG2	1:A:280:LYS:O	2.15	0.45
1:A:502:LEU:HD13	1:A:540:VAL:HA	1.99	0.45
1:B:16:LEU:HD11	1:B:31:SER:OG	2.16	0.45
1:B:116:SER:O	1:B:119:HIS:HB2	2.17	0.45
1:B:271:GLN:HE22	1:B:312:ASN:HB2	1.80	0.45
1:B:421:LEU:O	1:B:425:GLU:HG3	2.17	0.45
1:A:70:ALA:HB2	1:A:96:LEU:HD13	1.98	0.45
1:B:248:LEU:O	1:B:251:ALA:HB3	2.17	0.45
1:B:409:VAL:HG13	1:B:446:LEU:CD2	2.46	0.45
2:D:115:LEU:HD12	2:D:115:LEU:O	2.16	0.45
1:A:405:LEU:O	1:A:409:VAL:HG23	2.17	0.45
1:A:496:LEU:HD23	1:A:499:MET:CE	2.45	0.45
1:B:245:MET:CE	1:B:278:ILE:HG22	2.47	0.45
1:A:528:MET:C	1:A:530:GLY:N	2.70	0.45
1:B:539:ASN:HA	1:B:542:LYS:HD3	1.97	0.45
1:B:35:LEU:O	1:B:35:LEU:HG	2.16	0.45
1:B:102:THR:O	1:B:103:VAL:C	2.54	0.45
1:B:481:THR:CG2	1:B:482:ILE:HD13	2.47	0.45
1:A:427:MET:HE3	1:A:430:LEU:HD13	1.99	0.45
2:C:93:ASP:C	2:C:95:MET:N	2.70	0.45
1:A:176:ASP:O	1:A:182:ARG:NH1	2.47	0.44
1:A:296:ALA:O	1:A:298:VAL:N	2.50	0.44
1:A:372:GLN:C	1:A:374:LYS:N	2.71	0.44
1:B:42:LEU:H	1:B:42:LEU:CD2	2.29	0.44
1:B:101:GLU:O	1:B:104:VAL:HB	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:LEU:HD12	1:B:404:LEU:HD22	1.99	0.44
1:B:414:ASP:OD1	1:B:415:ALA:N	2.47	0.44
1:B:466:LEU:O	1:B:467:LYS:C	2.56	0.44
1:B:182:ARG:NE	1:B:215:ASP:OD2	2.43	0.44
1:B:317:CYS:O	1:B:318:ARG:C	2.56	0.44
1:B:467:LYS:O	1:B:471:GLU:HG3	2.17	0.44
2:D:98:LYS:O	2:D:99:GLN:HB2	2.16	0.44
1:A:424:ILE:HG12	1:A:450:TRP:CE3	2.53	0.44
2:C:115:LEU:HD13	2:C:141:PHE:CB	2.45	0.44
2:C:162:ASP:O	2:C:166:GLN:HG3	2.17	0.44
1:A:352:LEU:HA	1:A:355:ILE:CG2	2.48	0.44
1:B:178:THR:HG22	1:B:180:MET:CG	2.39	0.44
1:A:100:GLU:O	1:A:105:ARG:NH1	2.42	0.44
1:A:154:CYS:O	1:A:156:PRO:N	2.51	0.44
1:A:326:ILE:H	1:A:326:ILE:CD1	2.29	0.44
1:A:538:PHE:CD1	1:A:538:PHE:C	2.90	0.44
1:B:84:GLU:HB3	1:B:85:TYR:CD1	2.52	0.44
1:B:322:ILE:HG21	1:B:356:LEU:HD21	1.98	0.44
2:D:100:TRP:O	2:D:102:GLU:N	2.51	0.44
1:A:133:LYS:HG2	1:A:169:TYR:CE1	2.53	0.44
1:A:439:PHE:CD1	1:A:443:LEU:HB3	2.53	0.44
1:B:198:LEU:HD12	1:B:202:LYS:HE3	1.99	0.44
1:B:368:LEU:O	1:B:372:GLN:HG3	2.18	0.44
1:B:316:ASP:OD1	1:B:317:CYS:N	2.51	0.44
