Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:52 AM GMT

PDB ID	:	2J42
Title	:	LOW QUALITY CRYSTAL STRUCTURE OF THE TRANSPORT COMPONENT C2-II OF THE C2-TOXIN FROM CLOSTRIDIUM BOTULINUM
Authors	:	Schleberger, C.; Hochmann, H.; Barth, H.; Aktories, K.; Schulz, G.E.
Deposited on	:	2006-08-24
Resolution	:	3.13 Å(reported)

The following versions of software and data (see references (i)) 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 3.13 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	Percentile Ranks	Value
Rfree		0.471
Clashscore		80
Ramachandran outliers		14.3%
Sidechain outliers		26.6%
RSRZ outliers		23.6%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
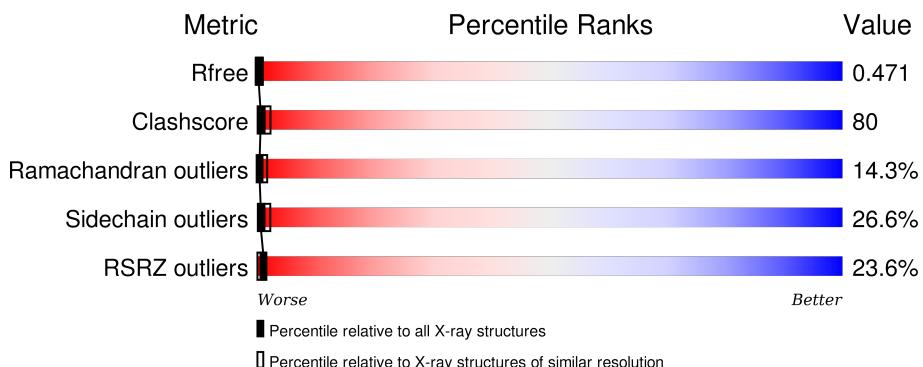
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1095 (3.18-3.10)
Clashscore	102246	1202 (3.18-3.10)
Ramachandran outliers	100387	1162 (3.18-3.10)
Sidechain outliers	100360	1162 (3.18-3.10)
RSRZ outliers	91569	1097 (3.18-3.10)

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	721	17% 15% 36% 17% • 30%
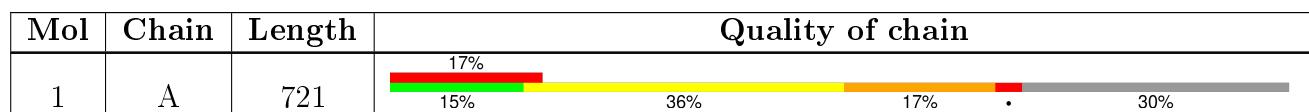
2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3948 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 C2 TOXIN COMPONENT-II.

| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	505	Total 3948	C 2493	N 654	O 786	S 15	0	0	1

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	357	ALA	GLY	CONFLICT	UNP O86171
A	494	LEU	PHE	CONFLICT	UNP O86171
A	495	PRO	SER	CONFLICT	UNP O86171
A	496	ASP	GLY	CONFLICT	UNP O86171
A	517	ARG	LYS	CONFLICT	UNP O86171
A	529	ARG	ALA	CONFLICT	UNP O86171
A	542	MET	LEU	CONFLICT	UNP O86171
A	556	ARG	SER	CONFLICT	UNP O86171
A	560	VAL	ASN	CONFLICT	UNP O86171
A	571	ASN	ASP	CONFLICT	UNP O86171
A	576	ASN	HIS	CONFLICT	UNP O86171

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: C2 TOXIN COMPONENT-II
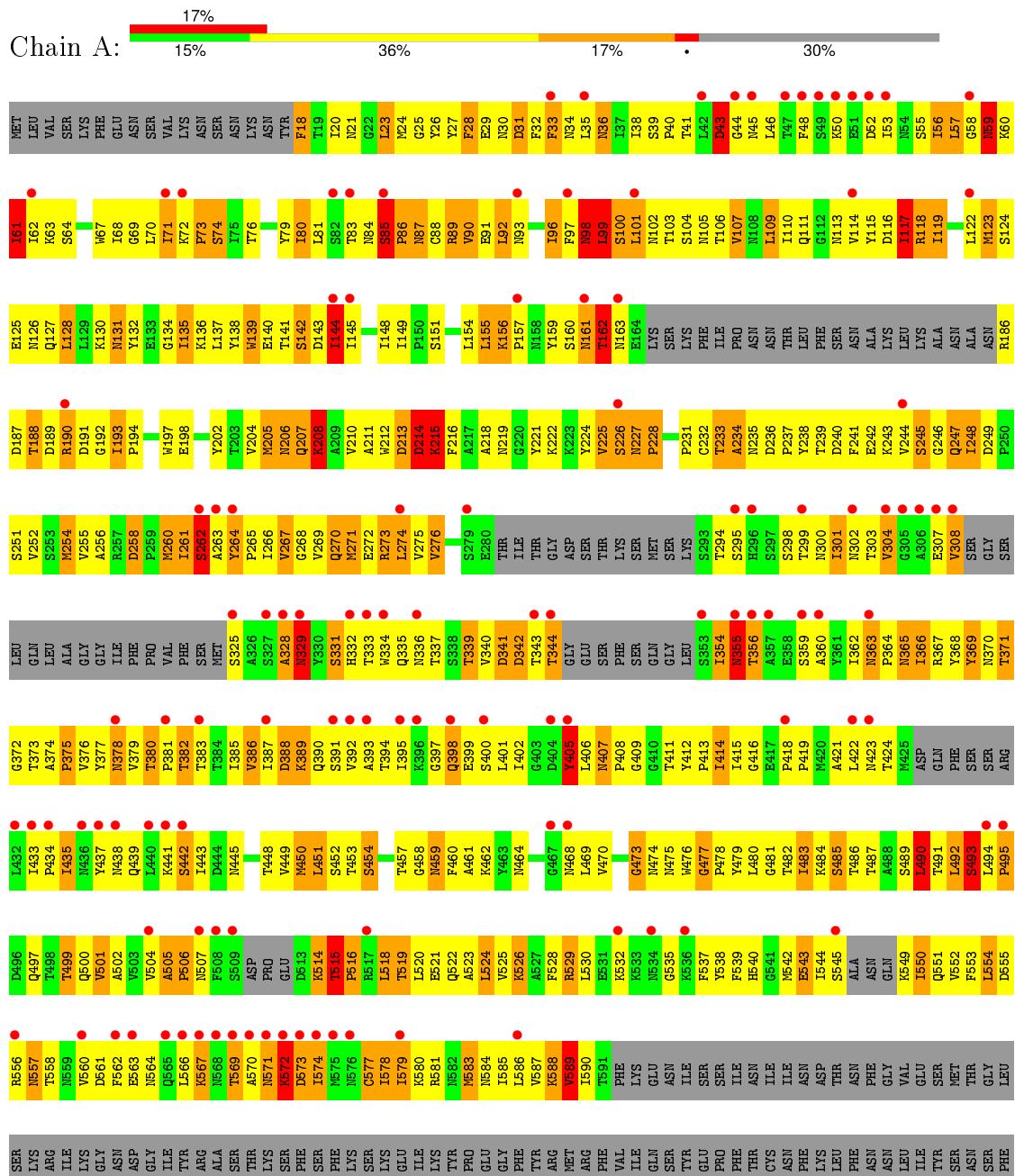
ASP ILE GLY TYR TYR ASP GLU PHE PHE TYR PHE TYR CYS ASN GLY SER LYS SER PHE PHE ASP ILE SER CYS ASP ILE ILE ASN SER ILE ASN ARG LEU SER GLY VAL PHE LEU ILE GLU LEU ASP LYS LEU ILE ILE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	104.40Å 104.40Å 153.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.13 61.76 – 3.13	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.13) 99.6 (61.76-3.13)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	4.99 (at 3.13Å)	Xtriage
Refinement program	TNT BUSTER/TNT	Depositor
R, R_{free}	0.413 , 0.433 0.443 , 0.471	Depositor DCC
R_{free} test set	773 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	84.0	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 90.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.48, <L^2> = 0.31$	Xtriage
Outliers	1 of 15485 reflections (0.006%)	Xtriage
F_o,F_c correlation	0.63	EDS
Total number of atoms	3948	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

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	0.26	0/4019	0.68	4/5461 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	85	SER	C-N-CD	-33.67	46.52	120.60
1	A	374	ALA	C-N-CD	-7.90	103.23	120.60
1	A	227	ASN	C-N-CD	-7.04	105.11	120.60
1	A	515	THR	C-N-CD	-6.37	106.58	120.60

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	3948	0	3888	629	0
All	All	3948	0	3888	629	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 80.

