W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:04 AM GMT

PDB ID	:	2ZE2
Title	:	Crystal structure of L100I/K103N mutant HIV-1 reverse transcriptase (RT) in complex with TMC278 (rilpivirine), a non-nucleoside RT inhibitor
Authors	:	Das, K.; Bauman, J.D.; Clark Jr., A.D.; Shatkin, A.J.; Arnold, E.
Deposited on	:	2007-12-05
Resolution	:	2.90 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	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 2.90 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.237
Clashscore		34
Ramachandran outliers		4.0%
Sidechain outliers		3.8%
RSRZ outliers		8.8%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
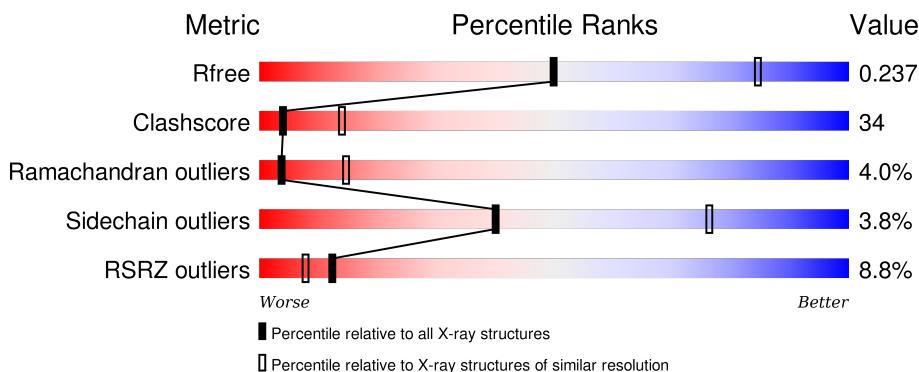
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	557	11% / 45% / 49% / · ·
2	B	428	6% / 43% / 48% / 6% ·
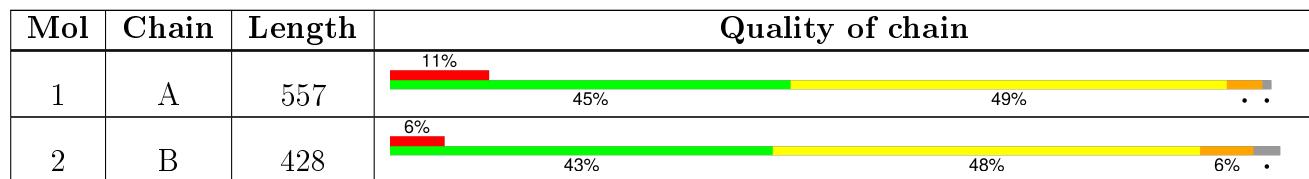
2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7958 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 Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	552	4489	2905	746	831	7	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	EXPRESSION TAG	UNP P03366
A	0	VAL	-	EXPRESSION TAG	UNP P03366
A	100	ILE	LEU	ENGINEERED	UNP P03366
A	103	ASN	LYS	ENGINEERED	UNP P03366
A	172	ALA	LYS	ENGINEERED	UNP P03366
A	173	ALA	LYS	ENGINEERED	UNP P03366
A	280	SER	CYS	ENGINEERED	UNP P03366

- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	416	3441	2244	568	622	7	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	ENGINEERED	UNP P03366

- Molecule 3 is 4-{[4-({4-[(E)-2-CYANOETHENYL]-2,6-DIMETHYLPHENYL}AMINO)PYRIMIDIN-2-YL]AMINO}BENZONITRILE (three-letter code: T27) (formula: $C_{22}H_{18}N_6$).
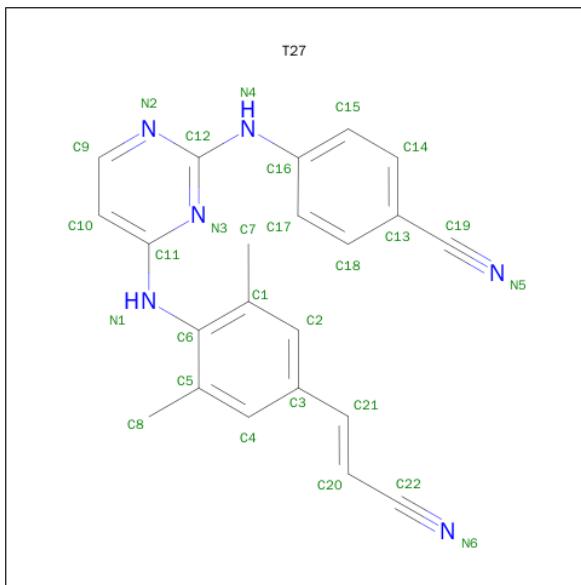
| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
3	A	1	28	22	6	0	0

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: Reverse transcriptase/ribonuclease H
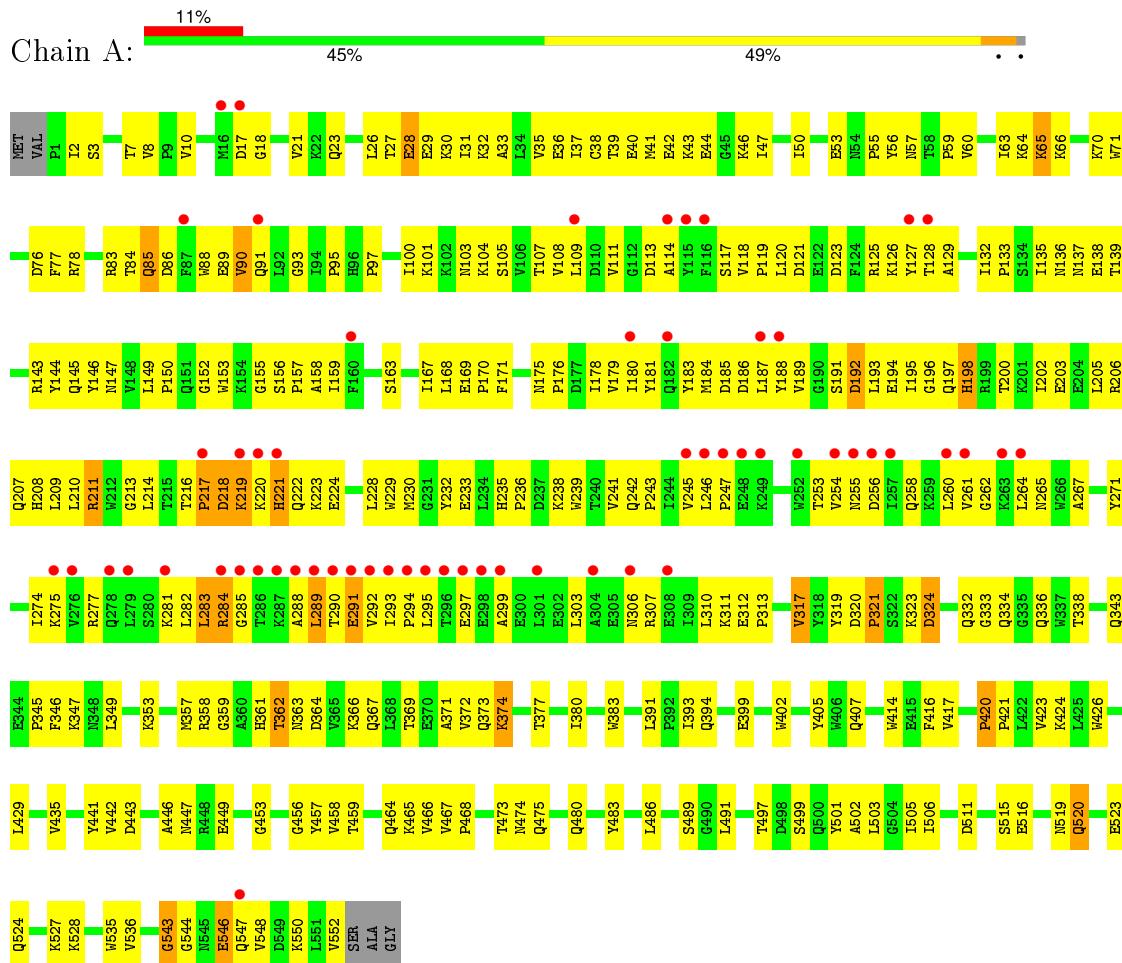
- Molecule 2: p51 RT
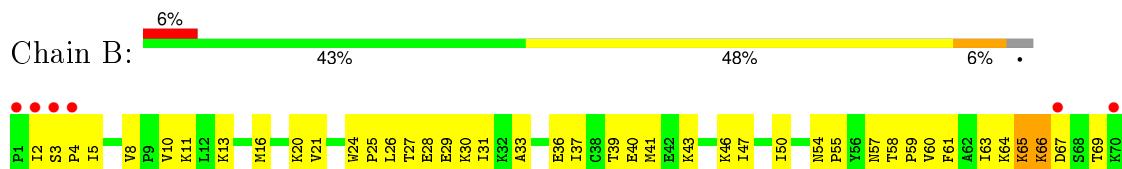
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	163.53Å 73.40Å 109.29Å 90.00° 100.60° 90.00°	Depositor
Resolution (Å)	40.00 – 2.90 43.51 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.7 (40.00-2.90) 98.7 (43.51-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.67 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.241 , 0.299 0.241 , 0.237	Depositor DCC
R_{free} test set	1403 reflections (4.99%)	DCC
Wilson B-factor (Å^2)	68.8	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 59.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.48$, $<L^2> = 0.31$	Xtriage
Outliers	0 of 28140 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7958	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section:
T27