1:B:366:LEU:O	1:B:367:PRO:C	2.56	0.44
1:A:556:LEU:O	1:A:560:VAL:HB	2.17	0.44
1:B:268:THR:HG21	1:B:308:GLU:HG2	2.00	0.44
1:B:372:GLN:C	1:B:374:LYS:N	2.71	0.44
1:B:405:LEU:O	1:B:409:VAL:HG23	2.18	0.44
1:B:560:VAL:HG12	1:B:561:LYS:N	2.33	0.44
1:A:42:LEU:HB3	1:A:46:ARG:CB	2.48	0.44
1:A:52:LEU:HB2	1:A:53:PRO:HD3	1.99	0.44
1:B:17:ILE:O	1:B:21:ARG:HG2	2.17	0.44
1:B:552:ASP:OD1	1:B:554:SER:HB3	2.18	0.44
1:B:565:GLU:C	1:B:567:LEU:N	2.72	0.44
1:A:35:LEU:O	1:A:35:LEU:CG	2.65	0.43
1:A:179:PRO:HD2	1:A:180:MET:CE	2.48	0.43
1:A:265:ASP:O	1:A:305:LYS:NZ	2.48	0.43
1:A:495:TYR:CD2	1:A:533:VAL:HG11	2.53	0.43
1:B:21:ARG:O	1:B:22:ASN:C	2.57	0.43
2:D:93:ASP:HB2	2:D:96:TYR:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:CYS:C	1:A:508:LEU:HD23	2.37	0.43
1:A:539:ASN:HA	1:A:542:LYS:HD3	2.00	0.43
1:A:584:THR:HG22	1:A:584:THR:O	2.17	0.43
1:B:99:VAL:HG12	1:B:101:GLU:N	2.31	0.43
1:B:300:ALA:O	1:B:301:ALA:C	2.56	0.43
1:B:427:MET:CE	1:B:430:LEU:HB3	2.46	0.43
1:B:521:MET:O	1:B:525:VAL:HG23	2.18	0.43
1:A:380:VAL:O	1:A:381:ARG:C	2.56	0.43
1:A:540:VAL:O	1:A:544:LEU:HG	2.18	0.43
1:A:565:GLU:C	1:A:567:LEU:N	2.70	0.43
1:B:61:ASP:HB3	1:B:65:VAL:HG21	1.98	0.43
1:B:519:LYS:O	1:B:519:LYS:CG	2.65	0.43
1:B:58:THR:CG2	1:B:59:ILE:H	2.11	0.43
1:B:78:THR:C	1:B:80:VAL:N	2.70	0.43
1:B:282:ASP:O	1:B:285:PRO:HD2	2.18	0.43
1:A:45:GLU:OE1	1:A:48:ARG:NH2	2.52	0.43
1:B:180:MET:CE	2:D:147:TRP:HA	2.48	0.43
1:B:317:CYS:O	1:B:320:ASN:N	2.51	0.43
1:B:487:LEU:HD22	1:B:524:THR:HG21	2.00	0.43
1:A:331:LYS:HG3	1:A:368:LEU:HD21	2.00	0.43
1:A:166:LEU:O	1:A:169:TYR:N	2.51	0.43
1:A:487:LEU:HD22	1:A:524:THR:CB	2.48	0.43
1:B:20:LEU:O	1:B:22:ASN:N	2.51	0.43
1:B:47:THR:HG23	1:B:51:LEU:HD23	2.01	0.43
2:C:134:VAL:HG11	2:C:147:TRP:HZ3	1.83	0.43
1:B:279:THR:HA	1:B:283:LEU:HG	2.01	0.43
2:C:120:MET:O	2:C:121:LYS:C	2.57	0.43
1:A:21:ARG:O	1:A:22:ASN:C	2.57	0.43
1:A:120:SER:OG	1:A:123:ASP:CG	2.57	0.43
1:A:154:CYS:O	1:A:156:PRO:HD2	2.19	0.43
1:A:390:CYS:SG	1:A:391:VAL:N	2.92	0.43
1:A:508:LEU:N	1:A:508:LEU:HD22	2.34	0.43
