Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:36 AM GMT

PDB ID	:	3BGR
Title	:	Crystal structure of K103N/Y181C 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	:	2007-11-27
Resolution	:	2.10 Å(reported)

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

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

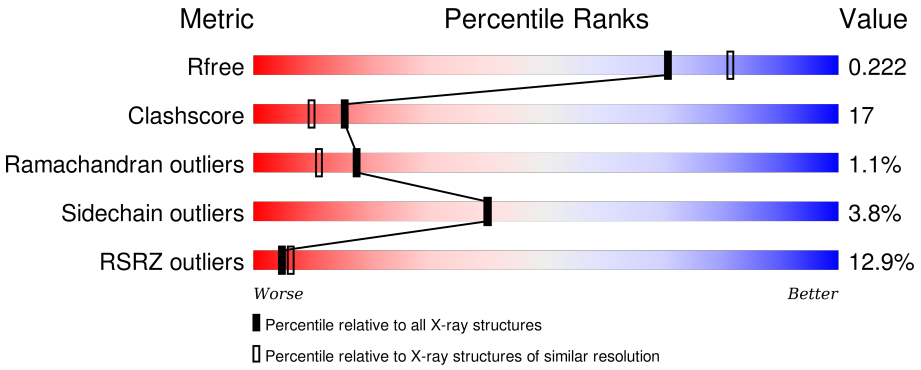
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	557	12% 68% 29%
2	B	428	14% 67% 27%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8415 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
1	A	554	Total	C	N	O	S	0	0	0
			4495	2907	748	832	8			

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	103	ASN	LYS	ENGINEERED	UNP P03366
A	172	ALA	LYS	ENGINEERED	UNP P03366
A	173	ALA	LYS	ENGINEERED	UNP P03366
A	181	CYS	TYR	ENGINEERED	UNP P03366
A	280	SER	CYS	ENGINEERED	UNP P03366

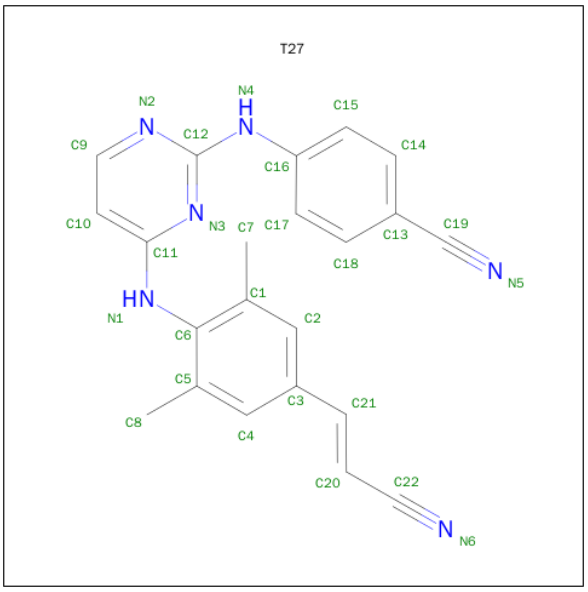
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	412	Total	C	N	O	S	0	0	0
			3413	2225	564	617	7			

There is a discrepancy between the modelled and reference sequences:

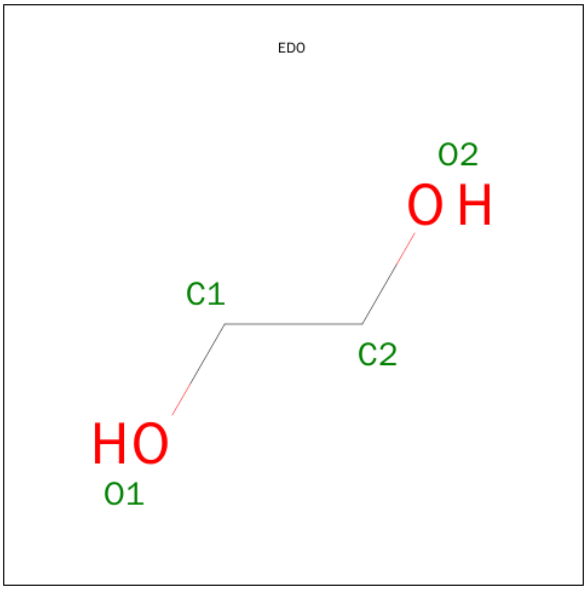
Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	ENGINEERED	UNP P03366

- 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
3	A	1	Total C N 28 22 6	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 4 2 2	0	0