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	0.45	0/4607	0.69	1/6263 (0.0%)
2	B	0.44	0/3541	0.70	1/4810 (0.0%)
All	All	0.45	0/8148	0.69	2/11073 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	91	GLN	N-CA-C	-6.44	93.62	111.00
1	A	546	GLU	N-CA-C	-6.41	93.70	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4489	0	4537	310	0
2	B	3441	0	3476	252	0
3	A	28	0	18	5	0
All	All	7958	0	8031	549	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 34.

All (549) 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)
2:B:94:ILE:HG21	2:B:181:TYR:CE1	1.80	1.17
2:B:94:ILE:HG21	2:B:181:TYR:HE1	0.99	1.14
1:A:206:ARG:HH12	1:A:218:ASP:HA	0.93	1.06
1:A:457:TYR:HA	1:A:547:GLN:HE22	1.11	1.05
1:A:206:ARG:NH1	1:A:218:ASP:HA	1.75	1.00
1:A:206:ARG:HH12	1:A:218:ASP:CA	1.76	0.99
1:A:57:ASN:HB2	1:A:143:ARG:HH12	1.27	0.97
2:B:94:ILE:CG2	2:B:181:TYR:HE1	1.77	0.95
2:B:361:HIS:CE1	2:B:366:LYS:HD3	2.02	0.95
1:A:219:LYS:HG2	1:A:219:LYS:O	1.67	0.94
2:B:425:LEU:O	2:B:428:GLN:HB3	1.73	0.89
1:A:303:LEU:HD21	1:A:307:ARG:HH21	1.38	0.89
1:A:457:TYR:HA	1:A:547:GLN:NE2	1.88	0.88
2:B:214:LEU:HB2	2:B:228:LEU:HD11	1.60	0.84
1:A:95:PRO:HD2	1:A:229:TRP:HH2	1.42	0.83
2:B:279:LEU:O	2:B:282:LEU:HG	1.78	0.81
1:A:31:ILE:O	1:A:35:VAL:HG23	1.80	0.81
1:A:202:ILE:O	1:A:206:ARG:HG3	1.82	0.79
1:A:65:LYS:HG3	1:A:66:LYS:H	1.46	0.79
2:B:66:LYS:HE2	2:B:230:MET:HG3	1.64	0.79
2:B:266:TRP:O	2:B:269:GLN:HG2	1.81	0.79
1:A:163:SER:O	1:A:167:ILE:HG13	1.83	0.78
1:A:456:GLY:HA3	1:A:550:LYS:NZ	1.99	0.78
1:A:57:ASN:HB2	1:A:143:ARG:NH1	1.99	0.77
1:A:28:GLU:O	1:A:32:LYS:HG3	1.84	0.77
1:A:90:VAL:HG21	2:B:140:PRO:HB3	1.67	0.76
2:B:361:HIS:HE1	2:B:366:LYS:HD3	1.48	0.75
2:B:93:GLY:O	2:B:94:ILE:HB	1.86	0.75
2:B:66:LYS:HG3	2:B:67:ASP:H	1.52	0.75
2:B:13:LYS:HB2	2:B:16:MET:SD	2.26	0.74
2:B:363:ASN:O	2:B:367:GLN:HG3	1.85	0.74
1:A:104:LYS:HG3	1:A:192:ASP:OD1	1.88	0.74
1:A:17:ASP:O	1:A:83:ARG:HD3	1.88	0.74
2:B:354:TYR:HE1	2:B:374:LYS:HD2	1.53	0.73
2:B:57:ASN:HA	2:B:129:ALA:O	1.87	0.73
2:B:170:PRO:HG2	2:B:208:HIS:CE1	2.23	0.72
1:A:543:GLY:HA2	2:B:284:ARG:HA	1.71	0.72
2:B:170:PRO:HG2	2:B:208:HIS:HE1	1.55	0.72
2:B:193:LEU:HD13	2:B:197:GLN:HG2	1.72	0.72
2:B:66:LYS:HG3	2:B:67:ASP:N	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:TYR:CD2	1:A:544:GLY:HA3	2.24	0.72
1:A:7:THR:HG21	1:A:121:ASP:HA	1.71	0.71
1:A:39:THR:O	1:A:43:LYS:HG2	1.91	0.71
1:A:543:GLY:HA3	2:B:283:LEU:C	2.12	0.70
1:A:255:ASN:ND2	1:A:289:LEU:HD13	2.06	0.70
2:B:354:TYR:CE1	2:B:374:LYS:HD2	2.26	0.70
1:A:443:ASP:HB3	1:A:547:GLN:OE1	1.91	0.70
2:B:356:ARG:NH1	2:B:367:GLN:OE1	2.25	0.70
1:A:186:ASP:HB2	1:A:188:TYR:CE1	2.27	0.70
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.74	0.70
2:B:107:THR:HA	2:B:232:TYR:O	1.92	0.70
1:A:64:LYS:HG2	1:A:70:LYS:O	1.92	0.69
2:B:66:LYS:CE	2:B:230:MET:HG3	2.23	0.69
2:B:425:LEU:HD12	2:B:428:GLN:CB	2.23	0.69
1:A:417:VAL:O	1:A:417:VAL:HG13	1.93	0.69
2:B:425:LEU:HD12	2:B:428:GLN:HB2	1.75	0.69
2:B:104:LYS:HG2	2:B:192:ASP:OD1	1.92	0.69
1:A:466:VAL:HG22	1:A:550:LYS:HZ3	1.58	0.68
1:A:136:ASN:O	1:A:138:GLU:HG3	1.94	0.68
1:A:218:ASP:OD1	1:A:220:LYS:HB2	1.93	0.68
1:A:107:THR:HG22	1:A:108:VAL:N	2.08	0.68
1:A:97:PRO:HA	1:A:100:ILE:HD12	1.75	0.68
1:A:246:LEU:HG	1:A:310:LEU:HD12	1.75	0.68
1:A:64:LYS:HG3	1:A:71:TRP:CE3	2.29	0.68
1:A:114:ALA:HB1	1:A:214:LEU:HD13	1.76	0.68
2:B:85:GLN:NE2	2:B:154:LYS:HB3	2.09	0.67
1:A:178:ILE:HD11	1:A:180:ILE:HD11	1.76	0.67
2:B:64:LYS:HD3	2:B:69:THR:HA	1.77	0.67
1:A:324:ASP:O	1:A:343:GLN:HG2	1.94	0.67
1:A:218:ASP:OD1	1:A:220:LYS:CB	2.43	0.67
1:A:543:GLY:HA3	2:B:283:LEU:O	1.95	0.67
2:B:214:LEU:HD23	2:B:214:LEU:H	1.60	0.67
2:B:312:GLU:HB3	2:B:313:PRO:HD2	1.76	0.66
1:A:246:LEU:HD11	1:A:306:ASN:HB3	1.76	0.66
1:A:235:HIS:HB3	1:A:236:PRO:HD2	1.77	0.66
2:B:108:VAL:O	2:B:231:GLY:HA2	1.95	0.66
1:A:456:GLY:HA3	1:A:550:LYS:HZ2	1.60	0.65
1:A:23:GLN:HE22	1:A:60:VAL:HG12	1.61	0.65
2:B:88:TRP:CD1	2:B:92:LEU:HD12	2.32	0.65
1:A:89:GLU:CD	1:A:158:ALA:HB2	2.18	0.64
2:B:81:ASN:HA	2:B:84:THR:HG22	1.79	0.64