1:B:58:THR:O	1:B:59:ILE:O	2.37	0.43
1:A:359:ASP:O	1:A:360:ASN:C	2.56	0.43
1:A:500:THR:O	1:A:503:PHE:HB2	2.18	0.43
1:A:535:ASN:HA	1:A:538:PHE:HD2	1.83	0.43
1:B:138:GLY:O	1:B:144:ARG:HD2	2.19	0.43
1:B:409:VAL:HG13	1:B:446:LEU:HD22	1.99	0.43
1:A:77:THR:O	1:A:82:GLY:HA2	2.19	0.42
1:A:80:VAL:HG22	1:A:80:VAL:O	2.19	0.42
1:B:206:ILE:HG13	1:B:243:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:LYS:HG3	1:B:362:ILE:HD11	2.01	0.42
1:B:383:ASN:O	1:B:386:SER:HB3	2.19	0.42
2:C:96:TYR:HA	2:C:114:LEU:HD13	2.01	0.42
1:A:69:LEU:HD12	1:A:69:LEU:O	2.18	0.42
1:A:577:TYR:HD1	1:A:577:TYR:O	2.02	0.42
1:B:51:LEU:O	1:B:54:PHE:HB3	2.19	0.42
1:B:267:PHE:HA	1:B:270:LEU:HD12	2.00	0.42
1:B:439:PHE:CD1	1:B:443:LEU:HB3	2.53	0.42
1:A:178:THR:HB	1:A:180:MET:HG2	2.00	0.42
1:A:405:LEU:N	1:A:406:PRO:CD	2.81	0.42
1:A:518:THR:HG23	1:A:555:THR:HG21	2.01	0.42
1:A:561:LYS:CD	1:A:588:LEU:HD22	2.40	0.42
1:B:46:ARG:O	1:B:47:THR:C	2.56	0.42
1:B:245:MET:O	1:B:246:PRO:C	2.55	0.42
2:C:102:GLU:O	2:C:103:CYS:C	2.58	0.42
1:A:67:LEU:HD12	1:A:107:LYS:HG3	2.01	0.42
1:A:125:GLU:CG	1:A:162:VAL:HG21	2.44	0.42
1:A:177:ASP:OD1	1:A:177:ASP:N	2.53	0.42
1:A:224:ALA:O	1:A:227:ALA:N	2.52	0.42
1:A:368:LEU:HD23	1:A:368:LEU:HA	1.83	0.42
1:B:43:GLY:H	1:B:46:ARG:HB2	1.84	0.42
1:B:107:LYS:HD3	1:B:110:GLU:OE1	2.19	0.42
2:D:164:ILE:HD13	2:D:164:ILE:HA	1.85	0.42
1:A:193:ALA:HB2	1:A:205:ILE:HD12	2.00	0.42
1:A:498:ARG:O	1:A:501:THR:HB	2.19	0.42
1:A:561:LYS:CG	1:A:588:LEU:HD13	2.49	0.42
1:B:291:MET:HB3	1:B:333:LEU:HD11	2.01	0.42
1:B:317:CYS:SG	1:B:318:ARG:N	2.93	0.42
1:A:11:TYR:CB	1:A:12:PRO:CD	2.97	0.42
1:A:436:VAL:CG1	1:A:437:GLU:N	2.81	0.42
1:B:38:ILE:N	1:B:38:ILE:CD1	2.82	0.42
1:B:128:PHE:O	1:B:131:LEU:N	2.49	0.42
1:A:412:ALA:HB1	1:A:450:TRP:CZ2	2.55	0.42
1:A:506:ASN:HD22	1:A:546:LYS:HG2	1.84	0.42
1:A:564:LEU:O	1:A:564:LEU:HD23	2.19	0.42
1:B:197:GLU:O	1:B:198:LEU:C	2.58	0.42
2:D:95:MET:O	2:D:114:LEU:HD13	2.19	0.42
2:D:100:TRP:CZ3	2:D:104:ALA:HB2	2.54	0.42
1:A:49:SER:OG	1:A:50:GLU:N	2.52	0.42