All (629) 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:83:THR:HG23	1:A:98:ASN:HD21	1.10	1.16
1:A:586:LEU:HD21	1:A:588:LYS:HE2	1.31	1.11
1:A:507:ASN:HB2	1:A:581:ARG:HD2	1.36	1.08
1:A:461:ALA:HB1	1:A:470:VAL:HG13	1.36	1.07
1:A:528:PHE:HB2	1:A:530:LEU:HD11	1.38	1.04
1:A:260:MET:HE2	1:A:526:LYS:HD2	1.38	1.04
1:A:337:THR:HG22	1:A:339:THR:HG23	1.38	1.02
1:A:414:ILE:HG23	1:A:416:GLY:H	1.21	1.02
1:A:70:LEU:HD13	1:A:114:VAL:HG11	1.41	1.01
1:A:543:GLU:HB2	1:A:549:LYS:HE3	1.44	1.00
1:A:267:VAL:HG12	1:A:268:GLY:H	1.28	0.99
1:A:554:LEU:HD23	1:A:585:ILE:HG12	1.44	0.99
1:A:386:VAL:HG13	1:A:391:SER:HA	1.43	0.98
1:A:492:LEU:HD13	1:A:587:VAL:HG12	1.45	0.98
1:A:379:VAL:HB	1:A:458:GLY:N	1.79	0.98
1:A:236:ASP:HB2	1:A:237:PRO:HD2	1.46	0.98
1:A:379:VAL:H	1:A:458:GLY:HA3	1.26	0.97
1:A:204:VAL:HG12	1:A:208:LYS:HG2	1.47	0.96
1:A:23:LEU:HG	1:A:154:LEU:HD22	1.47	0.95
1:A:586:LEU:HD12	1:A:587:VAL:H	1.30	0.95
1:A:28:PHE:HD2	1:A:35:LEU:H	1.15	0.94
1:A:274:LEU:HD23	1:A:274:LEU:H	1.33	0.93
1:A:298:SER:HB2	1:A:334:TRP:CZ2	2.04	0.92
1:A:328:ALA:HB3	1:A:484:LYS:HE2	1.52	0.92
1:A:335:GLN:HG2	1:A:336:ASN:H	1.33	0.92
1:A:462:LYS:HE3	1:A:473:GLY:HA3	1.51	0.91
1:A:30:ASN:HB2	1:A:34:ASN:HD22	1.38	0.89
1:A:53:ILE:HD11	1:A:130:LYS:HG2	1.55	0.89
1:A:238:TYR:CD2	1:A:248:ILE:HD11	2.09	0.88
1:A:29:GLU:HB2	1:A:36:ASN:ND2	1.89	0.88
1:A:366:ILE:HD13	1:A:422:LEU:HD21	1.54	0.87
1:A:71:ILE:HD11	1:A:92:LEU:HD21	1.56	0.87
1:A:83:THR:HG23	1:A:98:ASN:ND2	1.91	0.86
1:A:586:LEU:HD21	1:A:588:LYS:CE	2.04	0.86
1:A:23:LEU:CG	1:A:154:LEU:HD22	2.05	0.86
1:A:461:ALA:HB1	1:A:470:VAL:CG1	2.06	0.86
1:A:354:ILE:HD12	1:A:437:TYR:HE1	1.40	0.85
1:A:23:LEU:HD11	1:A:117:ILE:HD12	1.58	0.85
1:A:70:LEU:HD22	1:A:114:VAL:HG12	1.56	0.85
1:A:363:ASN:ND2	1:A:423:ASN:HB2	1.91	0.85
1:A:334:TRP:CD1	1:A:449:VAL:HG22	2.12	0.85
1:A:494:LEU:HD23	1:A:589:VAL:HG21	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:ARG:HG3	1:A:529:ARG:HH21	1.43	0.83
1:A:386:VAL:HG13	1:A:391:SER:CA	2.08	0.83
1:A:70:LEU:HB2	1:A:155:LEU:HG	1.61	0.82
1:A:276:VAL:HG13	1:A:362:ILE:CB	2.10	0.82
1:A:276:VAL:HG13	1:A:362:ILE:HB	1.60	0.82
1:A:72:LYS:HB3	1:A:114:VAL:HG22	1.62	0.81
1:A:387:ILE:CD1	1:A:449:VAL:HG12	2.10	0.81
1:A:136:LYS:HE2	1:A:148:ILE:HD11	1.60	0.81
1:A:343:THR:HG23	1:A:344:THR:HG22	1.61	0.81
1:A:365:ASN:HA	1:A:421:ALA:HA	1.60	0.81
1:A:125:GLU:HB3	1:A:127:GLN:NE2	1.96	0.81
1:A:79:TYR:CD1	1:A:109:LEU:HB2	2.16	0.81
1:A:558:THR:HA	1:A:561:ASP:HB2	1.63	0.81
1:A:234:ALA:HB1	1:A:262:SER:HA	1.62	0.81
1:A:71:ILE:CD1	1:A:92:LEU:HD21	2.11	0.80
1:A:276:VAL:HG13	1:A:362:ILE:CG1	2.11	0.80
1:A:563:GLU:O	1:A:567:LYS:HB2	1.81	0.80
1:A:26:TYR:CD2	1:A:38:ILE:HG12	2.17	0.79
1:A:265:PRO:HD3	1:A:476:TRP:CH2	2.17	0.79
1:A:407:ASN:ND2	1:A:407:ASN:N	2.29	0.79
1:A:407:ASN:ND2	1:A:407:ASN:H	1.79	0.79
1:A:117:ILE:HG22	1:A:118:ARG:H	1.47	0.79
1:A:79:TYR:HD1	1:A:109:LEU:HB2	1.46	0.78
1:A:530:LEU:HD22	1:A:537:PHE:CZ	2.18	0.78
1:A:407:ASN:HD22	1:A:407:ASN:N	1.82	0.78
1:A:387:ILE:HD11	1:A:449:VAL:HG12	1.66	0.78
1:A:232:CYS:SG	1:A:239:THR:HA	2.23	0.78
1:A:328:ALA:HB3	1:A:484:LYS:CE	2.12	0.78
1:A:328:ALA:HB3	1:A:484:LYS:CD	2.13	0.77
1:A:328:ALA:HB3	1:A:484:LYS:HD3	1.66	0.77
1:A:38:ILE:HB	1:A:208:LYS:NZ	1.99	0.77
1:A:86:PRO:HB3	1:A:123:MET:SD	2.24	0.77
1:A:411:THR:OG1	1:A:414:ILE:HA	1.85	0.76
1:A:232:CYS:SG	1:A:239:THR:HG22	2.24	0.76
1:A:80:ILE:HG13	1:A:140:GLU:O	1.84	0.76
1:A:493:SER:HA	1:A:497:GLN:O	1.85	0.76
1:A:494:LEU:HD13	1:A:539:PHE:CD2	2.20	0.76
1:A:335:GLN:HG2	1:A:336:ASN:N	2.01	0.76
1:A:439:GLN:O	1:A:443:ILE:HG13	1.85	0.76
1:A:269:VAL:HG11	1:A:366:ILE:HD12	1.66	0.76
1:A:379:VAL:N	1:A:458:GLY:HA3	1.99	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:ILE:HG23	1:A:416:GLY:N	1.99	0.75
1:A:67:TRP:CH2	1:A:135:ILE:HG21	2.21	0.75
1:A:459:ASN:HD22	1:A:459:ASN:N	1.84	0.75
1:A:155:LEU:HD13	1:A:468:ASN:OD1	1.87	0.75
1:A:149:ILE:HG21	1:A:154:LEU:HG	1.69	0.75
1:A:492:LEU:HD13	1:A:587:VAL:CG1	2.15	0.75
1:A:379:VAL:HB	1:A:458:GLY:CA	2.17	0.75
1:A:125:GLU:HB3	1:A:127:GLN:HE21	1.51	0.74
1:A:271:MET:HE1	1:A:274:LEU:HB3	1.70	0.74
1:A:380:THR:HB	1:A:397:GLY:HA3	1.70	0.74
1:A:579:ILE:HA	1:A:583:MET:HE3	1.69	0.74
1:A:224:TYR:CE2	1:A:244:VAL:HB	2.23	0.74
1:A:386:VAL:O	1:A:387:ILE:HD13	1.86	0.73
1:A:128:LEU:HB2	1:A:131:ASN:OD1	1.88	0.73
1:A:271:MET:HB3	1:A:334:TRP:CZ3	2.24	0.73
1:A:71:ILE:HG23	1:A:117:ILE:HD11	1.70	0.73
1:A:28:PHE:CD2	1:A:33:PHE:HA	2.23	0.73
1:A:543:GLU:HB2	1:A:549:LYS:CE	2.16	0.73
1:A:204:VAL:HG11	1:A:244:VAL:CG2	2.18	0.73
1:A:520:LEU:HB3	1:A:577:CYS:HB2	1.71	0.72
1:A:494:LEU:CD2	1:A:589:VAL:HG21	2.19	0.72
1:A:57:LEU:HG	1:A:58:GLY:H	1.53	0.72
1:A:99:LEU:N	1:A:99:LEU:HD13	2.05	0.72
1:A:110:ILE:HB	1:A:113:ASN:HD22	1.54	0.72
1:A:76:THR:OG1	1:A:110:ILE:HG23	1.90	0.72
1:A:494:LEU:HB2	1:A:495:PRO:HD3	1.70	0.72
1:A:256:ALA:HB2	1:A:373:THR:HB	1.71	0.71
1:A:354:ILE:HD12	1:A:437:TYR:CE1	2.24	0.71
1:A:532:LYS:HE3	1:A:535:GLY:HA2	1.72	0.71
1:A:44:GLY:HA3	1:A:148:ILE:HG23	1.72	0.71
1:A:519:THR:CG2	1:A:578:ILE:HD12	2.21	0.71
1:A:252:VAL:CG1	1:A:256:ALA:HB3	2.20	0.71
1:A:260:MET:HE2	1:A:526:LYS:CD	2.19	0.70
1:A:337:THR:CG2	1:A:339:THR:HG23	2.20	0.70
1:A:492:LEU:CG	1:A:493:SER:H	2.04	0.70
1:A:70:LEU:HB3	1:A:114:VAL:CG1	2.20	0.70
1:A:393:ALA:HB2	1:A:433:ILE:HG12	1.72	0.70
1:A:90:VAL:CG2	1:A:98:ASN:HB2	2.21	0.70
1:A:343:THR:HG23	1:A:344:THR:CG2	2.20	0.70