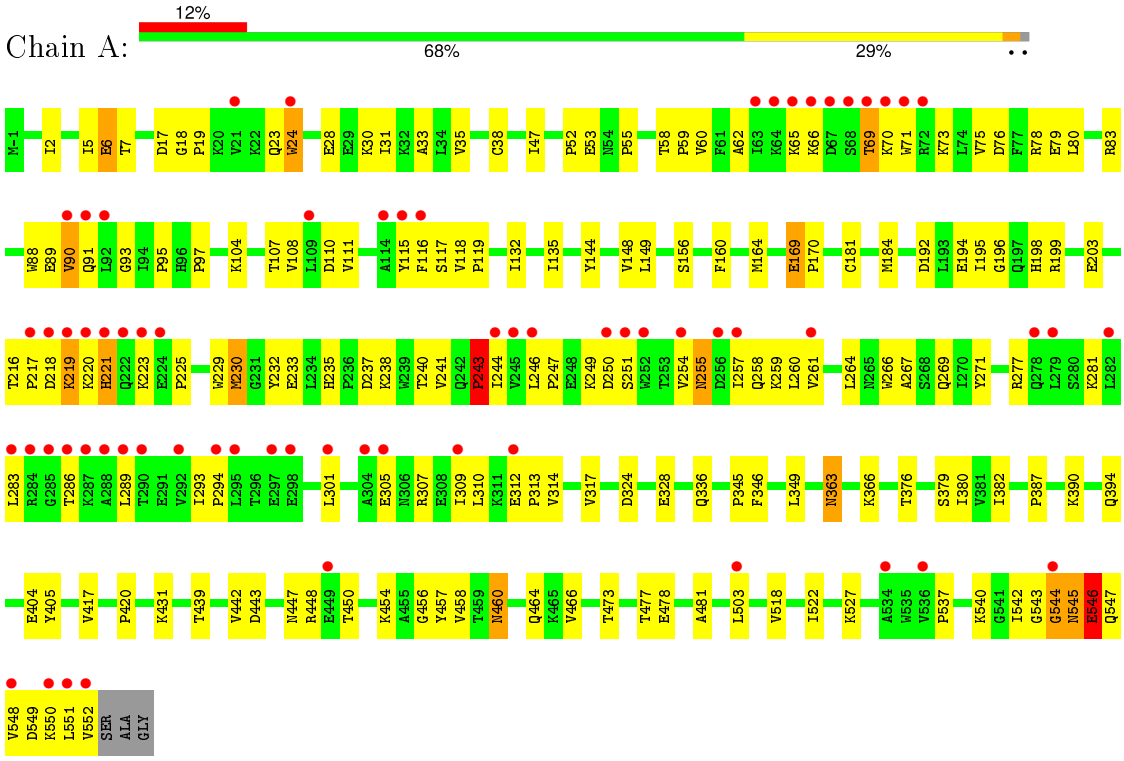
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	285	Total O 285 285	0	0
5	B	190	Total O 190 190	0	0

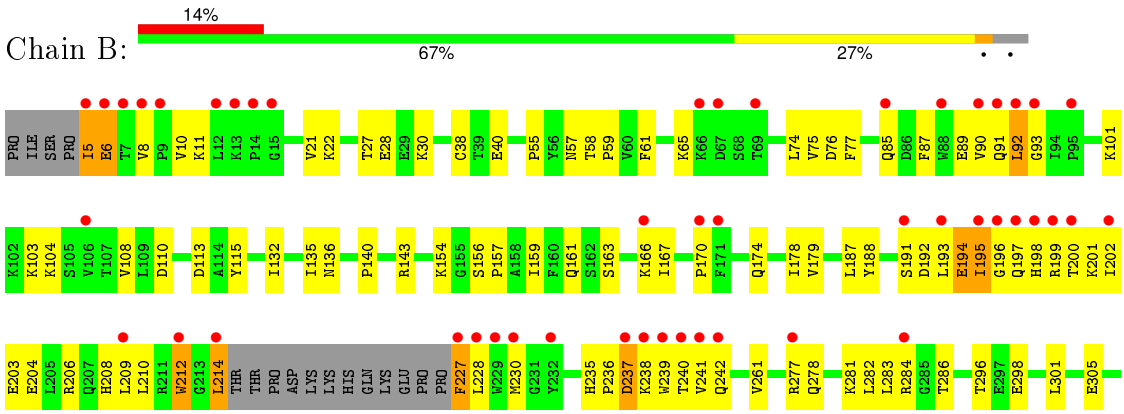
3 Residue-property plots (i)

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

- Molecule 1: Reverse transcriptase/ribonuclease H



- Molecule 2: p51 RT




E308
I309
H315
Y319
G335
Q336
Y339
K350
T351
G352
K353
Y354
A355
R356
M357
R358
G359
A360
H361
K366
Q367
L368
V372
K385
I393
E396
T397
W398
W401
A408
T409
W410
I411
V417
P420
P421
L422
Q428

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	162.84Å 73.18Å 108.92Å 90.00° 100.79° 90.00°	Depositor
Resolution (Å)	40.00 – 2.10 35.36 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.9 (40.00-2.10) 98.9 (35.36-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.228 , 0.269 0.229 , 0.222	Depositor DCC
R_{free} test set	2247 reflections (3.08%)	DCC
Wilson B-factor (Å^2)	41.5	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 52.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 72851 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8415	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, 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	0.41	0/4612	0.65	2/6271 (0.0%)
2	B	0.43	0/3511	0.65	1/4768 (0.0%)
All	All	0.42	0/8123	0.65	3/11039 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	220	LYS	N-CA-C	-10.00	84.00	111.00
1	A	219	LYS	N-CA-C	5.50	125.85	111.00
2	B	401	TRP	N-CA-C	5.38	125.53	111.00

