Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:19 AM GMT

PDB ID	:	2WON
Title	:	CRYSTAL STRUCTURE OF UK-453061 BOUND TO HIV-1 REVERSE TRANSCRIPTASE (WILD-TYPE).
Authors	:	Phillips, C.; Irving, S.L.; Knoechel, T.; Ringrose, H.
Deposited on	:	2009-07-27
Resolution	:	2.80 Å(reported)

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

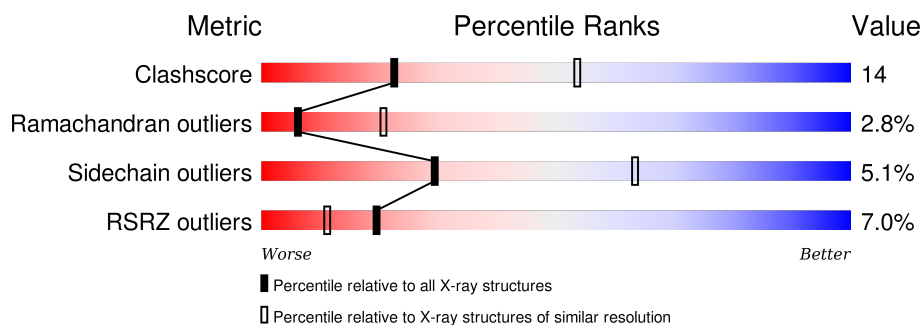|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.80 Å.

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

Metric	Percentile Ranks	Value
Clashscore		14
Ramachandran outliers		2.8%
Sidechain outliers		5.1%
RSRZ outliers		7.0%

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))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	560	7% 68% 28% •
2	B	440	7% 66% 25% • 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7944 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 HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	558	Total	C	N	O	S	0	0	1
			4537	2931	760	838	8			

- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	413	Total	C	N	O	S	0	0	1
			3384	2197	565	615	7			

- Molecule 3 is 5-{[3,5-DIETHYL-1-(2-HYDROXYETHYL)-1H-PYRAZOL-4-YL]OXY}BENZENE-1,3-DICARBONITRILE (three-letter code: ZZE) (formula: $C_{17}H_{18}N_4O_2$).
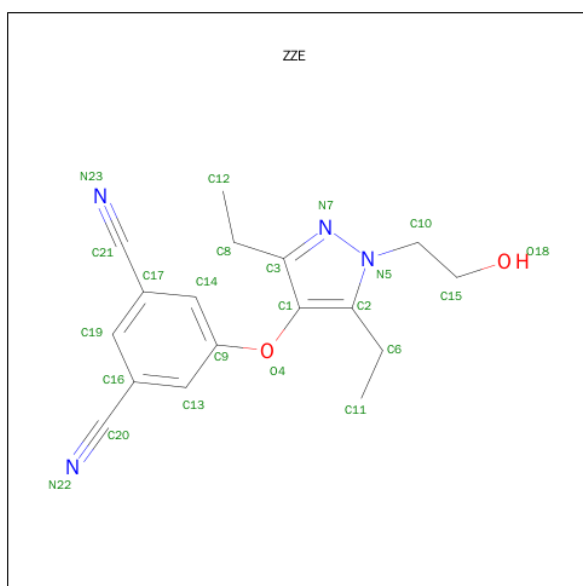

| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			23	17	4	2		

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: HIV-1 REVERSE TRANSCRIPTASE
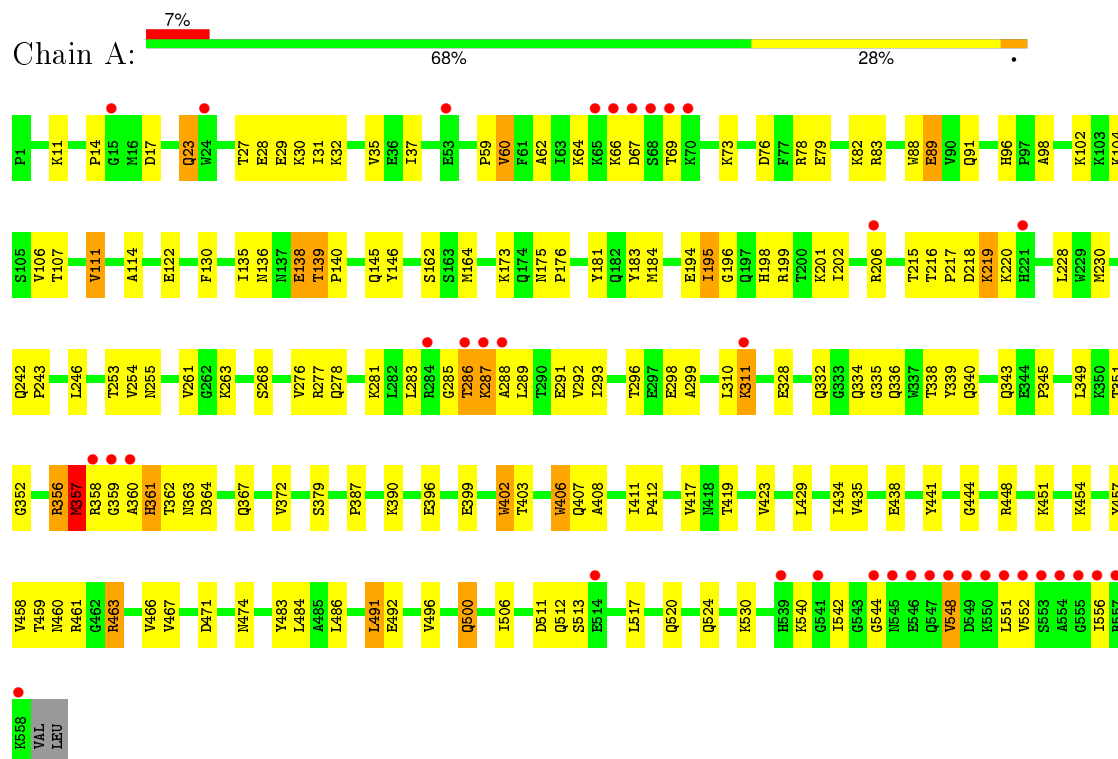
- Molecule 2: HIV-1 REVERSE TRANSCRIPTASE
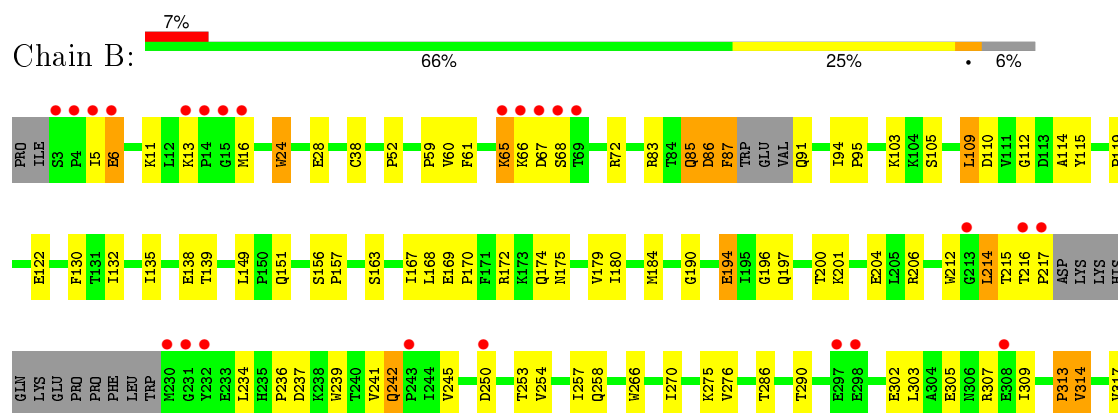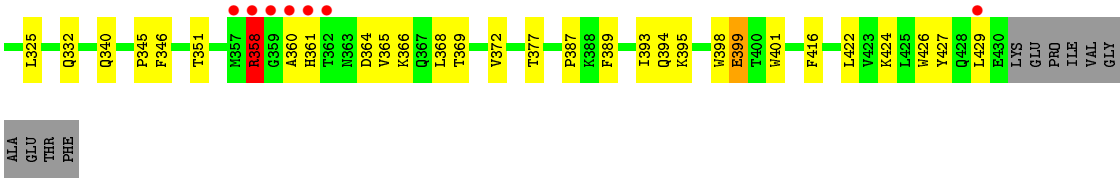
4   Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	117.49Å 154.25Å 154.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.88 – 2.80 24.88 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (24.88-2.80) 88.6 (24.88-2.80)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	4.38 (at 2.80Å)	Xtriage
Refinement program	BUSTER-TNT 2.9.2	Depositor
R, R_{free}	0.253 , 0.271 0.248 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	57.7	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 45.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.51$, $<L^2> = 0.34$	Xtriage
Outliers	0 of 32428 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7944	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: ZZE