1:A:386:VAL:C	1:A:387:ILE:HD13	2.12	0.70
1:A:155:LEU:HD12	1:A:156:LYS:O	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:THR:HA	1:A:578:ILE:HA	1.72	0.70
1:A:492:LEU:CD1	1:A:587:VAL:HG12	2.20	0.69
1:A:53:ILE:CD1	1:A:130:LYS:HG2	2.22	0.69
1:A:373:THR:CG2	1:A:501:VAL:HG22	2.23	0.69
1:A:50:LYS:HG2	1:A:132:TYR:CE2	2.27	0.69
1:A:202:TYR:O	1:A:224:TYR:HB2	1.91	0.69
1:A:71:ILE:O	1:A:114:VAL:HA	1.91	0.69
1:A:385:ILE:HD11	1:A:395:ILE:CD1	2.23	0.69
1:A:109:LEU:HD23	1:A:115:TYR:CD2	2.27	0.69
1:A:518:LEU:O	1:A:578:ILE:HG13	1.93	0.69
1:A:29:GLU:O	1:A:63:LYS:HG3	1.93	0.69
1:A:383:THR:HG21	1:A:451:LEU:HD23	1.76	0.68
1:A:266:ILE:CD1	1:A:372:GLY:HA2	2.24	0.68
1:A:204:VAL:HG11	1:A:244:VAL:HG23	1.74	0.68
1:A:30:ASN:CB	1:A:34:ASN:HD22	2.06	0.68
1:A:248:ILE:HG23	1:A:249:ASP:N	2.07	0.68
1:A:225:VAL:HG23	1:A:260:MET:CE	2.23	0.68
1:A:460:PHE:CZ	1:A:462:LYS:HG2	2.29	0.67
1:A:70:LEU:HD12	1:A:155:LEU:HD11	1.76	0.67
1:A:23:LEU:CD2	1:A:154:LEU:HD22	2.22	0.67
1:A:507:ASN:CB	1:A:581:ARG:HD2	2.21	0.67
1:A:59:ASN:OD1	1:A:59:ASN:N	2.22	0.67
1:A:24:MET:HG2	1:A:159:TYR:OH	1.95	0.67
1:A:35:LEU:HG	1:A:194:PRO:HG3	1.76	0.67
1:A:379:VAL:H	1:A:458:GLY:CA	2.04	0.67
1:A:243:LYS:NZ	1:A:261:ILE:O	2.28	0.67
1:A:276:VAL:O	1:A:294:THR:N	2.28	0.67
1:A:160:SER:N	1:A:242:GLU:OE2	2.28	0.67
1:A:219:ASN:HD22	1:A:221:TYR:HE2	1.41	0.67
1:A:329:ASN:ND2	1:A:329:ASN:H	1.92	0.66
1:A:266:ILE:HD12	1:A:372:GLY:HA2	1.77	0.66
1:A:492:LEU:HD12	1:A:493:SER:N	2.11	0.66
1:A:300:ASN:OD1	1:A:301:ILE:N	2.29	0.66
1:A:359:SER:OG	1:A:360:ALA:N	2.29	0.65
1:A:487:THR:HG22	1:A:504:VAL:HA	1.76	0.65
1:A:90:VAL:HG23	1:A:98:ASN:HB2	1.79	0.65
1:A:492:LEU:HD12	1:A:493:SER:H	1.62	0.65
1:A:98:ASN:C	1:A:99:LEU:HD22	2.16	0.65
1:A:401:LEU:HD12	1:A:401:LEU:O	1.97	0.65
1:A:118:ARG:O	1:A:119:ILE:HG13	1.95	0.65
1:A:101:LEU:HD22	1:A:102:ASN:H	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:GLN:HG3	1:A:401:LEU:HD21	1.77	0.65
1:A:343:THR:HG23	1:A:344:THR:N	2.12	0.64
1:A:556:ARG:HH21	1:A:556:ARG:HG2	1.62	0.64
1:A:255:VAL:O	1:A:261:ILE:HG21	1.96	0.64
1:A:117:ILE:O	1:A:118:ARG:HB2	1.95	0.64
1:A:363:ASN:HD22	1:A:423:ASN:HB2	1.61	0.64
1:A:271:MET:HG2	1:A:366:ILE:HG22	1.77	0.64
1:A:93:ASN:HD22	1:A:115:TYR:HB3	1.61	0.64
1:A:490:LEU:HD21	1:A:524:LEU:CD1	2.28	0.64
1:A:520:LEU:N	1:A:577:CYS:O	2.29	0.64
1:A:70:LEU:HD23	1:A:116:ASP:HA	1.79	0.64
1:A:46:LEU:N	1:A:46:LEU:HD23	2.12	0.64
1:A:89:ARG:HG2	1:A:90:VAL:N	2.12	0.64
1:A:269:VAL:HG11	1:A:366:ILE:CD1	2.27	0.64
1:A:38:ILE:HB	1:A:208:LYS:HZ1	1.60	0.64
1:A:61:ILE:HG22	1:A:126:ASN:HB3	1.78	0.64
1:A:264:TYR:CE1	1:A:266:ILE:HD11	2.33	0.64
1:A:462:LYS:CE	1:A:473:GLY:HA3	2.27	0.64
1:A:70:LEU:CD1	1:A:114:VAL:HG11	2.24	0.64
1:A:227:ASN:ND2	1:A:514:LYS:O	2.31	0.64
1:A:507:ASN:HB2	1:A:581:ARG:CD	2.23	0.63
1:A:459:ASN:N	1:A:459:ASN:ND2	2.45	0.63
1:A:89:ARG:NE	1:A:96:ILE:HG13	2.14	0.63
1:A:205:MET:O	1:A:207:GLN:N	2.29	0.63
1:A:365:ASN:OD1	1:A:365:ASN:N	2.30	0.63
1:A:551:GLN:HE21	1:A:590:ILE:HD13	1.63	0.63
1:A:492:LEU:CD1	1:A:493:SER:H	2.12	0.63
1:A:188:THR:HG22	1:A:189:ASP:N	2.12	0.63
1:A:26:TYR:HD2	1:A:38:ILE:HG12	1.64	0.62
1:A:328:ALA:CB	1:A:484:LYS:HE2	2.26	0.62
1:A:524:LEU:O	1:A:530:LEU:HD13	1.98	0.62
1:A:544:ILE:CD1	1:A:550:ILE:HD13	2.29	0.62
1:A:266:ILE:HD12	1:A:372:GLY:CA	2.30	0.62
1:A:56:ILE:O	1:A:60:LYS:HE3	2.00	0.62
1:A:586:LEU:HD12	1:A:587:VAL:N	2.09	0.62
1:A:385:ILE:HD12	1:A:393:ALA:O	1.99	0.62
1:A:580:LYS:H	1:A:583:MET:CE	2.13	0.62
1:A:483:ILE:HG22	1:A:484:LYS:N	2.15	0.62
1:A:375:PRO:HB3	1:A:408:PRO:HD3	1.81	0.62
1:A:490:LEU:HD12	1:A:528:PHE:HZ	1.65	0.62
1:A:529:ARG:HG3	1:A:529:ARG:NH2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:VAL:CG1	1:A:362:ILE:HB	2.29	0.62
1:A:93:ASN:ND2	1:A:115:TYR:HB3	2.15	0.61
1:A:491:THR:HG22	1:A:492:LEU:N	2.16	0.61
1:A:530:LEU:HD22	1:A:537:PHE:HZ	1.64	0.61
1:A:543:GLU:CB	1:A:549:LYS:HE3	2.25	0.61
1:A:71:ILE:HD13	1:A:117:ILE:HD13	1.82	0.61
1:A:271:MET:CE	1:A:274:LEU:HB3	2.30	0.61
1:A:387:ILE:HD12	1:A:449:VAL:HG12	1.82	0.61
1:A:70:LEU:HB2	1:A:155:LEU:CG	2.30	0.61
1:A:44:GLY:HA3	1:A:148:ILE:CG2	2.31	0.61
1:A:260:MET:HE1	1:A:526:LYS:NZ	2.15	0.61
1:A:387:ILE:CD1	1:A:449:VAL:HA	2.30	0.61
1:A:267:VAL:HG12	1:A:268:GLY:N	2.08	0.61
1:A:70:LEU:HB3	1:A:114:VAL:HG13	1.82	0.60
1:A:494:LEU:HD13	1:A:539:PHE:CG	2.36	0.60
1:A:515:THR:HG22	1:A:516:PRO:HD2	1.83	0.60
1:A:206:ASN:O	1:A:207:GLN:HG2	2.01	0.60
1:A:328:ALA:CB	1:A:484:LYS:HD3	2.32	0.60
1:A:492:LEU:HG	1:A:493:SER:H	1.65	0.60
1:A:109:LEU:HD23	1:A:115:TYR:CE2	2.36	0.60
1:A:53:ILE:HD12	1:A:60:LYS:HB3	1.84	0.60
1:A:71:ILE:HD11	1:A:92:LEU:CD2	2.29	0.59
1:A:235:ASN:HD22	1:A:482:THR:HB	1.67	0.59
1:A:434:PRO:O	1:A:435:ILE:HG23	2.01	0.59
1:A:219:ASN:HB2	1:A:221:TYR:CE2	2.38	0.59
1:A:81:LEU:HD11	1:A:92:LEU:CD1	2.33	0.59
1:A:583:MET:O	1:A:585:ILE:HG13	2.02	0.59
1:A:197:TRP:HZ3	1:A:208:LYS:NZ	2.00	0.59
1:A:204:VAL:HG12	1:A:208:LYS:CG	2.26	0.59
1:A:492:LEU:HD21	1:A:494:LEU:HD12	1.83	0.59
1:A:215:LYS:NZ	1:A:215:LYS:O	2.36	0.59
1:A:586:LEU:CD1	1:A:587:VAL:H	2.10	0.59
1:A:378:ASN:HB3	1:A:458:GLY:HA3	1.85	0.58
1:A:487:THR:HG22	1:A:504:VAL:CA	2.32	0.58
1:A:383:THR:CG2	1:A:451:LEU:HD23	2.33	0.58
1:A:162:THR:OG1	1:A:163:ASN:N	2.35	0.58
1:A:492:LEU:HD11	1:A:494:LEU:HG	1.84	0.58
1:A:264:TYR:CZ	1:A:266:ILE:HD11	2.39	0.58
1:A:551:GLN:NE2	1:A:590:ILE:HD13	2.18	0.58
1:A:530:LEU:HD22	1:A:537:PHE:CE2	2.39	0.58
1:A:255:VAL:HG12	1:A:529:ARG:HG3	1.85	0.58