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	4495	0	4544	165	0
2	B	3413	0	3443	124	0
3	A	28	0	18	1	0
4	B	4	0	6	0	0
5	A	285	0	0	9	0
5	B	190	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8415	0	8011	275	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (275) 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:466:VAL:HG22	1:A:550:LYS:HZ3	1.20	1.07
2:B:193:LEU:HD13	2:B:197:GLN:HE21	1.25	0.99
1:A:454:LYS:NZ	1:A:552:VAL:HB	1.80	0.96
2:B:242:GLN:HB2	2:B:351:THR:OG1	1.71	0.90
1:A:246:LEU:HB3	1:A:307:ARG:HH12	1.33	0.89
1:A:454:LYS:HZ2	1:A:552:VAL:HB	1.34	0.88
1:A:466:VAL:HG22	1:A:550:LYS:NZ	1.89	0.85
1:A:23:GLN:HE22	1:A:60:VAL:HG12	1.42	0.85
2:B:91:GLN:HB3	2:B:161:GLN:HE22	1.42	0.84
1:A:108:VAL:HB	1:A:221:HIS:HB2	1.58	0.83
2:B:30:LYS:HE3	5:B:617:HOH:O	1.78	0.83
1:A:115:TYR:OH	1:A:156:SER:HB3	1.82	0.80
1:A:458:VAL:HG12	1:A:464:GLN:HG2	1.64	0.79
1:A:246:LEU:HB3	1:A:307:ARG:NH1	1.98	0.78
2:B:195:ILE:HG12	2:B:199:ARG:HG3	1.67	0.77
2:B:10:VAL:HG22	2:B:87:PHE:HZ	1.51	0.75
1:A:246:LEU:HG	1:A:310:LEU:HD12	1.68	0.73
1:A:503:LEU:HD23	2:B:422:LEU:HD13	1.70	0.73
2:B:197:GLN:HA	2:B:200:THR:OG1	1.89	0.72
1:A:366:LYS:HE2	1:A:405:TYR:OH	1.89	0.72
1:A:90:VAL:HG23	5:B:619:HOH:O	1.89	0.72
1:A:543:GLY:CA	2:B:283:LEU:O	2.38	0.72
2:B:65:LYS:HE3	2:B:230:MET:HE1	1.70	0.71
1:A:456:GLY:HA3	1:A:550:LYS:NZ	2.05	0.71
1:A:6:GLU:H	1:A:6:GLU:CD	1.93	0.71
2:B:170:PRO:HB2	2:B:208:HIS:NE2	2.07	0.70
1:A:23:GLN:NE2	1:A:60:VAL:HG12	2.06	0.70
2:B:193:LEU:HD13	2:B:197:GLN:NE2	2.03	0.70
1:A:88:TRP:CD1	2:B:143:ARG:HD2	2.27	0.69
2:B:308:GLU:HG3	2:B:309:ILE:N	2.07	0.69
2:B:282:LEU:HD21	2:B:296:THR:HG23	1.76	0.67
1:A:90:VAL:HG21	2:B:140:PRO:HB3	1.76	0.67
1:A:24:TRP:HA	1:A:24:TRP:CE3	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:178:ILE:HG12	2:B:191:SER:HB3	1.76	0.66
1:A:65:LYS:O	1:A:66:LYS:HG2	1.94	0.66
1:A:543:GLY:N	2:B:283:LEU:O	2.28	0.66
1:A:89:GLU:C	1:A:91:GLN:H	1.99	0.65
1:A:254:VAL:HG13	1:A:283:LEU:HD22	1.77	0.65
2:B:277:ARG:HE	2:B:281:LYS:HE3	1.61	0.65
2:B:5:ILE:HD13	2:B:5:ILE:O	1.96	0.65
2:B:210:LEU:HA	2:B:214:LEU:C	2.18	0.64
2:B:196:GLY:O	2:B:200:THR:HG23	1.96	0.64
2:B:11:LYS:O	2:B:85:GLN:HG2	1.98	0.64
2:B:305:GLU:O	2:B:308:GLU:HG2	1.97	0.64
1:A:116:PHE:HD2	1:A:148:VAL:HG21	1.63	0.64
1:A:7:THR:HG22	1:A:119:PRO:HB2	1.80	0.64
1:A:164:MET:HA	1:A:164:MET:HE2	1.79	0.63
1:A:76:ASP:OD1	1:A:78:ARG:HD3	1.98	0.63
1:A:221:HIS:C	1:A:223:LYS:H	2.01	0.63
1:A:216:THR:O	1:A:217:PRO:C	2.36	0.62
1:A:439:THR:H	1:A:460:ASN:ND2	1.97	0.62
2:B:284:ARG:NH1	2:B:284:ARG:HB3	2.14	0.62
1:A:23:GLN:HE22	1:A:60:VAL:CG1	2.13	0.62
1:A:115:TYR:HA	1:A:160:PHE:CE2	2.35	0.61
1:A:544:GLY:HA3	2:B:286:THR:HG22	1.83	0.61
2:B:167:ILE:HG23	2:B:212:TRP:HB3	1.83	0.61
1:A:65:LYS:HG2	5:A:669:HOH:O	2.01	0.60
1:A:544:GLY:O	1:A:546:GLU:N	2.34	0.60
2:B:163:SER:O	2:B:167:ILE:HG13	2.01	0.60
1:A:544:GLY:O	1:A:546:GLU:HG3	2.02	0.60
1:A:328:GLU:HG3	1:A:390:LYS:HB2	1.84	0.60
1:A:254:VAL:HG11	1:A:286:THR:HB	1.83	0.60
2:B:195:ILE:HD11	2:B:199:ARG:HE	1.67	0.60
2:B:278:GLN:HE21	2:B:298:GLU:HB2	1.67	0.60
1:A:246:LEU:HD22	1:A:260:LEU:HD11	1.84	0.59