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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)
2:B:195:ILE:HG12	2:B:199:ARG:HH21	1.62	0.64
2:B:81:ASN:HA	2:B:84:THR:CG2	2.28	0.64
1:A:118:VAL:HG11	1:A:149:LEU:HD11	1.79	0.64
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.38	0.63
1:A:28:GLU:OE1	1:A:32:LYS:HE3	1.97	0.63
1:A:241:VAL:HG21	1:A:271:TYR:CE1	2.33	0.63
1:A:253:THR:HA	1:A:292:VAL:HA	1.81	0.63
2:B:298:GLU:N	2:B:298:GLU:OE1	2.28	0.63
1:A:311:LYS:HG3	1:A:312:GLU:N	2.13	0.63
1:A:202:ILE:HG21	1:A:219:LYS:HD2	1.80	0.63
2:B:239:TRP:CZ2	2:B:378:GLU:HG2	2.34	0.63
1:A:306:ASN:O	1:A:310:LEU:HG	1.99	0.63
2:B:154:LYS:HG2	2:B:184:MET:HE3	1.80	0.63
1:A:253:THR:HG23	1:A:255:ASN:H	1.63	0.63
1:A:101:LYS:HE2	1:A:321:PRO:HG3	1.80	0.63
1:A:546:GLU:O	1:A:546:GLU:HG3	1.98	0.62
2:B:214:LEU:HB2	2:B:228:LEU:CD1	2.28	0.62
2:B:63:ILE:HD13	2:B:74:LEU:HD22	1.81	0.62
2:B:214:LEU:HD12	2:B:228:LEU:HD22	1.81	0.62
1:A:311:LYS:O	1:A:313:PRO:HD3	2.00	0.62
1:A:228:LEU:CD2	1:A:233:GLU:HG2	2.29	0.62
1:A:26:LEU:HB2	1:A:31:ILE:CG1	2.29	0.62
1:A:274:ILE:HD11	1:A:310:LEU:HD21	1.82	0.62
2:B:72:ARG:HH11	2:B:72:ARG:HG3	1.64	0.62
1:A:284:ARG:HD3	1:A:284:ARG:N	2.15	0.61
1:A:457:TYR:CA	1:A:547:GLN:HE22	2.00	0.61
2:B:388:LYS:HD2	2:B:413:GLU:HB2	1.82	0.60
1:A:277:ARG:NH1	1:A:334:GLN:HB3	2.16	0.60
1:A:171:PHE:CD2	1:A:205:LEU:HD13	2.36	0.60
2:B:84:THR:HG21	2:B:153:TRP:HE1	1.66	0.60
2:B:240:THR:O	2:B:350:LYS:HD2	2.01	0.60
1:A:117:SER:O	1:A:119:PRO:HD3	2.01	0.60
1:A:281:LYS:O	1:A:282:LEU:HD23	2.02	0.60
1:A:206:ARG:HH22	1:A:218:ASP:N	2.00	0.60
1:A:267:ALA:HB1	1:A:271:TYR:CD1	2.37	0.60
1:A:536:VAL:CG1	2:B:258:GLN:HG2	2.31	0.60
1:A:311:LYS:HG3	1:A:312:GLU:HG2	1.83	0.59
2:B:332:GLN:HG3	2:B:338:THR:HG23	1.83	0.59
2:B:88:TRP:HD1	2:B:93:GLY:H	1.49	0.59
1:A:283:LEU:HD12	1:A:283:LEU:O	2.02	0.59
1:A:317:VAL:CG2	1:A:349:LEU:HD23	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:205:LEU:O	2:B:209:LEU:HG	2.02	0.59
1:A:50:ILE:HG13	1:A:143:ARG:HB3	1.83	0.59
2:B:103:LYS:HB3	2:B:191:SER:O	2.03	0.59
1:A:319:TYR:CD2	1:A:383:TRP:HD1	2.21	0.58
1:A:17:ASP:OD1	1:A:18:GLY:N	2.31	0.58
1:A:33:ALA:O	1:A:36:GLU:HB3	2.03	0.58
1:A:417:VAL:O	1:A:417:VAL:CG1	2.51	0.58
2:B:195:ILE:CD1	2:B:199:ARG:HH21	2.15	0.58
1:A:380:ILE:HG22	2:B:25:PRO:HB2	1.85	0.58
1:A:260:LEU:HD21	1:A:303:LEU:HD13	1.84	0.58
1:A:26:LEU:HD12	1:A:31:ILE:HG12	1.85	0.58
1:A:254:VAL:HG23	1:A:291:GLU:O	2.04	0.58
1:A:253:THR:H	1:A:256:ASP:HB2	1.68	0.58
1:A:284:ARG:HG2	1:A:285:GLY:H	1.68	0.58
2:B:8:VAL:O	2:B:10:VAL:HG23	2.03	0.58
1:A:229:TRP:HB2	3:A:556:T27:C22	2.33	0.58
2:B:191:SER:OG	2:B:198:HIS:ND1	2.37	0.58
2:B:195:ILE:CG1	2:B:199:ARG:HH21	2.16	0.57
1:A:391:LEU:HD12	1:A:414:TRP:CE3	2.39	0.57
1:A:104:LYS:HG3	1:A:192:ASP:CG	2.23	0.57
1:A:255:ASN:HB2	1:A:289:LEU:HB3	1.85	0.57
2:B:50:ILE:HG21	2:B:145:GLN:HB2	1.86	0.57
1:A:429:LEU:HD11	1:A:506:ILE:HG22	1.86	0.57
1:A:275:LYS:HE2	1:A:332:GLN:NE2	2.20	0.57
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.85	0.57
1:A:241:VAL:HG21	1:A:271:TYR:HE1	1.70	0.57
1:A:233:GLU:O	1:A:239:TRP:HA	2.03	0.57
1:A:456:GLY:HA3	1:A:550:LYS:HZ1	1.69	0.57
1:A:456:GLY:CA	1:A:550:LYS:NZ	2.67	0.57
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.39	0.57
1:A:246:LEU:HD22	1:A:260:LEU:HD11	1.88	0.56
1:A:264:LEU:HB3	1:A:274:ILE:CG2	2.36	0.56
1:A:40:GLU:O	1:A:43:LYS:HB2	2.05	0.56
2:B:116:PHE:CZ	2:B:151:GLN:HG3	2.40	0.56
2:B:65:LYS:HZ3	2:B:65:LYS:HA	1.69	0.56
1:A:111:VAL:C	1:A:113:ASP:H	2.06	0.56
1:A:443:ASP:CB	1:A:547:GLN:OE1	2.53	0.56
2:B:47:ILE:HD12	2:B:144:TYR:CD2	2.41	0.56
1:A:100:ILE:HG23	3:A:556:T27:C12	2.36	0.55
2:B:373:GLN:HE22	2:B:406:TRP:HA	1.71	0.55
2:B:379:SER:CB	2:B:387:PRO:HD3	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:VAL:HB	1:A:221:HIS:CB	2.36	0.55
1:A:260:LEU:HD21	1:A:303:LEU:CD1	2.35	0.55
2:B:89:GLU:O	2:B:91:GLN:HG2	2.06	0.55
2:B:167:ILE:HG23	2:B:212:TRP:CB	2.36	0.55
2:B:81:ASN:CA	2:B:84:THR:HG22	2.35	0.55
1:A:107:THR:CG2	1:A:108:VAL:N	2.69	0.55
1:A:457:TYR:CA	1:A:547:GLN:NE2	2.64	0.55
2:B:58:THR:N	2:B:129:ALA:O	2.40	0.55
1:A:194:GLU:HG3	1:A:197:GLN:H	1.71	0.55
2:B:305:GLU:O	2:B:309:ILE:HG13	2.06	0.55
2:B:178:ILE:HD11	2:B:201:LYS:HD3	1.88	0.55
1:A:466:VAL:HG22	1:A:550:LYS:NZ	2.21	0.55
1:A:56:TYR:O	1:A:129:ALA:HB3	2.07	0.55
1:A:254:VAL:HG12	1:A:289:LEU:HD23	1.88	0.54
2:B:73:LYS:NZ	2:B:130:PHE:CZ	2.70	0.54
2:B:105:SER:O	2:B:106:VAL:HG23	2.07	0.54
1:A:90:VAL:O	1:A:90:VAL:HG22	2.07	0.54
2:B:65:LYS:NZ	2:B:65:LYS:HA	2.22	0.54
2:B:88:TRP:HD1	2:B:92:LEU:HA	1.72	0.54
1:A:108:VAL:HB	1:A:221:HIS:HB2	1.87	0.54
1:A:8:VAL:O	1:A:10:VAL:HG23	2.08	0.54
1:A:228:LEU:HB3	1:A:242:GLN:OE1	2.07	0.54
2:B:20:LYS:HE2	2:B:55:PRO:HB2	1.90	0.54
1:A:57:ASN:CB	1:A:143:ARG:HH12	2.11	0.54
2:B:109:LEU:HB2	2:B:187:LEU:HB3	1.90	0.54
1:A:229:TRP:O	1:A:232:TYR:HD1	1.90	0.54
2:B:312:GLU:HB3	2:B:313:PRO:CD	2.37	0.54
1:A:235:HIS:CE1	1:A:238:LYS:HE3	2.43	0.54
1:A:118:VAL:CG1	1:A:149:LEU:HD11	2.38	0.54
1:A:220:LYS:O	1:A:222:GLN:N	2.41	0.54
2:B:112:GLY:HA2	2:B:185:ASP:HB3	1.90	0.54
2:B:270:ILE:HG12	2:B:346:PHE:HB3	1.89	0.54
2:B:180:ILE:HG12	2:B:189:VAL:HG22	1.90	0.54
2:B:249:LYS:HG3	2:B:252:TRP:CZ2	2.43	0.54
2:B:336:GLN:HB3	2:B:353:LYS:HZ3	1.73	0.54
1:A:200:THR:O	1:A:203:GLU:N	2.37	0.53
1:A:107:THR:CG2	1:A:108:VAL:H	2.21	0.53
1:A:536:VAL:HG11	2:B:258:GLN:HG2	1.91	0.53
2:B:270:ILE:HG22	2:B:271:TYR:CD1	2.44	0.53
1:A:107:THR:HG22	1:A:108:VAL:H	1.72	0.53
1:A:220:LYS:O	1:A:220:LYS:HG2	2.09	0.53