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Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:GLY:O	1:A:248:ILE:N	2.37	0.58
1:A:303:THR:HG21	1:A:331:SER:CB	2.34	0.58
1:A:28:PHE:HD2	1:A:34:ASN:H	1.50	0.58
1:A:477:GLY:C	1:A:479:TYR:H	2.08	0.58
1:A:235:ASN:HB3	1:A:482:THR:OG1	2.04	0.58
1:A:373:THR:HG21	1:A:501:VAL:HG22	1.86	0.57
1:A:558:THR:O	1:A:562:PHE:HB2	2.04	0.57
1:A:458:GLY:O	1:A:476:TRP:N	2.36	0.57
1:A:480:LEU:O	1:A:483:ILE:HB	2.05	0.57
1:A:57:LEU:HG	1:A:58:GLY:N	2.19	0.57
1:A:276:VAL:HG13	1:A:362:ILE:HG13	1.87	0.57
1:A:70:LEU:HD22	1:A:114:VAL:CG1	2.29	0.57
1:A:76:THR:HG23	1:A:110:ILE:CG1	2.35	0.57
1:A:387:ILE:HD12	1:A:449:VAL:HA	1.85	0.57
1:A:141:THR:OG1	1:A:142:SER:N	2.38	0.57
1:A:369:TYR:HD2	1:A:370:ASN:N	2.02	0.57
1:A:87:ASN:ND2	1:A:87:ASN:H	2.02	0.57
1:A:71:ILE:H	1:A:114:VAL:HG13	1.69	0.57
1:A:68:ILE:HG23	1:A:157:PRO:HG3	1.87	0.57
1:A:572:LYS:H	1:A:572:LYS:HD2	1.68	0.57
1:A:411:THR:HG1	1:A:414:ILE:HA	1.66	0.56
1:A:308:VAL:HG23	1:A:556:ARG:HD3	1.86	0.56
1:A:460:PHE:HB3	1:A:476:TRP:CE2	2.40	0.56
1:A:490:LEU:HD12	1:A:528:PHE:CZ	2.39	0.56
1:A:137:LEU:CD2	1:A:149:ILE:HD12	2.35	0.56
1:A:204:VAL:HG11	1:A:244:VAL:HG21	1.87	0.56
1:A:487:THR:HG22	1:A:504:VAL:N	2.20	0.56
1:A:60:LYS:HD3	1:A:130:LYS:CG	2.35	0.56
1:A:275:VAL:HG22	1:A:295:SER:CB	2.36	0.56
1:A:518:LEU:HD23	1:A:579:ILE:HB	1.87	0.56
1:A:476:TRP:O	1:A:479:TYR:HB2	2.06	0.56
1:A:43:ASP:OD1	1:A:43:ASP:N	2.39	0.56
1:A:80:ILE:O	1:A:139:TRP:HA	2.06	0.56
1:A:149:ILE:CG2	1:A:154:LEU:HG	2.36	0.56
1:A:274:LEU:CD2	1:A:274:LEU:H	2.15	0.55
1:A:204:VAL:O	1:A:204:VAL:HG23	2.06	0.55
1:A:558:THR:HG21	1:A:583:MET:SD	2.46	0.55
1:A:238:TYR:CD1	1:A:248:ILE:HG13	2.41	0.55
1:A:573:ASP:OD2	1:A:573:ASP:N	2.32	0.55
1:A:38:ILE:HB	1:A:208:LYS:CE	2.37	0.55
1:A:57:LEU:CG	1:A:58:GLY:H	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:LEU:O	1:A:569:THR:N	2.33	0.55
1:A:89:ARG:HG2	1:A:90:VAL:H	1.71	0.55
1:A:458:GLY:O	1:A:476:TRP:HB2	2.07	0.55
1:A:449:VAL:O	1:A:449:VAL:HG23	2.05	0.55
1:A:90:VAL:O	1:A:96:ILE:HA	2.07	0.55
1:A:28:PHE:CD1	1:A:28:PHE:N	2.74	0.55
1:A:81:LEU:HD11	1:A:92:LEU:HD11	1.88	0.55
1:A:233:THR:O	1:A:235:ASN:N	2.39	0.55
1:A:264:TYR:H	1:A:264:TYR:HD1	1.56	0.54
1:A:48:PHE:HE1	1:A:52:ASP:HB2	1.72	0.54
1:A:489:SER:O	1:A:490:LEU:HB2	2.07	0.54
1:A:137:LEU:HD21	1:A:149:ILE:HD12	1.90	0.54
1:A:236:ASP:HB2	1:A:237:PRO:CD	2.29	0.54
1:A:383:THR:HG21	1:A:451:LEU:CD2	2.37	0.54
1:A:255:VAL:CG1	1:A:529:ARG:HH21	2.20	0.54
1:A:276:VAL:HA	1:A:362:ILE:HA	1.89	0.54
1:A:53:ILE:HD12	1:A:60:LYS:CG	2.37	0.54
1:A:303:THR:HG21	1:A:331:SER:HB3	1.89	0.54
1:A:35:LEU:HG	1:A:194:PRO:CG	2.38	0.54
1:A:31:ASP:OD1	1:A:63:LYS:HD2	2.08	0.54
1:A:43:ASP:HB3	1:A:151:SER:OG	2.07	0.54
1:A:385:ILE:HA	1:A:450:MET:O	2.08	0.53
1:A:198:GLU:OE1	1:A:226:SER:HB3	2.08	0.53
1:A:60:LYS:HD3	1:A:130:LYS:HG3	1.89	0.53
1:A:89:ARG:HA	1:A:97:PHE:O	2.09	0.53
1:A:98:ASN:O	1:A:99:LEU:HD22	2.09	0.53
1:A:460:PHE:CE2	1:A:462:LYS:HE2	2.43	0.53
1:A:378:ASN:HB2	1:A:459:ASN:H	1.74	0.53
1:A:117:ILE:HG22	1:A:118:ARG:N	2.20	0.53
1:A:155:LEU:HD22	1:A:468:ASN:HD21	1.73	0.53
1:A:519:THR:HG22	1:A:578:ILE:HD12	1.91	0.53
1:A:494:LEU:HD13	1:A:539:PHE:CE2	2.44	0.53
1:A:53:ILE:CD1	1:A:60:LYS:HB3	2.38	0.53
1:A:294:THR:HG22	1:A:294:THR:O	2.06	0.53
1:A:72:LYS:HB3	1:A:114:VAL:CG2	2.36	0.53
1:A:23:LEU:HD21	1:A:154:LEU:HD22	1.90	0.53
1:A:233:THR:C	1:A:235:ASN:H	2.12	0.53
1:A:74:SER:HA	1:A:111:GLN:HG2	1.90	0.53
1:A:399:GLU:O	1:A:400:SER:HB2	2.09	0.53
1:A:413:PRO:HG2	1:A:418:PRO:O	2.09	0.53
1:A:333:THR:HG22	1:A:334:TRP:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:VAL:HG23	1:A:393:ALA:N	2.24	0.53
1:A:235:ASN:HD22	1:A:482:THR:CB	2.22	0.53
1:A:539:PHE:O	1:A:540:HIS:HB2	2.09	0.52
1:A:579:ILE:HD11	1:A:585:ILE:CD1	2.38	0.52
1:A:60:LYS:O	1:A:62:ILE:N	2.42	0.52
1:A:470:VAL:HG12	1:A:470:VAL:O	2.09	0.52
1:A:198:GLU:OE1	1:A:227:ASN:O	2.26	0.52
1:A:192:GLY:C	1:A:193:ILE:HG12	2.30	0.52
1:A:477:GLY:O	1:A:479:TYR:N	2.42	0.52
1:A:119:ILE:O	1:A:119:ILE:HG22	2.08	0.52
1:A:213:ASP:O	1:A:214:ASP:O	2.28	0.52
1:A:522:GLN:O	1:A:526:LYS:HG2	2.10	0.52
1:A:103:THR:O	1:A:104:SER:HB2	2.09	0.52
1:A:371:THR:OG1	1:A:500:GLN:N	2.37	0.52
1:A:143:ASP:C	1:A:145:ILE:H	2.12	0.52
1:A:490:LEU:HG	1:A:528:PHE:CE2	2.45	0.52
1:A:102:ASN:OD1	1:A:102:ASN:O	2.28	0.52
1:A:574:ILE:HG23	1:A:574:ILE:O	2.09	0.52
1:A:274:LEU:HD23	1:A:274:LEU:N	2.15	0.52
1:A:76:THR:HG23	1:A:110:ILE:HG12	1.92	0.52
1:A:144:ILE:O	1:A:144:ILE:HG22	2.10	0.52
1:A:272:GLU:O	1:A:273:ARG:HB3	2.08	0.52
1:A:499:THR:O	1:A:499:THR:HG22	2.09	0.52
1:A:362:ILE:CG2	1:A:433:ILE:HB	2.40	0.51
1:A:453:THR:O	1:A:454:SER:O	2.28	0.51
1:A:360:ALA:HB3	1:A:435:ILE:HG13	1.92	0.51
1:A:494:LEU:HB3	1:A:539:PHE:CE2	2.44	0.51
1:A:558:THR:O	1:A:562:PHE:N	2.43	0.51
1:A:28:PHE:CG	1:A:33:PHE:HA	2.45	0.51
1:A:356:THR:HA	1:A:437:TYR:CG	2.44	0.51
1:A:58:GLY:O	1:A:60:LYS:N	2.38	0.51
1:A:225:VAL:HG23	1:A:260:MET:SD	2.51	0.51
1:A:212:TRP:HB3	1:A:216:PHE:CD1	2.45	0.51
1:A:494:LEU:CB	1:A:495:PRO:HD3	2.39	0.51
1:A:379:VAL:HB	1:A:457:THR:C	2.30	0.51
1:A:385:ILE:HD11	1:A:395:ILE:HD11	1.93	0.51
1:A:251:SER:O	1:A:408:PRO:HG2	2.10	0.51
1:A:552:VAL:HG12	1:A:553:PHE:N	2.26	0.51
1:A:333:THR:CG2	1:A:334:TRP:N	2.74	0.51
1:A:300:ASN:C	1:A:301:ILE:HG13	2.30	0.51
1:A:255:VAL:CG2	1:A:373:THR:HG22	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ILE:CG2	1:A:118:ARG:H	2.11	0.51
1:A:25:GLY:CA	1:A:67:TRP:CD1	2.94	0.51
1:A:386:VAL:HG13	1:A:391:SER:N	2.26	0.51
1:A:48:PHE:CE1	1:A:52:ASP:HB2	2.46	0.51
1:A:304:VAL:O	1:A:304:VAL:HG12	2.11	0.51
1:A:378:ASN:CB	1:A:459:ASN:H	2.24	0.50
1:A:515:THR:HG22	1:A:516:PRO:CD	2.41	0.50
1:A:464:ASN:O	1:A:468:ASN:HA	2.11	0.50
1:A:269:VAL:CG1	1:A:366:ILE:HD12	2.37	0.50
1:A:560:VAL:O	1:A:564:ASN:OD1	2.30	0.50
1:A:271:MET:O	1:A:334:TRP:HZ3	1.94	0.50
1:A:97:PHE:CZ	1:A:105:ASN:HB3	2.47	0.50
1:A:587:VAL:HG12	1:A:587:VAL:O	2.11	0.50
1:A:46:LEU:HB2	1:A:135:ILE:HG23	1.93	0.50
1:A:267:VAL:HG13	1:A:406:LEU:CD2	2.42	0.50
1:A:368:TYR:CD1	1:A:412:TYR:HD1	2.29	0.50
1:A:208:LYS:HE3	1:A:208:LYS:C	2.32	0.50
1:A:56:ILE:O	1:A:57:LEU:O	2.29	0.50
1:A:71:ILE:HD13	1:A:117:ILE:CD1	2.41	0.50
1:A:38:ILE:O	1:A:207:GLN:O	2.29	0.50
1:A:76:THR:HA	1:A:110:ILE:HA	1.94	0.50
1:A:521:GLU:O	1:A:524:LEU:N	2.45	0.49
1:A:252:VAL:HG13	1:A:256:ALA:HB3	1.91	0.49
1:A:251:SER:HB2	1:A:375:PRO:HG3	1.93	0.49
1:A:38:ILE:HB	1:A:208:LYS:HE2	1.94	0.49
1:A:50:LYS:HG2	1:A:132:TYR:HE2	1.76	0.49
1:A:371:THR:O	1:A:371:THR:OG1	2.29	0.49
1:A:368:TYR:HB2	1:A:412:TYR:HB3	1.92	0.49
1:A:460:PHE:CD1	1:A:461:ALA:N	2.80	0.49
1:A:343:THR:C	1:A:344:THR:HG23	2.32	0.49
1:A:300:ASN:HD21	1:A:332:HIS:HB3	1.77	0.49
1:A:105:ASN:O	1:A:106:THR:OG1	2.28	0.49
1:A:491:THR:OG1	1:A:500:GLN:HG2	2.12	0.49
1:A:578:ILE:HG23	1:A:579:ILE:N	2.27	0.49
1:A:30:ASN:CB	1:A:34:ASN:ND2	2.75	0.49
1:A:132:TYR:C	1:A:134:GLY:H	2.14	0.49
1:A:74:SER:C	1:A:111:GLN:HG2	2.33	0.49
1:A:441:LYS:O	1:A:445:ASN:OD1	2.29	0.49
1:A:492:LEU:O	1:A:493:SER:HB3	2.12	0.49
1:A:493:SER:OG	1:A:493:SER:O	2.27	0.49