1:A:240:THR:HG23	1:A:241:VAL:O	2.02	0.59
1:A:217:PRO:O	1:A:219:LYS:HG2	2.03	0.59
1:A:260:LEU:O	1:A:264:LEU:HG	2.03	0.58
1:A:24:TRP:HA	1:A:24:TRP:HE3	1.68	0.58
1:A:460:ASN:H	1:A:460:ASN:HD22	1.50	0.58
1:A:116:PHE:C	1:A:118:VAL:H	2.07	0.58
1:A:108:VAL:HB	1:A:221:HIS:CB	2.33	0.58
2:B:65:LYS:CE	2:B:230:MET:HE1	2.33	0.58
1:A:307:ARG:HG2	1:A:307:ARG:HH11	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ASP:OD1	1:A:251:SER:N	2.37	0.57
1:A:543:GLY:O	1:A:545:ASN:N	2.36	0.57
2:B:193:LEU:O	2:B:198:HIS:HB2	2.05	0.57
2:B:336:GLN:HA	2:B:354:TYR:O	2.05	0.57
2:B:319:TYR:OH	2:B:385:LYS:HE2	2.03	0.56
1:A:312:GLU:OE1	1:A:314:VAL:HG22	2.05	0.56
1:A:544:GLY:CA	2:B:286:THR:HG22	2.35	0.56
1:A:258:GLN:HB3	1:A:283:LEU:HD13	1.87	0.56
1:A:548:VAL:HG23	1:A:549:ASP:N	2.20	0.56
1:A:301:LEU:O	1:A:305:GLU:HG3	2.06	0.56
1:A:246:LEU:CB	1:A:307:ARG:NH1	2.69	0.56
1:A:194:GLU:O	1:A:196:GLY:N	2.39	0.55
1:A:456:GLY:HA3	1:A:550:LYS:HZ1	1.70	0.55
1:A:317:VAL:HG23	1:A:349:LEU:HD23	1.87	0.55
1:A:90:VAL:CG2	2:B:140:PRO:HB3	2.36	0.55
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.47	0.55
1:A:31:ILE:O	1:A:35:VAL:HG23	2.07	0.55
2:B:421:PRO:HD2	5:B:466:HOH:O	2.07	0.54
1:A:454:LYS:HZ1	1:A:552:VAL:HB	1.66	0.54
1:A:69:THR:C	1:A:70:LYS:HG3	2.27	0.54
1:A:547:GLN:O	1:A:551:LEU:HG	2.07	0.54
2:B:242:GLN:HB2	2:B:351:THR:HG1	1.69	0.54
2:B:301:LEU:O	2:B:305:GLU:HG3	2.07	0.54
1:A:257:ILE:O	1:A:260:LEU:HB3	2.08	0.54
2:B:8:VAL:HG11	2:B:159:ILE:HG12	1.90	0.54
1:A:169:GLU:HB3	1:A:170:PRO:CD	2.38	0.54
2:B:195:ILE:CG1	2:B:199:ARG:HG3	2.36	0.53
2:B:360:ALA:HB2	2:B:366:LYS:HG2	1.89	0.53
1:A:458:VAL:HG12	1:A:464:GLN:CG	2.37	0.53
1:A:456:GLY:HA3	1:A:550:LYS:HZ2	1.72	0.53
2:B:202:ILE:O	2:B:206:ARG:N	2.39	0.53
2:B:91:GLN:HG3	2:B:93:GLY:H	1.72	0.53
2:B:89:GLU:HB2	2:B:91:GLN:HG2	1.91	0.52
1:A:448:ARG:HH11	1:A:448:ARG:HG3	1.73	0.52
2:B:163:SER:HA	2:B:166:LYS:HE2	1.90	0.52
1:A:221:HIS:C	1:A:223:LYS:N	2.63	0.52
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.92	0.52
1:A:254:VAL:HG22	1:A:286:THR:HG21	1.91	0.51
1:A:90:VAL:O	1:A:90:VAL:HG22	2.09	0.51
1:A:89:GLU:C	1:A:91:GLN:N	2.64	0.51
1:A:258:GLN:HB3	1:A:283:LEU:CD1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:228:LEU:HD23	5:B:462:HOH:O	2.08	0.51
1:A:246:LEU:HD12	1:A:307:ARG:HG2	1.92	0.51
1:A:17:ASP:OD2	1:A:18:GLY:N	2.40	0.51
1:A:277:ARG:HB2	1:A:336:GLN:CD	2.31	0.51
1:A:478:GLU:HG2	5:A:615:HOH:O	2.11	0.51
2:B:103:LYS:HE2	2:B:179:VAL:HG23	1.92	0.51
2:B:10:VAL:HG13	2:B:87:PHE:CE1	2.45	0.51
1:A:247:PRO:HB3	1:A:249:LYS:NZ	2.25	0.51
1:A:527:LYS:HE3	5:A:819:HOH:O	2.10	0.50
1:A:376:THR:O	1:A:380:ILE:HG12	2.11	0.50
2:B:278:GLN:NE2	2:B:298:GLU:CB	2.74	0.50
1:A:246:LEU:HG	1:A:310:LEU:CD1	2.40	0.50
1:A:313:PRO:HD2	5:A:661:HOH:O	2.11	0.50
1:A:235:HIS:HB3	5:A:748:HOH:O	2.11	0.50
1:A:266:TRP:O	1:A:269:GLN:HG2	2.11	0.50
1:A:235:HIS:HB2	1:A:238:LYS:O	2.12	0.50
2:B:209:LEU:HD22	2:B:214:LEU:HD11	1.94	0.50
2:B:195:ILE:HG12	2:B:199:ARG:CG	2.40	0.50
2:B:103:LYS:O	2:B:236:PRO:HG2	2.12	0.50
1:A:199:ARG:O	1:A:203:GLU:HG2	2.12	0.50
3:A:556:T27:H17	3:A:556:T27:N3	2.27	0.50