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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:543:GLY:CA	2:B:284:ARG:HA	2.36	0.53
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.90	0.53
1:A:424:LYS:HD3	1:A:426:TRP:CH2	2.43	0.53
1:A:254:VAL:HB	1:A:289:LEU:HA	1.90	0.53
2:B:163:SER:O	2:B:166:LYS:HG2	2.09	0.53
1:A:209:LEU:O	1:A:214:LEU:HB2	2.07	0.53
1:A:126:LYS:HE3	1:A:127:TYR:CE1	2.42	0.53
1:A:253:THR:HG23	1:A:256:ASP:H	1.73	0.53
2:B:358:ARG:NH2	2:B:370:GLU:OE1	2.40	0.53
2:B:13:LYS:HG2	2:B:86:ASP:HA	1.90	0.53
1:A:311:LYS:CG	1:A:312:GLU:N	2.71	0.53
2:B:163:SER:HA	2:B:166:LYS:HE2	1.90	0.53
1:A:363:ASN:HB2	1:A:511:ASP:OD2	2.09	0.53
2:B:84:THR:O	2:B:86:ASP:N	2.35	0.53
1:A:467:VAL:HG13	1:A:468:PRO:HD2	1.90	0.53
2:B:329:ILE:N	2:B:329:ILE:HD12	2.23	0.53
2:B:84:THR:C	2:B:86:ASP:H	2.10	0.52
2:B:28:GLU:HB2	2:B:135:ILE:HD11	1.91	0.52
1:A:178:ILE:CD1	1:A:180:ILE:HD11	2.39	0.52
1:A:7:THR:CG2	1:A:121:ASP:HA	2.39	0.52
1:A:483:TYR:HE1	1:A:524:GLN:HE21	1.57	0.52
1:A:258:GLN:O	1:A:261:VAL:HG12	2.09	0.52
1:A:357:MET:O	1:A:359:GLY:N	2.42	0.52
1:A:277:ARG:HB2	1:A:336:GLN:NE2	2.23	0.52
2:B:106:VAL:HG22	2:B:190:GLY:HA3	1.91	0.52
1:A:467:VAL:CG1	1:A:468:PRO:HD2	2.40	0.52
2:B:36:GLU:O	2:B:39:THR:HB	2.09	0.52
1:A:307:ARG:HG2	1:A:307:ARG:HH11	1.75	0.52
1:A:338:THR:HA	1:A:353:LYS:HA	1.91	0.52
2:B:272:PRO:O	2:B:274:ILE:N	2.42	0.52
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.45	0.52
1:A:206:ARG:HH12	1:A:218:ASP:C	2.12	0.52
2:B:124:PHE:CE1	2:B:127:TYR:HD1	2.28	0.52
1:A:253:THR:HG22	1:A:256:ASP:OD2	2.10	0.52
1:A:184:MET:CE	1:A:184:MET:HA	2.40	0.52
2:B:193:LEU:HD11	2:B:201:LYS:HD2	1.91	0.51
1:A:76:ASP:OD1	1:A:78:ARG:HG3	2.10	0.51
1:A:50:ILE:CG1	1:A:143:ARG:HB3	2.41	0.51
2:B:84:THR:HG21	2:B:153:TRP:NE1	2.24	0.51
1:A:179:VAL:O	1:A:189:VAL:HA	2.11	0.51
2:B:13:LYS:HE2	2:B:86:ASP:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:81:ASN:O	2:B:85:GLN:HG3	2.10	0.51
1:A:41:MET:O	1:A:44:GLU:N	2.42	0.51
1:A:464:GLN:O	1:A:465:LYS:HB2	2.10	0.51
1:A:523:GLU:O	1:A:527:LYS:HG3	2.09	0.51
1:A:441:TYR:CE2	1:A:544:GLY:HA3	2.44	0.51
1:A:64:LYS:HE2	1:A:70:LYS:O	2.09	0.51
2:B:25:PRO:O	2:B:26:LEU:HD23	2.10	0.51
2:B:246:LEU:CD1	2:B:264:LEU:HD21	2.40	0.51
1:A:253:THR:CG2	1:A:256:ASP:H	2.23	0.51
2:B:72:ARG:NH1	2:B:73:LYS:O	2.44	0.51
2:B:27:THR:OG1	2:B:30:LYS:HG3	2.09	0.51
2:B:88:TRP:CD1	2:B:92:LEU:HA	2.46	0.51
2:B:86:ASP:O	2:B:87:PHE:HB2	2.11	0.51
2:B:91:GLN:HA	2:B:161:GLN:NE2	2.26	0.50
2:B:41:MET:HE1	2:B:73:LYS:HD3	1.92	0.50
2:B:167:ILE:HG23	2:B:212:TRP:HB3	1.94	0.50
2:B:253:THR:O	2:B:257:ILE:HG12	2.11	0.50
1:A:2:ILE:CG2	1:A:3:SER:N	2.74	0.50
1:A:97:PRO:HG2	1:A:232:TYR:CD2	2.46	0.50
2:B:160:PHE:CD2	2:B:164:MET:HB2	2.46	0.50
1:A:219:LYS:C	1:A:221:HIS:H	2.14	0.50
2:B:50:ILE:HD12	2:B:54:ASN:HB3	1.94	0.50
1:A:506:ILE:O	1:A:506:ILE:HG22	2.10	0.50
2:B:156:SER:N	2:B:157:PRO:HD2	2.26	0.50
1:A:264:LEU:O	1:A:274:ILE:HG21	2.11	0.50
1:A:211:ARG:HG2	1:A:211:ARG:HH11	1.76	0.50
1:A:26:LEU:HB2	1:A:31:ILE:HD11	1.93	0.50
1:A:486:LEU:HB3	1:A:524:GLN:CG	2.41	0.50
1:A:399:GLU:HA	1:A:402:TRP:CD1	2.45	0.50
2:B:329:ILE:HD11	2:B:389:PHE:HD2	1.76	0.50
1:A:229:TRP:HB2	3:A:556:T27:N6	2.26	0.50
2:B:80:LEU:O	2:B:84:THR:HG22	2.12	0.50
1:A:30:LYS:HE2	1:A:71:TRP:CH2	2.47	0.50
2:B:373:GLN:NE2	2:B:406:TRP:HA	2.27	0.50
2:B:167:ILE:HG22	2:B:167:ILE:O	2.11	0.50
2:B:166:LYS:C	2:B:168:LEU:H	2.15	0.50
2:B:106:VAL:HA	2:B:190:GLY:HA2	1.93	0.50
1:A:245:VAL:HG22	1:A:246:LEU:N	2.26	0.50
1:A:456:GLY:CA	1:A:550:LYS:HZ1	2.24	0.49
1:A:7:THR:HG22	1:A:8:VAL:N	2.27	0.49
1:A:536:VAL:HG12	2:B:258:GLN:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:HIS:C	1:A:223:LYS:N	2.66	0.49
1:A:40:GLU:O	1:A:44:GLU:HG3	2.12	0.49
2:B:195:ILE:HD11	2:B:199:ARG:HH21	1.77	0.49
2:B:336:GLN:OE1	2:B:353:LYS:NZ	2.45	0.49