1:A:379:VAL:CG1	1:A:380:THR:N	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:GLY:HA2	1:A:67:TRP:CD1	2.48	0.48
1:A:375:PRO:HD3	1:A:408:PRO:HG3	1.95	0.48
1:A:214:ASP:OD1	1:A:214:ASP:N	2.45	0.48
1:A:26:TYR:HH	1:A:159:TYR:HH	1.55	0.48
1:A:38:ILE:HG21	1:A:241:PHE:CZ	2.48	0.48
1:A:85:SER:O	1:A:86:PRO:O	2.32	0.48
1:A:334:TRP:NE1	1:A:335:GLN:O	2.46	0.48
1:A:555:ASP:OD2	1:A:558:THR:OG1	2.31	0.48
1:A:341:ASP:O	1:A:342:ASP:HB2	2.13	0.48
1:A:89:ARG:HG3	1:A:96:ILE:HG23	1.95	0.48
1:A:46:LEU:HD13	1:A:67:TRP:CG	2.49	0.48
1:A:264:TYR:OH	1:A:502:ALA:HB2	2.13	0.48
1:A:270:GLN:HA	1:A:300:ASN:ND2	2.28	0.48
1:A:149:ILE:HG21	1:A:154:LEU:CG	2.41	0.48
1:A:266:ILE:HD13	1:A:372:GLY:HA2	1.94	0.48
1:A:30:ASN:HB2	1:A:34:ASN:ND2	2.19	0.48
1:A:27:TYR:HE2	1:A:67:TRP:CZ2	2.31	0.48
1:A:25:GLY:CA	1:A:67:TRP:HD1	2.26	0.48
1:A:219:ASN:ND2	1:A:221:TYR:HE2	2.10	0.48
1:A:571:ASN:O	1:A:573:ASP:N	2.46	0.48
1:A:38:ILE:HG21	1:A:241:PHE:CE1	2.49	0.48
1:A:393:ALA:CB	1:A:433:ILE:HG12	2.40	0.48
1:A:398:GLN:HB3	1:A:401:LEU:HD11	1.95	0.48
1:A:266:ILE:O	1:A:266:ILE:HG22	2.13	0.47
1:A:504:VAL:O	1:A:505:ALA:HB2	2.14	0.47
1:A:539:PHE:O	1:A:542:MET:HE3	2.14	0.47
1:A:67:TRP:CZ2	1:A:135:ILE:HG21	2.49	0.47
1:A:362:ILE:HG22	1:A:433:ILE:HB	1.95	0.47
1:A:387:ILE:O	1:A:389:LYS:N	2.47	0.47
1:A:359:SER:O	1:A:360:ALA:HB2	2.14	0.47
1:A:373:THR:HG23	1:A:501:VAL:HG22	1.97	0.47
1:A:395:ILE:HG12	1:A:422:LEU:HD22	1.96	0.47
1:A:244:VAL:HG22	1:A:245:SER:N	2.30	0.47
1:A:238:TYR:CG	1:A:248:ILE:HD11	2.48	0.47
1:A:530:LEU:HB2	1:A:537:PHE:CZ	2.49	0.47
1:A:79:TYR:CE1	1:A:109:LEU:HB2	2.50	0.47
1:A:570:ALA:O	1:A:573:ASP:OD2	2.33	0.47
1:A:189:ASP:O	1:A:190:ARG:HB2	2.14	0.47
1:A:267:VAL:CG1	1:A:268:GLY:H	2.11	0.47
1:A:245:SER:HB2	1:A:247:GLN:OE1	2.14	0.47
1:A:233:THR:HG22	1:A:504:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LYS:NZ	1:A:219:ASN:HD21	2.13	0.47
1:A:45:ASN:OD1	1:A:136:LYS:HG2	2.15	0.46
1:A:67:TRP:HE3	1:A:119:ILE:CG2	2.28	0.46
1:A:392:VAL:CG2	1:A:393:ALA:N	2.77	0.46
1:A:518:LEU:HG	1:A:519:THR:N	2.29	0.46
1:A:402:ILE:HD12	1:A:405:TYR:HA	1.96	0.46
1:A:383:THR:HA	1:A:453:THR:HA	1.97	0.46
1:A:382:THR:O	1:A:382:THR:HG22	2.13	0.46
1:A:255:VAL:HG12	1:A:529:ARG:HH21	1.79	0.46
1:A:491:THR:HG22	1:A:492:LEU:H	1.80	0.46
1:A:586:LEU:HD21	1:A:588:LYS:NZ	2.30	0.46
1:A:69:GLY:O	1:A:117:ILE:HG13	2.16	0.46
1:A:24:MET:CE	1:A:247:GLN:NE2	2.79	0.46
1:A:555:ASP:OD1	1:A:557:ASN:HB2	2.16	0.46
1:A:214:ASP:O	1:A:216:PHE:N	2.48	0.46
1:A:556:ARG:HG2	1:A:556:ARG:NH2	2.29	0.46
1:A:544:ILE:HD13	1:A:550:ILE:HD13	1.98	0.46
1:A:492:LEU:HD21	1:A:494:LEU:CD1	2.46	0.46
1:A:28:PHE:CD2	1:A:34:ASN:N	2.84	0.46
1:A:356:THR:HA	1:A:437:TYR:CD2	2.51	0.46
1:A:518:LEU:HD21	1:A:523:ALA:HB2	1.98	0.45
1:A:35:LEU:O	1:A:36:ASN:HB2	2.14	0.45
1:A:25:GLY:HA3	1:A:67:TRP:CD1	2.51	0.45
1:A:70:LEU:HD23	1:A:116:ASP:CA	2.43	0.45
1:A:363:ASN:HD22	1:A:363:ASN:HA	1.60	0.45
1:A:32:PHE:CD2	1:A:122:LEU:HD11	2.51	0.45
1:A:530:LEU:CB	1:A:537:PHE:CZ	2.99	0.45
1:A:578:ILE:CG2	1:A:579:ILE:N	2.79	0.45
1:A:383:THR:O	1:A:394:THR:HG23	2.17	0.45
1:A:90:VAL:HG23	1:A:97:PHE:C	2.37	0.45
1:A:189:ASP:OD1	1:A:189:ASP:N	2.44	0.45
1:A:233:THR:C	1:A:235:ASN:N	2.69	0.45
1:A:32:PHE:CE2	1:A:122:LEU:HD11	2.51	0.45
1:A:492:LEU:CG	1:A:493:SER:N	2.75	0.45
1:A:225:VAL:HG23	1:A:260:MET:HE1	1.97	0.45
1:A:260:MET:CE	1:A:526:LYS:HZ2	2.29	0.45
1:A:92:LEU:HD12	1:A:107:VAL:HG11	1.98	0.45
1:A:387:ILE:HD12	1:A:448:THR:O	2.16	0.45
1:A:579:ILE:HD11	1:A:585:ILE:HD12	1.98	0.45
1:A:159:TYR:HB2	1:A:242:GLU:HG3	1.97	0.45
1:A:38:ILE:O	1:A:38:ILE:HG22	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:PHE:HD2	1:A:34:ASN:N	2.14	0.45
1:A:34:ASN:O	1:A:35:LEU:HB2	2.15	0.45
1:A:506:PRO:HD3	1:A:515:THR:HB	1.99	0.45
1:A:260:MET:CE	1:A:526:LYS:NZ	2.80	0.45
1:A:53:ILE:HD12	1:A:60:LYS:CB	2.47	0.45
1:A:70:LEU:HB3	1:A:114:VAL:HG11	1.97	0.45
1:A:240:ASP:O	1:A:244:VAL:HG13	2.17	0.45
1:A:369:TYR:CD2	1:A:370:ASN:N	2.82	0.45
1:A:490:LEU:CD1	1:A:528:PHE:CZ	3.00	0.45
1:A:483:ILE:O	1:A:487:THR:OG1	2.30	0.45
1:A:307:GLU:N	1:A:307:GLU:OE2	2.50	0.45
1:A:88:CYS:O	1:A:99:LEU:HD13	2.16	0.45
1:A:573:ASP:O	1:A:574:ILE:HG22	2.16	0.45
1:A:525:VAL:HG22	1:A:530:LEU:O	2.17	0.44
1:A:74:SER:CA	1:A:111:GLN:HG2	2.47	0.44
1:A:506:PRO:O	1:A:581:ARG:HG3	2.17	0.44
1:A:269:VAL:HG22	1:A:368:TYR:CD2	2.52	0.44
1:A:197:TRP:O	1:A:202:TYR:HD1	1.99	0.44
1:A:255:VAL:CG1	1:A:529:ARG:NH2	2.81	0.44
1:A:88:CYS:O	1:A:98:ASN:HB3	2.18	0.44
1:A:519:THR:HG23	1:A:578:ILE:HD12	1.97	0.44
1:A:89:ARG:CZ	1:A:96:ILE:HG13	2.47	0.44
1:A:215:LYS:NZ	1:A:219:ASN:OD1	2.51	0.44
1:A:441:LYS:O	1:A:441:LYS:HG2	2.18	0.44
1:A:487:THR:CG2	1:A:504:VAL:HA	2.44	0.44
1:A:50:LYS:HA	1:A:53:ILE:HG12	1.99	0.44
1:A:303:THR:HG21	1:A:331:SER:HB2	1.99	0.44
1:A:243:LYS:NZ	1:A:258:ASP:O	2.50	0.44
1:A:395:ILE:HG12	1:A:422:LEU:CD2	2.47	0.44
1:A:39:SER:CB	1:A:207:GLN:NE2	2.81	0.44
1:A:529:ARG:CG	1:A:529:ARG:NH2	2.79	0.44
1:A:362:ILE:O	1:A:362:ILE:HG23	2.17	0.44
1:A:550:ILE:O	1:A:550:ILE:HG12	2.18	0.44
1:A:145:ILE:O	1:A:145:ILE:HG22	2.17	0.44
1:A:18:PHE:O	1:A:21:ASN:HB2	2.18	0.44
1:A:155:LEU:CB	1:A:468:ASN:ND2	2.81	0.43
1:A:69:GLY:HA2	1:A:157:PRO:HD3	2.00	0.43
1:A:29:GLU:HB2	1:A:36:ASN:HD21	1.75	0.43
1:A:586:LEU:CD1	1:A:587:VAL:N	2.77	0.43
1:A:489:SER:OG	1:A:490:LEU:N	2.51	0.43
1:A:70:LEU:HD13	1:A:114:VAL:CG1	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ALA:HB3	1:A:236:ASP:OD2	2.18	0.43
1:A:586:LEU:CG	1:A:587:VAL:N	2.81	0.43
1:A:331:SER:OG	1:A:452:SER:HA	2.18	0.43
1:A:105:ASN:O	1:A:105:ASN:ND2	2.52	0.43
1:A:491:THR:CG2	1:A:492:LEU:N	2.80	0.43
1:A:387:ILE:HD11	1:A:449:VAL:CG1	2.45	0.43
1:A:438:ASN:O	1:A:442:SER:OG	2.35	0.43
1:A:97:PHE:HZ	1:A:105:ASN:HB3	1.81	0.43
1:A:586:LEU:O	1:A:587:VAL:HG23	2.17	0.43
1:A:580:LYS:N	1:A:583:MET:CE	2.80	0.43
1:A:355:ASN:OD1	1:A:355:ASN:N	2.52	0.43
1:A:87:ASN:ND2	1:A:87:ASN:N	2.66	0.43
1:A:161:ASN:OD1	1:A:231:PRO:HG2	2.18	0.43
1:A:555:ASP:HB3	1:A:584:ASN:HB3	2.00	0.43
1:A:219:ASN:HB2	1:A:221:TYR:CZ	2.53	0.43
1:A:23:LEU:O	1:A:41:THR:OG1	2.30	0.43
1:A:262:SER:OG	1:A:263:ALA:N	2.51	0.43
1:A:555:ASP:OD2	1:A:584:ASN:O	2.36	0.43
1:A:191:ASP:OD1	1:A:193:ILE:HG13	2.18	0.43
1:A:132:TYR:O	1:A:134:GLY:N	2.41	0.43
1:A:125:GLU:CB	1:A:127:GLN:HE21	2.28	0.43
1:A:266:ILE:HD12	1:A:372:GLY:HA3	2.01	0.42
1:A:215:LYS:HZ1	1:A:219:ASN:HD21	1.66	0.42
1:A:189:ASP:HB3	1:A:228:PRO:O	2.19	0.42
1:A:72:LYS:HE2	1:A:468:ASN:ND2	2.35	0.42
1:A:202:TYR:HE1	1:A:226:SER:HB2	1.84	0.42
1:A:63:LYS:CD	1:A:126:ASN:HD21	2.32	0.42
1:A:386:VAL:HG12	1:A:390:GLN:C	2.40	0.42
1:A:193:ILE:HA	1:A:194:PRO:HD3	1.79	0.42
1:A:73:PRO:HG2	1:A:110:ILE:O	2.19	0.42
1:A:260:MET:CE	1:A:526:LYS:HD2	2.28	0.42
1:A:197:TRP:HZ3	1:A:208:LYS:HZ1	1.66	0.42
1:A:83:THR:HB	1:A:136:LYS:O	2.20	0.42
1:A:460:PHE:HB3	1:A:476:TRP:NE1	2.34	0.42
1:A:24:MET:HE3	1:A:247:GLN:NE2	2.35	0.42
1:A:210:VAL:HG22	1:A:211:ALA:H	1.83	0.42
1:A:378:ASN:HB3	1:A:379:VAL:H	1.66	0.42
1:A:107:VAL:O	1:A:107:VAL:HG13	2.20	0.42
1:A:101:LEU:HD22	1:A:102:ASN:N	2.33	0.42
1:A:275:VAL:HG22	1:A:295:SER:HA	2.01	0.42
1:A:143:ASP:O	1:A:145:ILE:N	2.52	0.42