2:B:203:GLU:HA	2:B:203:GLU:OE2	2.12	0.49
2:B:305:GLU:O	2:B:308:GLU:CG	2.60	0.49
2:B:282:LEU:CD2	2:B:296:THR:HG23	2.41	0.49
1:A:448:ARG:NH1	1:A:448:ARG:HG3	2.28	0.49
2:B:195:ILE:CG2	2:B:196:GLY:N	2.75	0.49
2:B:308:GLU:HG3	2:B:309:ILE:H	1.77	0.49
1:A:30:LYS:O	1:A:33:ALA:HB3	2.13	0.49
2:B:284:ARG:HB3	2:B:284:ARG:HH11	1.78	0.49
2:B:200:THR:O	2:B:204:GLU:HB2	2.12	0.49
1:A:542:ILE:HG23	2:B:283:LEU:HD13	1.95	0.48
2:B:360:ALA:HB2	2:B:366:LYS:CG	2.43	0.48
1:A:543:GLY:H	2:B:283:LEU:HB3	1.78	0.48
2:B:278:GLN:HE21	2:B:298:GLU:CB	2.26	0.48
2:B:198:HIS:O	2:B:202:ILE:HG12	2.13	0.48
1:A:254:VAL:HA	1:A:283:LEU:HD21	1.96	0.48
1:A:116:PHE:C	1:A:118:VAL:N	2.66	0.48
1:A:543:GLY:C	1:A:545:ASN:H	2.16	0.48
1:A:73:LYS:HE2	1:A:75:VAL:HG23	1.96	0.48
1:A:89:GLU:O	1:A:91:GLN:N	2.46	0.47
1:A:118:VAL:HG11	1:A:149:LEU:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:VAL:HG13	1:A:283:LEU:CD2	2.44	0.47
2:B:8:VAL:HG13	2:B:8:VAL:O	2.13	0.47
1:A:366:LYS:HE2	1:A:405:TYR:CZ	2.50	0.47
1:A:52:PRO:HD2	1:A:53:GLU:OE2	2.14	0.47
2:B:195:ILE:HG23	2:B:196:GLY:N	2.29	0.47
1:A:458:VAL:CG2	2:B:286:THR:HG21	2.45	0.47
2:B:61:PHE:CZ	2:B:74:LEU:HD23	2.48	0.47
1:A:233:GLU:OE1	1:A:243:PRO:HD3	2.15	0.47
1:A:546:GLU:OE1	1:A:546:GLU:N	2.48	0.47
2:B:65:LYS:HZ3	2:B:110:ASP:CB	2.27	0.47
1:A:258:GLN:O	1:A:261:VAL:HB	2.14	0.47
2:B:167:ILE:HG23	2:B:212:TRP:CB	2.45	0.47
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.96	0.47
1:A:277:ARG:O	1:A:281:LYS:HB2	2.14	0.47
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.50	0.47
1:A:518:VAL:O	1:A:522:ILE:HG13	2.16	0.46
1:A:229:TRP:CE2	1:A:230:MET:HG3	2.51	0.46
1:A:28:GLU:HG3	1:A:135:ILE:HD12	1.96	0.46
2:B:241:VAL:C	2:B:242:GLN:HG2	2.36	0.46
1:A:89:GLU:OE2	1:A:89:GLU:HA	2.15	0.46
1:A:97:PRO:HG2	1:A:232:TYR:CD2	2.51	0.46
1:A:443:ASP:OD1	1:A:547:GLN:CD	2.54	0.46
2:B:167:ILE:HG22	2:B:167:ILE:O	2.14	0.46
2:B:356:ARG:NH2	5:B:589:HOH:O	2.48	0.46
2:B:197:GLN:CA	2:B:200:THR:OG1	2.63	0.46
1:A:293:ILE:HA	1:A:294:PRO:HD3	1.77	0.46
2:B:368:LEU:O	2:B:372:VAL:HG23	2.16	0.46
2:B:91:GLN:OE1	2:B:161:GLN:OE1	2.34	0.45
2:B:278:GLN:NE2	2:B:298:GLU:HB2	2.31	0.45
1:A:230:MET:HA	1:A:230:MET:CE	2.46	0.45
1:A:537:PRO:HD2	1:A:542:ILE:CD1	2.47	0.45
1:A:417:VAL:O	1:A:417:VAL:HG13	2.17	0.45
2:B:57:ASN:OD1	2:B:143:ARG:NH2	2.50	0.45
1:A:271:TYR:CE2	1:A:314:VAL:HG23	2.51	0.45
1:A:2:ILE:O	1:A:2:ILE:HG13	2.17	0.45
1:A:543:GLY:HA2	2:B:283:LEU:O	2.16	0.45
1:A:58:THR:HG23	1:A:76:ASP:O	2.16	0.45
2:B:75:VAL:HG11	2:B:77:PHE:CZ	2.52	0.45
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.16	0.45
1:A:246:LEU:CD1	1:A:307:ARG:HG2	2.47	0.45
2:B:393:ILE:HD13	2:B:398:TRP:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:ILE:HD11	2:B:261:VAL:HG11	1.99	0.45
2:B:194:GLU:H	2:B:194:GLU:HG2	1.31	0.45
2:B:202:ILE:HG22	2:B:206:ARG:NH1	2.32	0.45
1:A:110:ASP:OD2	1:A:111:VAL:N	2.49	0.45
2:B:200:THR:O	2:B:204:GLU:N	2.43	0.44
2:B:104:LYS:HB2	2:B:192:ASP:HA	1.98	0.44
1:A:420:PRO:HG3	5:A:803:HOH:O	2.17	0.44
2:B:115:TYR:OH	2:B:157:PRO:HB3	2.18	0.44
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.53	0.44