1:A:568:THR:HG22	1:A:580:GLN:HB2	2.00	0.42
1:B:34:LYS:C	1:B:36:SER:N	2.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:LEU:O	1:B:92:PRO:HD2	2.20	0.42
1:B:317:CYS:O	1:B:320:ASN:HB2	2.20	0.42
1:A:140:TRP:CD1	1:A:140:TRP:N	2.85	0.42
1:A:310:CYS:HB3	1:A:322:ILE:HD11	2.02	0.42
1:B:29:LEU:C	1:B:31:SER:N	2.72	0.42
1:B:222:LEU:HD23	1:B:262:MET:HG3	2.02	0.42
1:B:237:GLN:HE21	1:B:237:GLN:HB3	1.57	0.42
1:B:365:LEU:HD23	1:B:368:LEU:HD12	2.02	0.42
1:B:552:ASP:O	1:B:554:SER:N	2.53	0.42
1:B:562:PRO:C	1:B:564:LEU:H	2.23	0.42
1:A:46:ARG:HA	1:A:49:SER:OG	2.20	0.42
1:A:98:THR:O	1:A:98:THR:CG2	2.66	0.42
1:A:412:ALA:HB1	1:A:450:TRP:HZ2	1.84	0.42
1:B:178:THR:CG2	1:B:180:MET:CG	2.98	0.42
1:B:352:LEU:O	1:B:355:ILE:HB	2.19	0.42
1:B:474:GLY:O	1:B:477:TRP:HB3	2.19	0.42
1:A:133:LYS:HE2	1:A:169:TYR:CE1	2.55	0.41
1:A:333:LEU:HD22	1:A:341:VAL:CG1	2.49	0.41
1:A:355:ILE:CG2	1:A:356:LEU:N	2.83	0.41
1:A:456:TYR:HD1	1:A:457:ALA:N	2.17	0.41
1:A:508:LEU:CD2	1:A:508:LEU:N	2.83	0.41
1:B:353:SER:HB3	1:B:394:VAL:HG21	2.01	0.41
1:B:571:GLN:O	1:B:572:ASP:C	2.59	0.41
1:A:112:LEU:HD13	1:A:150:LEU:CD1	2.50	0.41
1:A:427:MET:HE3	1:A:430:LEU:CD1	2.50	0.41
1:B:502:LEU:HD13	1:B:540:VAL:HA	2.02	0.41
1:B:561:LYS:CD	1:B:588:LEU:HD22	2.50	0.41
1:A:224:ALA:O	1:A:227:ALA:HB3	2.20	0.41
1:A:482:ILE:O	1:A:483:ILE:C	2.59	0.41
1:B:180:MET:HG2	1:B:180:MET:H	1.63	0.41
1:B:257:TRP:CB	1:B:295:GLU:HG3	2.50	0.41
1:B:284:VAL:O	1:B:285:PRO:C	2.55	0.41
2:C:134:VAL:HG11	2:C:147:TRP:CZ3	2.55	0.41
1:A:214:SER:HA	1:A:221:ARG:HD2	2.00	0.41
1:A:284:VAL:HB	1:A:285:PRO:HD3	2.02	0.41
1:A:369:PHE:O	1:A:373:LEU:HD22	2.20	0.41
1:A:390:CYS:O	1:A:391:VAL:C	2.59	0.41
1:A:565:GLU:O	1:A:567:LEU:N	2.53	0.41
1:B:282:ASP:C	1:B:285:PRO:HD2	2.41	0.41
1:B:336:ASP:O	1:B:342:LYS:HE2	2.20	0.41
2:C:135:TRP:CZ3	2:C:139:TYR:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:THR:HG22	1:A:105:ARG:CZ	2.50	0.41
1:A:417:TRP:HB3	1:A:455:VAL:HG11	2.02	0.41
1:A:576:LYS:O	1:A:577:TYR:C	2.59	0.41
1:B:16:LEU:O	1:B:20:LEU:N	2.53	0.41
1:B:179:PRO:HG3	1:B:182:ARG:HH22	1.86	0.41