1:A:489:SER:O	1:A:528:LYS:NZ	2.46	0.49
1:A:361:HIS:O	1:A:362:THR:OG1	2.28	0.49
1:A:281:LYS:O	1:A:281:LYS:HG2	2.12	0.49
1:A:297:GLU:OE1	1:A:297:GLU:HA	2.13	0.49
1:A:446:ALA:HA	1:A:453:GLY:HA3	1.94	0.49
1:A:89:GLU:OE1	1:A:158:ALA:HB2	2.13	0.49
2:B:46:LYS:HZ2	2:B:116:PHE:HD1	1.60	0.49
2:B:361:HIS:NE2	2:B:366:LYS:HD3	2.28	0.49
2:B:209:LEU:HD13	2:B:214:LEU:HD11	1.95	0.49
2:B:120:LEU:HD11	2:B:124:PHE:HD2	1.78	0.49
1:A:303:LEU:O	1:A:307:ARG:HG3	2.12	0.48
2:B:209:LEU:O	2:B:214:LEU:HG	2.14	0.48
1:A:64:LYS:HE3	1:A:71:TRP:CD1	2.49	0.48
2:B:3:SER:HA	2:B:117:SER:O	2.13	0.48
2:B:4:PRO:CD	2:B:118:VAL:HG22	2.43	0.48
2:B:206:ARG:CZ	2:B:229:TRP:HA	2.43	0.48
2:B:319:TYR:OH	2:B:385:LYS:HD3	2.13	0.48
2:B:378:GLU:O	2:B:382:ILE:HG12	2.13	0.48
1:A:171:PHE:CE2	1:A:205:LEU:HB2	2.49	0.48
1:A:424:LYS:HE2	1:A:426:TRP:CE3	2.48	0.48
1:A:90:VAL:HG21	2:B:140:PRO:CB	2.42	0.48
1:A:520:GLN:O	1:A:524:GLN:HB2	2.14	0.48
1:A:109:LEU:HB2	1:A:187:LEU:HB3	1.95	0.48
2:B:423:VAL:CG1	2:B:427:TYR:CD1	2.96	0.48
1:A:442:VAL:HG12	1:A:457:TYR:HB3	1.96	0.48
2:B:87:PHE:CZ	2:B:89:GLU:HB3	2.49	0.48
1:A:228:LEU:HD21	1:A:233:GLU:HG2	1.96	0.48
2:B:29:GLU:HG3	2:B:30:LYS:N	2.28	0.48
1:A:27:THR:HG22	1:A:29:GLU:OE1	2.14	0.48
1:A:90:VAL:HG13	1:A:91:GLN:NE2	2.29	0.48
1:A:235:HIS:ND1	1:A:238:LYS:HE3	2.27	0.48
1:A:171:PHE:CE2	1:A:205:LEU:HD13	2.49	0.48
2:B:155:GLY:C	2:B:157:PRO:HD2	2.33	0.48
2:B:423:VAL:O	2:B:424:LYS:C	2.52	0.48
2:B:84:THR:HG23	2:B:85:GLN:N	2.29	0.48
1:A:317:VAL:HG11	1:A:347:LYS:HB3	1.96	0.48
2:B:112:GLY:CA	2:B:185:ASP:HB3	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ASP:OD1	1:A:220:LYS:HB3	2.13	0.47
2:B:154:LYS:HG2	2:B:184:MET:CE	2.43	0.47
2:B:350:LYS:NZ	2:B:378:GLU:OE1	2.47	0.47
1:A:458:VAL:HG22	2:B:286:THR:HG21	1.96	0.47
2:B:331:LYS:HB2	2:B:337:TRP:CZ3	2.49	0.47
2:B:50:ILE:CG2	2:B:145:GLN:HB2	2.44	0.47
1:A:457:TYR:C	1:A:457:TYR:CD1	2.88	0.47
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.14	0.47
2:B:315:HIS:CD2	2:B:316:GLY:N	2.83	0.47
2:B:368:LEU:O	2:B:371:ALA:HB3	2.14	0.47
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.97	0.47
2:B:110:ASP:OD2	2:B:227:PHE:CE1	2.67	0.47
2:B:72:ARG:NH2	2:B:151:GLN:NE2	2.63	0.47
1:A:333:GLY:O	1:A:334:GLN:HB2	2.14	0.47
1:A:53:GLU:O	1:A:55:PRO:HD3	2.14	0.47
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.96	0.47
2:B:425:LEU:O	2:B:428:GLN:CB	2.55	0.47
2:B:39:THR:HG23	2:B:43:LYS:HE3	1.96	0.47
2:B:40:GLU:OE1	2:B:40:GLU:N	2.45	0.47
1:A:221:HIS:ND1	1:A:221:HIS:O	2.48	0.47
2:B:358:ARG:HD3	2:B:358:ARG:N	2.29	0.47
1:A:31:ILE:HG23	1:A:133:PRO:O	2.15	0.47
1:A:267:ALA:O	1:A:271:TYR:HD1	1.98	0.47
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.97	0.47
1:A:188:TYR:N	1:A:188:TYR:CD1	2.83	0.47
1:A:320:ASP:OD2	1:A:323:LYS:HE2	2.14	0.47
1:A:205:LEU:O	1:A:208:HIS:N	2.48	0.47
2:B:345:PRO:O	2:B:346:PHE:HB2	2.15	0.47
2:B:260:LEU:HD21	2:B:303:LEU:HD13	1.97	0.47
2:B:242:GLN:OE1	2:B:242:GLN:HA	2.14	0.47
2:B:210:LEU:HA	2:B:214:LEU:C	2.36	0.46
1:A:499:SER:HB3	1:A:502:ALA:HB3	1.96	0.46
2:B:330:GLN:HE21	2:B:330:GLN:HB2	1.56	0.46
2:B:181:TYR:HB3	2:B:188:TYR:HB2	1.97	0.46
1:A:303:LEU:HD21	1:A:307:ARG:NH2	2.18	0.46
2:B:194:GLU:O	2:B:198:HIS:N	2.48	0.46
2:B:202:ILE:O	2:B:205:LEU:N	2.46	0.46
2:B:13:LYS:CG	2:B:86:ASP:HA	2.45	0.46
1:A:114:ALA:HA	1:A:214:LEU:HD22	1.97	0.46
1:A:320:ASP:OD2	1:A:323:LYS:HG3	2.15	0.46
2:B:80:LEU:HG	2:B:84:THR:HB	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:LYS:NZ	2:B:116:PHE:HB3	2.30	0.46
2:B:92:LEU:O	2:B:93:GLY:C	2.53	0.46
2:B:357:MET:C	2:B:358:ARG:HD3	2.36	0.46
1:A:29:GLU:O	1:A:33:ALA:N	2.45	0.46
2:B:65:LYS:HD3	2:B:72:ARG:HD3	1.98	0.46
1:A:111:VAL:C	1:A:113:ASP:N	2.68	0.46
2:B:33:ALA:O	2:B:37:ILE:HG13	2.15	0.46
1:A:435:VAL:HA	2:B:290:THR:HG21	1.97	0.46