2:B:90:VAL:O	2:B:90:VAL:HG12	2.18	0.44
2:B:65:LYS:HZ3	2:B:110:ASP:CG	2.20	0.44
1:A:540:LYS:HA	1:A:540:LYS:HD3	1.78	0.44
2:B:6:GLU:HA	2:B:6:GLU:OE1	2.17	0.44
2:B:235:HIS:CG	2:B:238:LYS:HE2	2.53	0.44
2:B:167:ILE:HG12	2:B:212:TRP:CE3	2.53	0.44
2:B:335:GLY:O	2:B:355:ALA:HA	2.17	0.43
1:A:307:ARG:HG2	1:A:307:ARG:NH1	2.32	0.43
1:A:548:VAL:HG23	1:A:549:ASP:H	1.82	0.43
1:A:30:LYS:HD3	1:A:62:ALA:HB3	2.01	0.43
1:A:118:VAL:HA	1:A:119:PRO:HD3	1.84	0.43
2:B:238:LYS:HG3	2:B:238:LYS:O	2.18	0.43
1:A:79:GLU:O	1:A:83:ARG:HD2	2.18	0.43
2:B:87:PHE:O	2:B:89:GLU:OE1	2.37	0.43
2:B:428:GLN:OXT	2:B:428:GLN:CD	2.57	0.43
1:A:237:ASP:OD1	5:A:748:HOH:O	2.21	0.43
2:B:91:GLN:O	2:B:92:LEU:HB2	2.19	0.43
2:B:101:LYS:O	2:B:236:PRO:HB2	2.18	0.43
1:A:382:ILE:O	2:B:136:ASN:HB2	2.19	0.43
1:A:95:PRO:HA	2:B:136:ASN:O	2.18	0.43
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.59	0.43
1:A:545:ASN:ND2	5:A:597:HOH:O	2.52	0.42
1:A:59:PRO:HG2	1:A:76:ASP:HB3	2.01	0.42
1:A:246:LEU:CB	1:A:307:ARG:HH12	2.17	0.42
1:A:107:THR:OG1	1:A:198:HIS:NE2	2.40	0.42
2:B:27:THR:OG1	2:B:30:LYS:HG3	2.18	0.42
1:A:473:THR:O	1:A:477:THR:HG23	2.19	0.42
2:B:197:GLN:O	2:B:201:LYS:HG2	2.19	0.42
1:A:255:ASN:ND2	1:A:259:LYS:HE3	2.34	0.42
2:B:156:SER:N	2:B:157:PRO:HD2	2.35	0.42
2:B:58:THR:HG23	2:B:76:ASP:O	2.19	0.42
1:A:547:GLN:O	1:A:551:LEU:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ILE:HG13	1:A:267:ALA:HB2	2.01	0.42
2:B:10:VAL:HG13	2:B:87:PHE:HE1	1.82	0.42
1:A:194:GLU:C	1:A:196:GLY:N	2.73	0.42
1:A:442:VAL:HB	1:A:481:ALA:HB1	2.01	0.42
1:A:454:LYS:HZ1	1:A:552:VAL:CG1	2.33	0.42
1:A:246:LEU:HD21	1:A:264:LEU:HD21	2.02	0.42
2:B:396:GLU:CD	2:B:396:GLU:H	2.23	0.42
1:A:454:LYS:HZ1	1:A:552:VAL:CB	2.31	0.41
1:A:404:GLU:OE1	1:A:431:LYS:NZ	2.53	0.41
2:B:28:GLU:HB2	2:B:135:ILE:HD11	2.02	0.41
2:B:278:GLN:NE2	2:B:298:GLU:HB3	2.35	0.41
2:B:240:THR:O	2:B:240:THR:HG23	2.20	0.41
2:B:339:TYR:CZ	2:B:352:GLY:HA3	2.55	0.41
2:B:91:GLN:HB3	2:B:161:GLN:NE2	2.23	0.41
1:A:104:LYS:HE2	1:A:192:ASP:O	2.20	0.41
2:B:195:ILE:O	2:B:196:GLY:C	2.58	0.41
1:A:312:GLU:OE1	1:A:314:VAL:CG2	2.67	0.41
1:A:28:GLU:HG3	1:A:135:ILE:HG23	2.03	0.41
2:B:154:LYS:O	2:B:157:PRO:HD2	2.21	0.41
2:B:350:LYS:HD2	5:B:615:HOH:O	2.20	0.41
1:A:454:LYS:NZ	1:A:552:VAL:CB	2.66	0.41
2:B:187:LEU:HA	2:B:187:LEU:HD12	1.95	0.41
1:A:47:ILE:HD12	1:A:144:TYR:CD2	2.56	0.41
2:B:420:PRO:HA	2:B:421:PRO:HD3	1.85	0.41
1:A:547:GLN:C	1:A:551:LEU:HG	2.42	0.41
1:A:71:TRP:HB2	5:A:721:HOH:O	2.20	0.41
1:A:194:GLU:C	1:A:196:GLY:H	2.24	0.40
1:A:217:PRO:O	1:A:218:ASP:C	2.58	0.40
2:B:298:GLU:N	2:B:298:GLU:OE1	2.31	0.40
2:B:104:LYS:HA	2:B:237:ASP:HB3	2.03	0.40
1:A:457:TYR:C	1:A:457:TYR:CD1	2.95	0.40
1:A:363:ASN:OD1	1:A:363:ASN:C	2.59	0.40
1:A:345:PRO:O	1:A:346:PHE:HB2	2.21	0.40
1:A:19:PRO:HD3	1:A:80:LEU:HD13	2.04	0.40
1:A:379:SER:CB	1:A:387:PRO:HD3	2.51	0.40
1:A:5:ILE:HD12	1:A:117:SER:O	2.22	0.40
2:B:227:PHE:N	5:B:580:HOH:O	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	552/557 (99%)	512 (93%)	32 (6%)	8 (1%)	14 7
2	B	408/428 (95%)	376 (92%)	29 (7%)	3 (1%)	26 21
All	All	960/985 (98%)	888 (92%)	61 (6%)	11 (1%)	17 11