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Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ILE:O	1:A:97:PHE:CD1	2.73	0.42
1:A:266:ILE:O	1:A:267:VAL:O	2.37	0.42
1:A:275:VAL:HG22	1:A:295:SER:OG	2.19	0.42
1:A:490:LEU:HD12	1:A:490:LEU:C	2.40	0.42
1:A:554:LEU:HD23	1:A:585:ILE:CG1	2.31	0.42
1:A:552:VAL:HG12	1:A:553:PHE:H	1.85	0.42
1:A:241:PHE:O	1:A:245:SER:OG	2.29	0.42
1:A:341:ASP:N	1:A:341:ASP:OD1	2.53	0.42
1:A:99:LEU:HB2	1:A:100:SER:H	1.69	0.41
1:A:386:VAL:CG1	1:A:391:SER:N	2.83	0.41
1:A:26:TYR:OH	1:A:159:TYR:OH	2.29	0.41
1:A:53:ILE:C	1:A:55:SER:H	2.22	0.41
1:A:216:PHE:C	1:A:218:ALA:N	2.73	0.41
1:A:260:MET:CE	1:A:526:LYS:CD	2.95	0.41
1:A:406:LEU:CD1	1:A:412:TYR:CB	2.98	0.41
1:A:238:TYR:CG	1:A:248:ILE:HG13	2.55	0.41
1:A:136:LYS:CE	1:A:148:ILE:HD11	2.39	0.41
1:A:235:ASN:ND2	1:A:482:THR:HB	2.32	0.41
1:A:460:PHE:CE1	1:A:462:LYS:HG2	2.55	0.41
1:A:70:LEU:O	1:A:71:ILE:HG23	2.19	0.41
1:A:276:VAL:HG13	1:A:362:ILE:CD1	2.49	0.41
1:A:242:GLU:HA	1:A:247:GLN:OE1	2.21	0.41
1:A:31:ASP:OD1	1:A:63:LYS:HB3	2.20	0.41
1:A:232:CYS:SG	1:A:238:TYR:O	2.78	0.41
1:A:359:SER:HA	1:A:435:ILE:O	2.20	0.41
1:A:402:ILE:O	1:A:402:ILE:HG13	2.19	0.41
1:A:490:LEU:CD1	1:A:528:PHE:CE2	3.03	0.41
1:A:261:ILE:HG12	1:A:526:LYS:HB2	2.03	0.41
1:A:149:ILE:HG22	1:A:154:LEU:HD12	2.02	0.41
1:A:551:GLN:HG2	1:A:590:ILE:HG23	2.02	0.41
1:A:99:LEU:N	1:A:99:LEU:CD1	2.76	0.41
1:A:515:THR:HA	1:A:516:PRO:HD3	1.64	0.41
1:A:149:ILE:CG2	1:A:154:LEU:CD1	2.99	0.41
1:A:586:LEU:HD11	1:A:588:LYS:HZ3	1.86	0.41
1:A:406:LEU:CD1	1:A:412:TYR:HB3	2.51	0.41
1:A:242:GLU:HB3	1:A:247:GLN:O	2.21	0.41
1:A:60:LYS:HD3	1:A:130:LYS:HG2	2.02	0.41
1:A:215:LYS:NZ	1:A:219:ASN:ND2	2.69	0.41
1:A:377:TYR:HB2	1:A:459:ASN:O	2.21	0.41
1:A:393:ALA:CB	1:A:433:ILE:CD1	2.99	0.41
1:A:485:SER:O	1:A:581:ARG:HD3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:TRP:CE3	1:A:119:ILE:CG2	3.04	0.40
1:A:244:VAL:CG2	1:A:245:SER:N	2.82	0.40
1:A:110:ILE:HG22	1:A:111:GLN:N	2.35	0.40
1:A:24:MET:SD	1:A:40:PRO:HB3	2.62	0.40
1:A:48:PHE:CZ	1:A:53:ILE:CG2	3.05	0.40
1:A:248:ILE:HG12	1:A:249:ASP:H	1.86	0.40
1:A:355:ASN:HB2	1:A:356:THR:H	1.52	0.40
1:A:490:LEU:HG	1:A:528:PHE:CZ	2.56	0.40
1:A:558:THR:CG2	1:A:583:MET:SD	3.09	0.40
1:A:462:LYS:NZ	1:A:474:ASN:H	2.19	0.40
1:A:260:MET:HE1	1:A:526:LYS:HZ2	1.82	0.40
1:A:482:THR:O	1:A:486:THR:HG23	2.21	0.40
1:A:370:ASN:O	1:A:409:GLY:HA2	2.22	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	489/721 (68%)	311 (64%)	108 (22%)	70 (14%)	0 1