1:A:221:HIS:O	1:A:223:LYS:O	2.33	0.46
2:B:84:THR:CG2	2:B:153:TRP:HE1	2.28	0.46
1:A:292:VAL:O	1:A:292:VAL:HG23	2.15	0.46
2:B:246:LEU:HD13	2:B:264:LEU:HD21	1.98	0.46
1:A:516:GLU:HA	1:A:519:ASN:HD22	1.81	0.46
1:A:206:ARG:NH2	1:A:216:THR:OG1	2.44	0.46
1:A:253:THR:HG23	1:A:255:ASN:N	2.30	0.46
2:B:194:GLU:OE1	2:B:194:GLU:N	2.49	0.46
1:A:420:PRO:HA	1:A:421:PRO:C	2.37	0.46
1:A:26:LEU:HB2	1:A:31:ILE:HG13	1.98	0.46
2:B:337:TRP:HE1	2:B:367:GLN:NE2	2.14	0.46
1:A:77:PHE:CE1	1:A:150:PRO:HB3	2.51	0.46
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.51	0.46
1:A:114:ALA:CB	1:A:214:LEU:HD13	2.45	0.46
2:B:249:LYS:HB3	2:B:249:LYS:NZ	2.31	0.46
2:B:319:TYR:CZ	2:B:321:PRO:HA	2.51	0.46
1:A:548:VAL:O	1:A:552:VAL:HG23	2.16	0.46
2:B:47:ILE:HG22	2:B:145:GLN:O	2.16	0.45
2:B:252:TRP:CE3	2:B:257:ILE:HD13	2.51	0.45
2:B:315:HIS:CD2	2:B:316:GLY:H	2.34	0.45
1:A:23:GLN:NE2	1:A:60:VAL:HG12	2.29	0.45
1:A:377:THR:O	1:A:380:ILE:N	2.50	0.45
2:B:28:GLU:O	2:B:31:ILE:N	2.50	0.45
1:A:261:VAL:HG13	1:A:262:GLY:N	2.31	0.45
2:B:90:VAL:HG22	2:B:90:VAL:O	2.16	0.45
1:A:47:ILE:HD12	1:A:144:TYR:CD2	2.52	0.45
2:B:128:THR:OG1	2:B:146:TYR:HB2	2.17	0.45
2:B:171:PHE:CD2	2:B:205:LEU:HD13	2.51	0.45
1:A:2:ILE:HG22	1:A:3:SER:N	2.31	0.45
2:B:136:ASN:O	2:B:137:ASN:HB2	2.16	0.45
2:B:151:GLN:HB3	2:B:151:GLN:HE21	1.58	0.45
1:A:486:LEU:HB3	1:A:524:GLN:HG2	1.97	0.45
2:B:24:TRP:HZ2	2:B:61:PHE:CD2	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:SER:HG	1:A:198:HIS:HD1	1.65	0.45
2:B:88:TRP:HD1	2:B:93:GLY:N	2.13	0.45
2:B:64:LYS:HD3	2:B:69:THR:CA	2.45	0.45
1:A:265:ASN:OD1	1:A:353:LYS:NZ	2.48	0.45
1:A:107:THR:HG23	1:A:219:LYS:HG3	1.99	0.44
1:A:84:THR:O	1:A:85:GLN:O	2.34	0.44
2:B:94:ILE:HG23	2:B:94:ILE:O	2.17	0.44
2:B:336:GLN:HB3	2:B:353:LYS:NZ	2.33	0.44
1:A:369:THR:O	1:A:373:GLN:HG2	2.17	0.44
1:A:307:ARG:HG2	1:A:307:ARG:NH1	2.32	0.44
1:A:282:LEU:HA	1:A:284:ARG:NH1	2.33	0.44
2:B:136:ASN:O	2:B:137:ASN:CB	2.66	0.44
2:B:297:GLU:OE1	2:B:297:GLU:HA	2.17	0.44
2:B:358:ARG:CB	2:B:361:HIS:HD2	2.31	0.44
1:A:253:THR:N	1:A:256:ASP:HB2	2.31	0.44
1:A:64:LYS:HE3	1:A:71:TRP:CG	2.53	0.44
2:B:166:LYS:C	2:B:168:LEU:N	2.71	0.44
2:B:77:PHE:O	2:B:81:ASN:HB2	2.17	0.44
1:A:39:THR:O	1:A:42:GLU:HG2	2.18	0.44
1:A:150:PRO:HB2	1:A:153:TRP:HB2	1.98	0.44
2:B:60:VAL:HG13	2:B:60:VAL:O	2.18	0.44
1:A:491:LEU:HD23	1:A:491:LEU:HA	1.78	0.44
2:B:322:SER:OG	2:B:323:LYS:N	2.51	0.44
2:B:254:VAL:O	2:B:258:GLN:HB2	2.17	0.44
1:A:288:ALA:C	1:A:290:THR:H	2.21	0.44
1:A:155:GLY:O	1:A:159:ILE:HG13	2.18	0.44
2:B:149:LEU:HA	2:B:150:PRO:HD3	1.84	0.44
2:B:171:PHE:HZ	2:B:201:LYS:O	2.01	0.44
1:A:91:GLN:C	1:A:93:GLY:H	2.21	0.44
1:A:311:LYS:CG	1:A:312:GLU:H	2.31	0.44
2:B:72:ARG:HH11	2:B:72:ARG:CG	2.30	0.44
1:A:277:ARG:HH11	1:A:334:GLN:HB3	1.81	0.44
1:A:217:PRO:O	1:A:218:ASP:OD1	2.36	0.44
2:B:367:GLN:O	2:B:368:LEU:C	2.56	0.44
2:B:169:GLU:N	2:B:170:PRO:HD2	2.32	0.44
1:A:282:LEU:HA	1:A:284:ARG:HH12	1.82	0.44
2:B:308:GLU:OE2	2:B:311:LYS:HE3	2.18	0.44
1:A:50:ILE:CG2	1:A:145:GLN:HG2	2.47	0.43
2:B:89:GLU:O	2:B:90:VAL:HG12	2.18	0.43
1:A:153:TRP:HB3	1:A:156:SER:OG	2.18	0.43
1:A:366:LYS:HE2	1:A:405:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:PRO:O	1:A:346:PHE:HB2	2.17	0.43
1:A:206:ARG:NH1	1:A:218:ASP:C	2.71	0.43
1:A:261:VAL:CG1	1:A:262:GLY:N	2.81	0.43
2:B:13:LYS:HD2	2:B:16:MET:SD	2.59	0.43
2:B:94:ILE:CG2	2:B:181:TYR:CE1	2.67	0.43
1:A:107:THR:CG2	1:A:219:LYS:HG3	2.48	0.43
1:A:246:LEU:CD1	1:A:306:ASN:HB3	2.46	0.43
2:B:208:HIS:CD2	2:B:208:HIS:C	2.92	0.43
2:B:420:PRO:HA	2:B:421:PRO:HD2	1.95	0.43
1:A:26:LEU:HB2	1:A:31:ILE:CD1	2.49	0.43
1:A:456:GLY:C	1:A:550:LYS:HZ1	2.22	0.43
1:A:64:LYS:HE2	1:A:70:LYS:C	2.39	0.43
1:A:320:ASP:HA	1:A:321:PRO:HD2	1.81	0.43
1:A:253:THR:HG22	1:A:256:ASP:CG	2.39	0.43
1:A:332:GLN:N	1:A:336:GLN:O	2.50	0.43