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	ILE
1	A	544	GLY
2	B	355	ALA
1	A	90	VAL
1	A	545	ASN
2	B	195	ILE
2	B	359	GLY
1	A	243	PRO
1	A	546	GLU
1	A	225	PRO
1	A	93	GLY

5.3.2 Protein sidechains

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	493/495 (100%)	475 (96%)	18 (4%)	41 41
2	B	374/390 (96%)	359 (96%)	15 (4%)	38 38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	867/885 (98%)	834 (96%)	33 (4%)	40 40

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

Mol	Chain	Res	Type
1	A	6	GLU
1	A	24	TRP
1	A	55	PRO
1	A	69	THR
1	A	169	GLU
1	A	181	CYS
1	A	184	MET
1	A	221	HIS
1	A	230	MET
1	A	243	PRO
1	A	255	ASN
1	A	289	LEU
1	A	309	ILE
1	A	324	ASP
1	A	363	ASN
1	A	394	GLN
1	A	460	ASN
1	A	546	GLU
2	B	5	ILE
2	B	6	GLU
2	B	22	LYS
2	B	40	GLU
2	B	55	PRO
2	B	92	LEU
2	B	113	ASP
2	B	174	GLN
2	B	194	GLU
2	B	212	TRP
2	B	214	LEU
2	B	227	PHE
2	B	237	ASP
2	B	315	HIS
2	B	417	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	174	GLN
1	A	255	ASN
1	A	306	ASN
1	A	394	GLN
1	A	460	ASN
1	A	475	GLN
1	A	487	GLN
1	A	524	GLN
1	A	545	ASN
2	B	174	GLN
2	B	197	GLN
2	B	278	GLN
2	B	330	GLN
2	B	340	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 ligands are 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	1.65	6 (20%)	37,40,40	1.25	2 (5%)
4	EDO	B	429	-	3,3,3	0.41	0	2,2,2	0.49	0