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	PHE
1	A	57	LEU
1	A	85	SER
1	A	86	PRO
1	A	213	ASP
1	A	214	ASP
1	A	215	LYS
1	A	247	GLN

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Mol	Chain	Res	Type
1	A	262	SER
1	A	267	VAL
1	A	329	ASN
1	A	454	SER
1	A	493	SER
1	A	543	GLU
1	A	572	LYS
1	A	589	VAL
1	A	36	ASN
1	A	43	ASP
1	A	61	ILE
1	A	98	ASN
1	A	107	VAL
1	A	118	ARG
1	A	144	ILE
1	A	234	ALA
1	A	248	ILE
1	A	304	VAL
1	A	328	ALA
1	A	342	ASP
1	A	405	TYR
1	A	477	GLY
1	A	490	LEU
1	A	557	ASN
1	A	571	ASN
1	A	59	ASN
1	A	84	ASN
1	A	131	ASN
1	A	378	ASN
1	A	381	PRO
1	A	388	ASP
1	A	478	PRO
1	A	31	ASP
1	A	100	SER
1	A	119	ILE
1	A	161	ASN
1	A	162	THR
1	A	187	ASP
1	A	206	ASN
1	A	207	GLN
1	A	254	MET
1	A	273	ARG

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Mol	Chain	Res	Type
1	A	355	ASN
1	A	481	GLY
1	A	506	PRO
1	A	529	ARG
1	A	588	LYS
1	A	73	PRO
1	A	99	LEU
1	A	208	LYS
1	A	375	PRO
1	A	516	PRO
1	A	117	ILE
1	A	473	GLY
1	A	475	ASN
1	A	574	ILE
1	A	483	ILE
1	A	228	PRO
1	A	419	PRO
1	A	364	PRO
1	A	495	PRO
1	A	505	ALA