1:A:2:ILE:HD13	1:A:213:GLY:HA3	2.00	0.43
2:B:339:TYR:O	2:B:340:GLN:HG3	2.19	0.43
2:B:72:ARG:HG3	2:B:73:LYS:N	2.34	0.43
2:B:423:VAL:CG1	2:B:427:TYR:HD1	2.31	0.43
2:B:369:THR:HG21	2:B:405:TYR:HB2	2.01	0.43
1:A:374:LYS:C	1:A:374:LYS:HD2	2.39	0.43
1:A:132:ILE:O	1:A:133:PRO:C	2.55	0.43
2:B:63:ILE:HD13	2:B:74:LEU:CD2	2.49	0.43
1:A:319:TYR:CG	1:A:383:TRP:CD1	3.07	0.43
2:B:28:GLU:CB	2:B:135:ILE:HD11	2.49	0.43
1:A:219:LYS:C	1:A:221:HIS:N	2.72	0.42
2:B:65:LYS:HB3	2:B:65:LYS:HZ2	1.83	0.42
2:B:120:LEU:HD11	2:B:124:PHE:CD2	2.54	0.42
1:A:230:MET:HA	1:A:230:MET:HE2	2.01	0.42
1:A:277:ARG:CB	1:A:336:GLN:NE2	2.83	0.42
2:B:8:VAL:HB	2:B:159:ILE:HD12	2.00	0.42
1:A:371:ALA:O	1:A:372:VAL:C	2.56	0.42
1:A:63:ILE:HG22	1:A:64:LYS:N	2.33	0.42
2:B:195:ILE:HG12	2:B:199:ARG:NH2	2.31	0.42
1:A:362:THR:CG2	1:A:367:GLN:HE21	2.33	0.42
2:B:393:ILE:HD13	2:B:398:TRP:HB2	2.02	0.42
2:B:5:ILE:HG22	2:B:5:ILE:O	2.19	0.42
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.54	0.42
1:A:447:ASN:ND2	1:A:449:GLU:OE2	2.53	0.42
1:A:473:THR:C	1:A:475:GLN:H	2.23	0.42
1:A:103:ASN:H	3:A:556:T27:H15	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:238:LYS:O	2:B:239:TRP:HD1	2.02	0.42
1:A:194:GLU:C	1:A:196:GLY:H	2.23	0.42
1:A:265:ASN:OD1	1:A:353:LYS:CE	2.67	0.42
1:A:128:THR:HB	1:A:146:TYR:HD2	1.84	0.42
1:A:27:THR:O	1:A:28:GLU:C	2.57	0.42
2:B:178:ILE:HD11	2:B:201:LYS:CD	2.50	0.42
2:B:239:TRP:CH2	2:B:378:GLU:HG2	2.53	0.42
1:A:480:GLN:NE2	1:A:483:TYR:HD2	2.17	0.42
2:B:3:SER:HA	2:B:4:PRO:HD3	1.86	0.42
1:A:207:GLN:O	1:A:210:LEU:HB3	2.20	0.42
1:A:216:THR:HA	1:A:217:PRO:HD3	1.80	0.42
1:A:120:LEU:O	1:A:121:ASP:C	2.58	0.42
2:B:104:LYS:HA	2:B:237:ASP:OD2	2.20	0.42
1:A:135:ILE:HG22	1:A:136:ASN:ND2	2.35	0.42
1:A:366:LYS:HE2	1:A:405:TYR:CE1	2.55	0.42
1:A:136:ASN:O	1:A:137:ASN:C	2.58	0.41
2:B:2:ILE:O	2:B:117:SER:HB2	2.19	0.41
2:B:46:LYS:HD3	2:B:116:PHE:HB3	2.02	0.41
1:A:458:VAL:O	1:A:458:VAL:HG13	2.20	0.41
1:A:473:THR:O	1:A:475:GLN:N	2.53	0.41
1:A:394:GLN:OE1	1:A:416:PHE:CE2	2.73	0.41
2:B:356:ARG:NE	2:B:359:GLY:O	2.52	0.41
2:B:115:TYR:OH	2:B:157:PRO:HB3	2.19	0.41
2:B:206:ARG:NH1	2:B:229:TRP:HA	2.35	0.41
1:A:168:LEU:C	1:A:170:PRO:HD2	2.40	0.41
1:A:277:ARG:HB2	1:A:336:GLN:CD	2.40	0.41
2:B:47:ILE:HA	2:B:145:GLN:O	2.20	0.41
2:B:320:ASP:O	2:B:322:SER:N	2.52	0.41
1:A:88:TRP:CD1	2:B:143:ARG:HD2	2.56	0.41
2:B:93:GLY:O	2:B:94:ILE:CB	2.59	0.41
1:A:247:PRO:HD2	1:A:260:LEU:HD13	2.01	0.41
1:A:260:LEU:O	1:A:264:LEU:HG	2.20	0.41
1:A:295:LEU:HD12	1:A:299:ALA:HB3	2.01	0.41
1:A:393:ILE:O	1:A:393:ILE:HG23	2.21	0.41
1:A:275:LYS:HG2	1:A:332:GLN:OE1	2.21	0.41
1:A:175:ASN:N	1:A:176:PRO:HD3	2.35	0.41
2:B:39:THR:HG22	2:B:40:GLU:N	2.36	0.41
2:B:200:THR:O	2:B:202:ILE:N	2.54	0.41
2:B:13:LYS:CE	2:B:86:ASP:HA	2.50	0.41
1:A:41:MET:HG2	1:A:46:LYS:HD2	2.02	0.41
1:A:77:PHE:HE1	1:A:150:PRO:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:GLU:OE2	1:A:158:ALA:HB2	2.21	0.41
2:B:319:TYR:CE2	2:B:321:PRO:HG3	2.56	0.41
2:B:84:THR:C	2:B:86:ASP:N	2.73	0.41
2:B:125:ARG:O	2:B:145:GLN:HG3	2.21	0.41
1:A:183:TYR:O	1:A:184:MET:HB2	2.21	0.41
2:B:388:LYS:CD	2:B:413:GLU:HB2	2.49	0.40
1:A:194:GLU:OE2	1:A:197:GLN:HG3	2.21	0.40
2:B:10:VAL:HG12	2:B:11:LYS:N	2.36	0.40
2:B:163:SER:O	2:B:167:ILE:HG13	2.21	0.40
1:A:18:GLY:HA3	1:A:56:TYR:CE1	2.57	0.40
2:B:156:SER:N	2:B:157:PRO:CD	2.85	0.40
1:A:458:VAL:HG13	2:B:286:THR:CG2	2.51	0.40
2:B:136:ASN:HD22	2:B:138:GLU:HG3	1.87	0.40
1:A:293:ILE:HA	1:A:294:PRO:HD3	1.96	0.40
2:B:233:GLU:CD	2:B:233:GLU:H	2.24	0.40
3:A:556:T27:H17	3:A:556:T27:N3	2.37	0.40
1:A:548:VAL:O	1:A:548:VAL:HG12	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	550/557 (99%)	448 (82%)	80 (14%)	22 (4%)	4	15
2	B	412/428 (96%)	337 (82%)	59 (14%)	16 (4%)	4	15
All	All	962/985 (98%)	785 (82%)	139 (14%)	38 (4%)	4	15