1:B:323:MET:HE2	1:B:323:MET:HB2	1.94	0.41
2:D:122:HIS:NE2	2:D:133:LEU:HD12	2.35	0.41
1:A:546:LYS:C	1:A:548:GLY:H	2.24	0.41
1:B:377:CYS:HA	1:B:378:PRO:HD3	1.86	0.41
1:B:522:LEU:N	1:B:523:PRO:CD	2.83	0.41
2:D:129:ARG:HD3	2:D:131:ASP:HB2	2.02	0.41
1:A:16:LEU:O	1:A:19:GLU:HB2	2.21	0.41
1:A:119:HIS:ND1	1:A:123:ASP:HB3	2.35	0.41
1:A:272:LYS:O	1:A:272:LYS:HG2	2.21	0.41
1:A:439:PHE:HZ	1:A:447:CYS:HG	1.65	0.41
1:B:59:ILE:CD1	1:B:69:LEU:HD22	2.51	0.41
1:B:438:PHE:C	1:B:438:PHE:CD1	2.94	0.41
1:A:63:ASP:HA	1:A:66:LEU:HD12	2.01	0.41
1:A:420:ARG:O	1:A:421:LEU:C	2.59	0.41
1:A:437:GLU:N	1:A:437:GLU:CD	2.73	0.41
1:B:16:LEU:O	1:B:19:GLU:N	2.54	0.41
1:B:180:MET:HE1	2:D:147:TRP:HA	2.03	0.41
1:B:587:SER:C	1:B:588:LEU:HG	2.41	0.41
2:D:134:VAL:CG1	2:D:147:TRP:CZ3	3.04	0.41
1:A:47:THR:CG2	1:A:51:LEU:HD23	2.45	0.41
1:A:482:ILE:C	1:A:484:PRO:HD2	2.41	0.41
1:B:29:LEU:CD2	1:B:33:LYS:HG3	2.51	0.41
1:B:405:LEU:CD1	1:B:409:VAL:HG23	2.51	0.41
1:B:427:MET:CE	1:B:427:MET:HA	2.51	0.41
1:B:527:ARG:HG2	1:B:527:ARG:NH1	2.36	0.41
1:B:537:ARG:HE	1:B:537:ARG:HB2	1.71	0.41
1:B:544:LEU:HD23	1:B:544:LEU:HA	1.93	0.41
1:B:580:GLN:HE21	1:B:580:GLN:HB2	1.60	0.41
2:D:102:GLU:CB	2:D:107:MET:HB2	2.51	0.41
1:B:23:GLU:N	1:B:23:GLU:OE1	2.54	0.41
1:B:451:LEU:HD12	1:B:451:LEU:HA	1.85	0.41
1:B:482:ILE:O	1:B:483:ILE:C	2.60	0.41
1:B:560:VAL:O	1:B:561:LYS:C	2.59	0.41
1:B:565:GLU:O	1:B:568:THR:N	2.49	0.41
2:C:144:PHE:CD2	2:C:160:TRP:HB2	2.56	0.41
1:A:377:CYS:HA	1:A:378:PRO:HD3	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:TRP:C	1:A:452:VAL:N	2.74	0.40
1:B:179:PRO:O	1:B:180:MET:C	2.59	0.40
1:B:270:LEU:O	1:B:274:VAL:HG23	2.22	0.40
1:B:516:ILE:HD13	2:C:101:PRO:HG3	2.02	0.40
1:B:565:GLU:O	1:B:567:LEU:N	2.54	0.40
2:D:115:LEU:HD13	2:D:141:PHE:HB2	2.03	0.40
1:B:29:LEU:HD23	1:B:33:LYS:CG	2.51	0.40
1:B:42:LEU:HB3	1:B:46:ARG:HB2	2.03	0.40
1:B:52:LEU:C	1:B:54:PHE:N	2.74	0.40
1:B:535:ASN:HA	1:B:538:PHE:CE2	2.56	0.40
1:B:538:PHE:CD1	1:B:542:LYS:HD2	2.56	0.40
1:A:178:THR:HA	1:A:179:PRO:HD3	1.95	0.40