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	451/648 (70%)	331 (73%)	120 (27%)	0	2

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	PHE
1	A	20	ILE
1	A	23	LEU
1	A	28	PHE
1	A	43	ASP
1	A	56	ILE

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Mol	Chain	Res	Type
1	A	59	ASN
1	A	61	ILE
1	A	64	SER
1	A	71	ILE
1	A	74	SER
1	A	80	ILE
1	A	87	ASN
1	A	89	ARG
1	A	90	VAL
1	A	91	GLU
1	A	92	LEU
1	A	96	ILE
1	A	98	ASN
1	A	99	LEU
1	A	101	LEU
1	A	109	LEU
1	A	117	ILE
1	A	123	MET
1	A	124	SER
1	A	128	LEU
1	A	135	ILE
1	A	138	TYR
1	A	139	TRP
1	A	142	SER
1	A	144	ILE
1	A	155	LEU
1	A	156	LYS
1	A	162	THR
1	A	186	ARG
1	A	188	THR
1	A	190	ARG
1	A	193	ILE
1	A	205	MET
1	A	208	LYS
1	A	214	ASP
1	A	215	LYS
1	A	222	LYS
1	A	225	VAL
1	A	226	SER
1	A	233	THR
1	A	245	SER
1	A	254	MET

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Mol	Chain	Res	Type
1	A	258	ASP
1	A	260	MET
1	A	261	ILE
1	A	262	SER
1	A	264	TYR
1	A	270	GLN
1	A	271	MET
1	A	274	LEU
1	A	276	VAL
1	A	299	THR
1	A	301	ILE
1	A	302	ASN
1	A	308	VAL
1	A	325	SER
1	A	329	ASN
1	A	331	SER
1	A	339	THR
1	A	340	VAL
1	A	341	ASP
1	A	344	THR
1	A	354	ILE
1	A	355	ASN
1	A	356	THR
1	A	363	ASN
1	A	365	ASN
1	A	366	ILE
1	A	367	ARG
1	A	369	TYR
1	A	371	THR
1	A	376	VAL
1	A	380	THR
1	A	382	THR
1	A	386	VAL
1	A	388	ASP
1	A	389	LYS
1	A	398	GLN
1	A	405	TYR
1	A	407	ASN
1	A	414	ILE
1	A	415	ILE
1	A	424	THR
1	A	435	ILE

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Mol	Chain	Res	Type
1	A	442	SER
1	A	450	MET
1	A	451	LEU
1	A	459	ASN
1	A	469	LEU
1	A	485	SER
1	A	490	LEU
1	A	492	LEU
1	A	493	SER
1	A	499	THR
1	A	501	VAL
1	A	514	LYS
1	A	515	THR
1	A	518	LEU
1	A	519	THR
1	A	524	LEU
1	A	526	LYS
1	A	538	TYR
1	A	545	SER
1	A	550	ILE
1	A	554	LEU
1	A	567	LYS
1	A	569	THR
1	A	572	LYS
1	A	573	ASP
1	A	577	CYS
1	A	578	ILE
1	A	579	ILE
1	A	583	MET
1	A	589	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	87	ASN
1	A	93	ASN
1	A	98	ASN
1	A	105	ASN
1	A	113	ASN
1	A	126	ASN
1	A	127	GLN

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Mol	Chain	Res	Type
1	A	200	ASN
1	A	207	GLN
1	A	247	GLN
1	A	302	ASN
1	A	329	ASN
1	A	363	ASN
1	A	407	ASN
1	A	423	ASN
1	A	455	GLN
1	A	459	ASN
1	A	468	ASN
1	A	500	GLN
1	A	551	GLN
1	A	571	ASN
1	A	576	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	505/721 (70%)	1.36	119 (23%)	1	0	22, 43, 63, 71	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	344	THR	8.3
1	A	48	PHE	7.0
1	A	328	ALA	7.0
1	A	359	SER	6.9
1	A	305	GLY	6.7
1	A	440	LEU	6.4
1	A	566	LEU	6.3
1	A	343	THR	5.9
1	A	50	LYS	5.7
1	A	49	SER	5.4
1	A	353	SER	5.3
1	A	47	THR	5.0
1	A	295	SER	5.0
1	A	437	TYR	5.0
1	A	556	ARG	4.8
1	A	438	ASN	4.8
1	A	306	ALA	4.6
1	A	378	ASN	4.5
1	A	562	PHE	4.4
1	A	62	ILE	4.3
1	A	161	ASN	4.1
1	A	395	ILE	4.1
1	A	334	TRP	4.1
1	A	327	SER	4.0
1	A	398	GLN	3.9
1	A	545	SER	3.9
1	A	433	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	83	THR	3.8
1	A	400	SER	3.8
1	A	383	THR	3.7
1	A	575	MET	3.7
1	A	423	ASN	3.7
1	A	333	THR	3.6
1	A	58	GLY	3.6
1	A	571	ASN	3.4
1	A	405	TYR	3.4
1	A	494	LEU	3.4
1	A	363	ASN	3.4
1	A	244	VAL	3.4
1	A	391	SER	3.4
1	A	360	ALA	3.3
1	A	534	ASN	3.3
1	A	418	PRO	3.3
1	A	44	GLY	3.3
1	A	53	ILE	3.2
1	A	325	SER	3.2
1	A	536	LYS	3.2
1	A	51	GLU	3.2
1	A	304	VAL	3.2
1	A	392	VAL	3.2
1	A	226	SER	3.2
1	A	573	ASP	3.1
1	A	532	LYS	3.1
1	A	432	LEU	3.1
1	A	509	SER	3.1
1	A	71	ILE	3.0
1	A	567	LYS	3.0
1	A	495	PRO	3.0
1	A	434	PRO	3.0
1	A	468	ASN	3.0
1	A	569	THR	3.0
1	A	296	HIS	2.9
1	A	441	LYS	2.9
1	A	302	ASN	2.9
1	A	568	ASN	2.9
1	A	97	PHE	2.9
1	A	442	SER	2.8
1	A	52	ASP	2.8
1	A	396	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	307	GLU	2.8
1	A	144	ILE	2.8
1	A	274	LEU	2.7
1	A	508	PHE	2.7
1	A	356	THR	2.7
1	A	387	ILE	2.7
1	A	163	ASN	2.7
1	A	586	LEU	2.7
1	A	299	THR	2.7
1	A	507	ASN	2.7
1	A	329	ASN	2.6
1	A	517	ARG	2.6
1	A	563	GLU	2.6
1	A	560	VAL	2.5
1	A	570	ALA	2.5
1	A	422	LEU	2.5
1	A	565	GLN	2.5
1	A	101	LEU	2.5
1	A	85	SER	2.5
1	A	42	LEU	2.4
1	A	122	LEU	2.4
1	A	393	ALA	2.4
1	A	404	ASP	2.3
1	A	436	ASN	2.3
1	A	264	TYR	2.3
1	A	576	ASN	2.3
1	A	262	SER	2.3
1	A	93	ASN	2.3
1	A	572	LYS	2.3
1	A	381	PRO	2.2
1	A	357	ALA	2.2
1	A	82	SER	2.2
1	A	308	VAL	2.2
1	A	355	ASN	2.2
1	A	574	ILE	2.2
1	A	336	ASN	2.2
1	A	579	ILE	2.2
1	A	263	ALA	2.1
1	A	332	HIS	2.1
1	A	114	VAL	2.1
1	A	467	GLY	2.1
1	A	504	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	33	PHE	2.1
1	A	145	ILE	2.1
1	A	35	LEU	2.1
1	A	190	ARG	2.1
1	A	72	LYS	2.1
1	A	279	SER	2.0
1	A	45	ASN	2.0
1	A	157	PRO	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.