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	GLN

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Mol	Chain	Res	Type
1	A	90	VAL
2	B	66	LYS
2	B	273	GLY
2	B	286	THR
1	A	65	LYS
1	A	217	PRO
1	A	291	GLU
1	A	358	ARG
1	A	543	GLY
2	B	94	ILE
2	B	200	THR
2	B	424	LYS
1	A	219	LYS
1	A	221	HIS
1	A	289	LEU
1	A	474	ASN
2	B	81	ASN
2	B	85	GLN
2	B	93	GLY
2	B	201	LYS
2	B	272	PRO
2	B	321	PRO
1	A	198	HIS
1	A	362	THR
2	B	362	THR
1	A	321	PRO
2	B	116	PHE
1	A	152	GLY
2	B	236	PRO
1	A	169	GLU
1	A	195	ILE
1	A	243	PRO
1	A	317	VAL
1	A	37	ILE
1	A	224	GLU
2	B	90	VAL
1	A	420	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	492/495 (99%)	474 (96%)	18 (4%)	41	77
2	B	378/390 (97%)	363 (96%)	15 (4%)	38	74
All	All	870/885 (98%)	837 (96%)	33 (4%)	40	76

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	GLU
1	A	86	ASP
1	A	105	SER
1	A	123	ASP
1	A	139	THR
1	A	185	ASP
1	A	192	ASP
1	A	193	LEU
1	A	211	ARG
1	A	218	ASP
1	A	283	LEU
1	A	284	ARG
1	A	324	ASP
1	A	374	LYS
1	A	459	THR
1	A	497	THR
1	A	515	SER
1	A	520	GLN
2	B	65	LYS
2	B	72	ARG
2	B	185	ASP
2	B	194	GLU
2	B	233	GLU
2	B	249	LYS
2	B	258	GLN
2	B	282	LEU
2	B	286	THR
2	B	300	GLU
2	B	313	PRO
2	B	330	GLN
2	B	340	GLN

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Mol	Chain	Res	Type
2	B	356	ARG
2	B	358	ARG

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

Mol	Chain	Res	Type
1	A	91	GLN
1	A	136	ASN
1	A	151	GLN
1	A	182	GLN
1	A	197	GLN
1	A	235	HIS
1	A	306	ASN
1	A	336	GLN
1	A	474	ASN
1	A	475	GLN
1	A	480	GLN
1	A	507	GLN
1	A	520	GLN
1	A	524	GLN
1	A	545	ASN
2	B	85	GLN
2	B	96	HIS
2	B	136	ASN
2	B	151	GLN
2	B	161	GLN
2	B	182	GLN
2	B	208	HIS
2	B	278	GLN
2	B	315	HIS
2	B	330	GLN
2	B	340	GLN
2	B	373	GLN

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)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	T27	A	556	-	30,30,30	2.16	12 (40%)	37,40,40	1.41	5 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	T27	A	556	-	-	0/13/14/14	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	556	T27	C12-N2	2.14	1.37	1.34
3	A	556	T27	C2-C3	2.25	1.43	1.39
3	A	556	T27	C11-N1	2.52	1.43	1.38
3	A	556	T27	C18-C17	2.57	1.43	1.38
3	A	556	T27	C4-C5	2.64	1.43	1.39
3	A	556	T27	C15-C16	2.73	1.43	1.39
3	A	556	T27	C15-C14	2.79	1.43	1.38
3	A	556	T27	C6-C1	2.95	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	556	T27	C2-C1	3.40	1.44	1.39
3	A	556	T27	C12-N4	3.58	1.42	1.36
3	A	556	T27	C17-C16	3.92	1.45	1.39
3	A	556	T27	C6-C5	4.77	1.47	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	556	T27	N2-C12-N3	-4.88	121.47	126.67
3	A	556	T27	C5-C6-C1	-2.41	118.05	121.54
3	A	556	T27	C1-C6-N1	2.05	121.45	119.31
3	A	556	T27	C16-N4-C12	2.28	135.24	129.19
3	A	556	T27	C12-N3-C11	2.42	120.86	116.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	556	T27	5	0

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	552/557 (99%)	0.48	59 (10%)	8	4	24, 79, 129, 151	0
2	B	416/428 (97%)	0.35	26 (6%)	23	17	28, 67, 123, 151	0
All	All	968/985 (98%)	0.42	85 (8%)	12	8	24, 72, 128, 151	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	2	ILE	11.3
2	B	1	PRO	10.4
1	A	257	ILE	10.2
2	B	231	GLY	9.7
2	B	227	PHE	9.2
1	A	252	TRP	5.9
1	A	292	VAL	5.4
1	A	247	PRO	5.3
2	B	3	SER	4.9
2	B	360	ALA	4.8
1	A	279	LEU	4.7
1	A	290	THR	4.7
1	A	263	LYS	4.6
1	A	295	LEU	4.5
2	B	230	MET	4.5
1	A	261	VAL	4.4
1	A	219	LYS	4.3
1	A	245	VAL	4.0
1	A	182	GLN	4.0
1	A	248	GLU	3.9
2	B	4	PRO	3.8
1	A	109	LEU	3.8
1	A	284	ARG	3.8
1	A	256	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	297	GLU	3.7
2	B	232	TYR	3.6
2	B	91	GLN	3.6
1	A	127	TYR	3.6
1	A	278	GLN	3.6
1	A	260	LEU	3.5
1	A	287	LYS	3.5
1	A	87	PHE	3.4
2	B	209	LEU	3.4
1	A	289	LEU	3.3
2	B	357	MET	3.3
1	A	298	GLU	3.3
1	A	160	PHE	3.2
1	A	286	THR	3.2
1	A	294	PRO	3.2
1	A	115	TYR	3.2
1	A	291	GLU	3.1
2	B	67	ASP	3.1
2	B	229	TRP	3.1
1	A	304	ALA	3.0
1	A	114	ALA	2.9
1	A	276	VAL	2.9
1	A	246	LEU	2.9
1	A	187	LEU	2.8
1	A	255	ASN	2.8
1	A	299	ALA	2.8
1	A	306	ASN	2.8
1	A	296	THR	2.8
1	A	275	LYS	2.8
2	B	172	LYS	2.7
1	A	217	PRO	2.7
1	A	221	HIS	2.7
1	A	188	TYR	2.6
2	B	180	ILE	2.6
2	B	86	ASP	2.6
1	A	220	LYS	2.6
1	A	116	PHE	2.6
1	A	281	LYS	2.5
2	B	109	LEU	2.5
1	A	254	VAL	2.5
1	A	17	ASP	2.5
2	B	84	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	293	ILE	2.4
1	A	264	LEU	2.3
1	A	16	MET	2.3
1	A	288	ALA	2.3
1	A	128	THR	2.3
2	B	189	VAL	2.3
2	B	188	TYR	2.3
1	A	249	LYS	2.2
2	B	87	PHE	2.2
1	A	180	ILE	2.2
2	B	212	TRP	2.2
1	A	285	GLY	2.1
1	A	308	GLU	2.1
1	A	91	GLN	2.1
1	A	547	GLN	2.1
2	B	150	PRO	2.0
1	A	301	LEU	2.0
2	B	70	LYS	2.0
2	B	95	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)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
3	T27	A	556	28/28	0.84	0.28	0.31	69,80,88,90	0

6.5 Other polymers (i)

There are no such residues in this entry.