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
4	EDO	B	429	-	-	0/1/1/1	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	556	T27	C15-C16	2.31	1.43	1.39
3	A	556	T27	C12-N4	2.35	1.40	1.36
3	A	556	T27	C15-C14	2.58	1.43	1.38
3	A	556	T27	C2-C1	2.81	1.43	1.39
3	A	556	T27	C17-C16	2.90	1.44	1.39
3	A	556	T27	C6-C5	4.37	1.47	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	556	T27	N2-C12-N3	-4.29	122.10	126.67
3	A	556	T27	C12-N3-C11	2.08	120.27	116.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	556	T27	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	554/557 (99%)	0.57	67 (12%) 6 7	26, 54, 103, 127	0
2	B	412/428 (96%)	0.75	58 (14%) 4 5	26, 51, 108, 118	0
All	All	966/985 (98%)	0.65	125 (12%) 5 6	26, 52, 107, 127	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	286	THR	15.6
2	B	92	LEU	13.9
2	B	240	THR	9.8
2	B	357	MET	8.8
2	B	90	VAL	8.2
2	B	193	LEU	7.7
1	A	69	THR	7.3
2	B	5	ILE	7.3
1	A	290	THR	7.1
1	A	283	LEU	6.4
1	A	257	ILE	6.3
1	A	91	GLN	6.3
1	A	67	ASP	6.3
1	A	285	GLY	6.2
1	A	552	VAL	6.1
2	B	229	TRP	5.9
2	B	230	MET	5.9
1	A	68	SER	5.7
2	B	358	ARG	5.4
1	A	222	GLN	5.3
2	B	197	GLN	5.3
1	A	220	LYS	5.2
1	A	221	HIS	5.2
1	A	70	LYS	5.1

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Mol	Chain	Res	Type	RSRZ
2	B	238	LYS	4.9
2	B	214	LEU	4.8
2	B	356	ARG	4.7
1	A	298	GLU	4.7
2	B	93	GLY	4.6
1	A	219	LYS	4.6
1	A	252	TRP	4.5
2	B	241	VAL	4.5
1	A	24	TRP	4.5
1	A	295	LEU	4.4
2	B	284	ARG	4.4
1	A	301	LEU	4.4
2	B	66	LYS	4.3
1	A	66	LYS	4.3
1	A	254	VAL	4.3
2	B	95	PRO	4.2
1	A	72	ARG	4.2
1	A	250	ASP	3.9
1	A	245	VAL	3.9
1	A	309	ILE	3.8
2	B	227	PHE	3.8
1	A	297	GLU	3.7
1	A	282	LEU	3.7
1	A	65	LYS	3.7
1	A	287	LYS	3.7
2	B	88	TRP	3.7
2	B	359	GLY	3.6
1	A	551	LEU	3.6
1	A	289	LEU	3.6
1	A	292	VAL	3.5
2	B	408	ALA	3.5
1	A	284	ARG	3.5
1	A	116	PHE	3.5
1	A	223	LYS	3.4
2	B	212	TRP	3.4
2	B	200	THR	3.3
2	B	191	SER	3.3
1	A	312	GLU	3.3
1	A	548	VAL	3.3
2	B	7	THR	3.2
2	B	209	LEU	3.2
1	A	288	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	410	TRP	3.2
2	B	69	THR	3.2
1	A	90	VAL	3.2
2	B	196	GLY	3.1
2	B	239	TRP	3.1
1	A	115	TYR	3.1
2	B	202	ILE	3.1
2	B	361	HIS	3.0
2	B	9	PRO	3.0
2	B	91	GLN	3.0
1	A	64	LYS	3.0
1	A	92	LEU	3.0
2	B	6	GLU	2.9
1	A	261	VAL	2.9
1	A	449	GLU	2.9
1	A	71	TRP	2.8
2	B	409	THR	2.7
1	A	503	LEU	2.6
2	B	237	ASP	2.6
1	A	294	PRO	2.5
2	B	67	ASP	2.5
2	B	195	ILE	2.5
2	B	198	HIS	2.5
1	A	246	LEU	2.4
2	B	8	VAL	2.4
1	A	21	VAL	2.4
1	A	63	ILE	2.4
1	A	218	ASP	2.4
2	B	411	ILE	2.3
1	A	544	GLY	2.3
2	B	199	ARG	2.3
2	B	277	ARG	2.3
2	B	85	GLN	2.3
1	A	224	GLU	2.3
1	A	550	LYS	2.3
2	B	232	TYR	2.3
2	B	166	LYS	2.3
1	A	534	ALA	2.3
1	A	305	GLU	2.2
1	A	536	VAL	2.2
2	B	106	VAL	2.2
2	B	228	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	304	ALA	2.1
2	B	315	HIS	2.1
1	A	279	LEU	2.1
2	B	242	GLN	2.1
1	A	244	ILE	2.1
2	B	14	PRO	2.1
2	B	13	LYS	2.1
2	B	15	GLY	2.1
2	B	171	PHE	2.1
1	A	109	LEU	2.0
1	A	114	ALA	2.0
2	B	12	LEU	2.0
1	A	256	ASP	2.0
1	A	278	GLN	2.0
1	A	217	PRO	2.0
2	B	170	PRO	2.0
1	A	251	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	T27	A	556	28/28	0.94	0.13	-0.20	40,46,53,58	0
4	EDO	B	429	4/4	0.93	0.25	-	53,58,59,60	0

6.5 Other polymers (i)

There are no such residues in this entry.