1:A:231:ILE:O	1:A:234:LEU:N	2.53	0.40
1:A:389:ASP:OD2	1:A:389:ASP:N	2.37	0.40
1:B:13:ILE:O	1:B:17:ILE:HG13	2.21	0.40
1:B:372:GLN:O	1:B:374:LYS:N	2.54	0.40
1:B:487:LEU:HD11	1:B:520:HIS:O	2.22	0.40
1:B:552:ASP:C	1:B:554:SER:N	2.75	0.40
2:C:148:PHE:O	2:C:149:GLY:C	2.59	0.40
1:A:151:PHE:CD2	1:A:170:PHE:HB2	2.56	0.40
1:A:168:GLN:O	1:A:171:ARG:HB3	2.22	0.40
1:A:362:ILE:HD13	1:A:399:GLN:HG3	2.03	0.40
1:A:561:LYS:HB2	1:A:588:LEU:HD13	2.04	0.40
1:B:370:LEU:HA	1:B:370:LEU:HD13	1.83	0.40
1:B:372:GLN:C	1:B:374:LYS:H	2.24	0.40
1:B:529:ALA:HA	1:B:540:VAL:HG11	2.03	0.40
1:B:552:ASP:C	1:B:554:SER:H	2.24	0.40
2:C:102:GLU:CG	2:C:107:MET:HB2	2.52	0.40
1:A:186:ALA:C	1:A:188:LYS:N	2.74	0.40
1:A:455:VAL:O	1:A:458:ILE:HB	2.21	0.40
1:A:522:LEU:HD22	1:A:551:LEU:CD2	2.51	0.40
1:B:11:TYR:CB	1:B:12:PRO:HD3	2.48	0.40
1:B:437:GLU:H	1:B:437:GLU:CD	2.24	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	577/580 (100%)	417 (72%)	111 (19%)	49 (8%)	1	5
1	B	577/580 (100%)	446 (77%)	90 (16%)	41 (7%)	1	7
2	C	78/88 (89%)	59 (76%)	14 (18%)	5 (6%)	1	9
2	D	78/88 (89%)	65 (83%)	8 (10%)	5 (6%)	1	9
All	All	1310/1336 (98%)	987 (75%)	223 (17%)	100 (8%)	1	6

All (100) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	ASP
1	A	155	TYR
1	A	198	LEU
1	A	274	VAL
1	A	318	ARG
1	A	389	ASP
1	A	391	VAL
1	B	59	ILE
1	B	61	ASP
1	B	76	PHE
1	B	79	LEU
1	B	80	VAL
1	B	317	CYS
1	B	318	ARG
1	B	358	LYS
1	B	414	ASP
1	B	510	GLU
2	C	100	TRP
2	C	135	TRP
2	D	100	TRP
1	A	80	VAL
1	A	94	GLU

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Mol	Chain	Res	Type
1	A	128	PHE
1	A	138	GLY
1	A	148	CYS
1	A	254	ASP
1	A	315	ALA
1	A	394	VAL
1	A	441	GLU
1	A	551	LEU
1	B	22	ASN
1	B	35	LEU
1	B	94	GLU
1	B	254	ASP
1	B	389	ASP
1	B	535	ASN
2	D	135	TRP
1	A	11	TYR
1	A	22	ASN
1	A	59	ILE
1	A	79	LEU
1	A	176	ASP
1	A	353	SER
1	A	373	LEU
1	A	440	ASP
1	A	484	PRO
1	A	515	ASP
1	A	523	PRO
1	A	547	ILE
1	A	560	VAL
1	A	571	GLN
1	B	11	TYR
1	B	148	CYS
1	B	198	LEU
1	B	316	ASP
1	B	456	TYR
1	B	571	GLN
1	B	587	SER
2	C	99	GLN
2	C	102	GLU
1	A	21	ARG
1	A	41	ALA
1	A	76	PHE
1	A	83	PRO

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Mol	Chain	Res	Type
1	A	154	CYS
1	A	271	GLN
1	A	529	ALA
1	B	41	ALA
1	B	73	LEU
1	B	83	PRO
1	B	301	ALA
1	B	315	ALA
1	B	441	GLU
1	B	475	LYS
1	B	577	TYR
1	A	55	LEU
1	A	57	ASP
1	A	86	VAL
1	A	97	ALA
1	A	201	VAL
1	A	587	SER
1	B	306	VAL
1	B	320	ASN
1	B	484	PRO
1	B	553	ASN
1	B	563	ILE
1	A	320	ASN
1	B	572	ASP
2	D	99	GLN
1	A	306	VAL
1	A	432	GLY
1	B	562	PRO
2	C	101	PRO
1	A	563	ILE
1	B	560	VAL
2	D	101	PRO
2	D	136	VAL
1	A	104	VAL
1	B	483	ILE
1	B	327	LEU

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	507/507 (100%)	467 (92%)	40 (8%)	12 37
1	B	507/507 (100%)	462 (91%)	45 (9%)	9 32
2	C	73/81 (90%)	68 (93%)	5 (7%)	16 44
2	D	73/81 (90%)	64 (88%)	9 (12%)	4 20
All	All	1160/1176 (99%)	1061 (92%)	99 (8%)	10 35

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	GLU
1	A	40	LEU
1	A	76	PHE
1	A	84	GLU
1	A	90	LEU
1	A	131	LEU
1	A	145	THR
1	A	146	SER
1	A	153	VAL
1	A	175	SER
1	A	177	ASP
1	A	178	THR
1	A	180	MET
1	A	214	SER
1	A	237	GLN
1	A	278	ILE
1	A	294	CYS
1	A	297	GLU
1	A	313	LEU
1	A	316	ASP
1	A	370	LEU
1	A	373	LEU
1	A	382	LEU
1	A	389	ASP
1	A	395	ILE
1	A	399	GLN
1	A	405	LEU
1	A	411	LEU
1	A	418	ARG
1	A	429	LEU

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Mol	Chain	Res	Type
1	A	430	LEU
1	A	437	GLU
1	A	438	PHE
1	A	443	LEU
1	A	444	ASN
1	A	455	VAL
1	A	476	GLU
1	A	508	LEU
1	A	538	PHE
1	A	577	TYR
1	B	23	GLU
1	B	36	SER
1	B	76	PHE
1	B	84	GLU
1	B	101	GLU
1	B	106	ASP
1	B	115	ILE
1	B	116	SER
1	B	141	PHE
1	B	142	THR
1	B	175	SER
1	B	176	ASP
1	B	180	MET
1	B	198	LEU
1	B	217	GLN
1	B	219	SER
1	B	222	LEU
1	B	237	GLN
1	B	263	VAL
1	B	278	ILE
1	B	294	CYS
1	B	297	GLU
1	B	320	ASN
1	B	332	GLU
1	B	370	LEU
1	B	373	LEU
1	B	389	ASP
1	B	390	CYS
1	B	399	GLN
1	B	405	LEU
1	B	411	LEU
1	B	413	GLU

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Mol	Chain	Res	Type
1	B	418	ARG
1	B	429	LEU
1	B	437	GLU
1	B	438	PHE
1	B	443	LEU
1	B	448	MET
1	B	451	LEU
1	B	455	VAL
1	B	476	GLU
1	B	481	THR
1	B	538	PHE
1	B	549	PRO
1	B	577	TYR
2	C	115	LEU
2	C	125	ARG
2	C	128	TYR
2	C	131	ASP
2	C	151	ASP
2	D	105	LYS
2	D	115	LEU
2	D	118	LEU
2	D	125	ARG
2	D	128	TYR
2	D	131	ASP
2	D	151	ASP
2	D	158	LEU
2	D	168	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	200	ASN
1	A	211	ASN
1	A	271	GLN
1	A	392	ASN
1	A	399	GLN
1	A	444	ASN
1	A	465	ASN
1	A	497	HIS
1	A	506	ASN
1	A	580	GLN
1	B	119	HIS

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Mol	Chain	Res	Type
1	B	168	GLN
1	B	200	ASN
1	B	211	ASN
1	B	237	GLN
1	B	271	GLN
1	B	288	GLN
1	B	338	ASN
1	B	383	ASN
1	B	392	ASN
1	B	399	GLN
1	B	433	GLN
1	B	444	ASN
1	B	465	ASN
1	B	506	ASN
1	B	514	GLN
1	B	580	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	579/580 (99%)	0.16	36 (6%) 20 20	17, 77, 147, 180	0
1	B	579/580 (99%)	-0.10	6 (1%) 82 82	15, 55, 142, 175	0
2	C	80/88 (90%)	-0.11	0 100 100	29, 54, 97, 117	0
2	D	80/88 (90%)	0.03	1 (1%) 77 77	28, 60, 98, 111	0
All	All	1318/1336 (98%)	0.02	43 (3%) 46 44	15, 65, 143, 180	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	13	ILE	8.5
1	A	11	TYR	8.3
1	A	12	PRO	6.9
1	B	14	ALA	6.6
1	A	10	LEU	6.4
1	A	14	ALA	6.4
1	A	13	ILE	5.6
1	A	35	LEU	5.1
1	A	32	ILE	4.1
1	B	17	ILE	3.9
1	A	57	ASP	3.5
1	A	23	GLU	3.3
1	A	164	ALA	3.3
1	A	192	PHE	3.2
1	A	165	GLU	3.1
1	A	18	ASP	3.0
1	A	17	ILE	2.9
1	A	161	ALA	2.9
1	A	53	PRO	2.8
1	A	36	SER	2.8
1	B	11	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	30	ASN	2.8
1	A	31	SER	2.6
1	B	12	PRO	2.6
1	A	150	LEU	2.5
1	A	15	VAL	2.5
1	A	66	LEU	2.4
1	A	544	LEU	2.4
1	A	52	LEU	2.4
1	A	151	PHE	2.4
1	A	502	LEU	2.4
1	A	89	LEU	2.3
1	A	168	GLN	2.3
1	A	38	ILE	2.3
1	A	16	LEU	2.2
1	A	29	LEU	2.2
1	A	59	ILE	2.1
1	A	132	VAL	2.1
1	A	566	LYS	2.1
1	A	50	GLU	2.1
2	D	94	ALA	2.0
1	A	535	ASN	2.0
1	B	23	GLU	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
3	ZN	C	175	1/1	0.99	0.12	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	D	175	1/1	0.99	0.13	57,57,57,57	0
3	ZN	D	176	1/1	0.99	0.10	38,38,38,38	0
3	ZN	C	176	1/1	1.00	0.12	40,40,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.