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	0.37	0/4654	0.58	0/6323
2	B	0.35	0/3477	0.55	0/4724
All	All	0.36	0/8131	0.57	0/11047

There are no bond length outliers.

There are no bond angle outliers.

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	4537	0	4590	130	0
2	B	3384	0	3417	98	0
3	A	23	0	18	2	0
All	All	7944	0	8025	218	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 14.

All (218) 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:139:THR:HB	1:A:140:PRO:HD2	1.38	1.05
1:A:23:GLN:HE22	1:A:60:VAL:H	1.02	0.95
2:B:13:LYS:HB2	2:B:16:MET:HG3	1.57	0.86
1:A:23:GLN:NE2	1:A:60:VAL:H	1.74	0.86
1:A:296:THR:HG23	1:A:299:ALA:H	1.42	0.84
1:A:278:GLN:HG2	1:A:298:GLU:HB3	1.61	0.82
2:B:85:GLN:HA	2:B:87:PHE:N	1.99	0.78
1:A:111:VAL:HG12	1:A:111:VAL:O	1.82	0.78
1:A:372:VAL:HG11	1:A:411:ILE:HG23	1.66	0.77
1:A:500:GLN:NE2	2:B:422:LEU:HG	2.01	0.75
2:B:5:ILE:HG22	2:B:6:GLU:H	1.52	0.74
2:B:360:ALA:HB2	2:B:366:LYS:HD2	1.69	0.74
1:A:175:ASN:OD1	1:A:201:LYS:HE3	1.87	0.74
1:A:328:GLU:HG2	1:A:390:LYS:HB2	1.70	0.72
2:B:13:LYS:HD2	2:B:16:MET:HE3	1.72	0.71
1:A:138:GLU:HG2	1:A:139:THR:N	2.04	0.71
2:B:85:GLN:HA	2:B:87:PHE:H	1.55	0.71
1:A:111:VAL:O	1:A:111:VAL:CG1	2.39	0.71
2:B:13:LYS:HZ1	2:B:85:GLN:HG2	1.57	0.70
1:A:311:LYS:HA	1:A:311:LYS:HE2	1.72	0.70
1:A:461:ARG:HH11	1:A:461:ARG:HG3	1.57	0.69
2:B:86:ASP:HA	2:B:91:GLN:HB2	1.77	0.67
1:A:362:THR:HG22	1:A:363:ASN:N	2.10	0.67
1:A:458:VAL:HG12	1:A:548:VAL:HG22	1.76	0.67
1:A:500:GLN:HE22	2:B:422:LEU:HG	1.59	0.67
1:A:492:GLU:HG2	1:A:530:LYS:HB2	1.78	0.66
1:A:263:LYS:HA	1:A:263:LYS:HE2	1.78	0.66
1:A:27:THR:CG2	1:A:29:GLU:HG2	2.26	0.65
1:A:412:PRO:HG3	2:B:401:TRP:HZ2	1.61	0.65
2:B:114:ALA:HB2	2:B:214:LEU:HD13	1.78	0.64
1:A:139:THR:HB	1:A:140:PRO:CD	2.21	0.64
2:B:24:TRP:HE1	2:B:59:PRO:HB3	1.62	0.64
1:A:551:LEU:HD23	1:A:551:LEU:H	1.63	0.64
1:A:277:ARG:HB3	1:A:336:GLN:OE1	1.98	0.64
1:A:451:LYS:HE2	1:A:471:ASP:HA	1.80	0.64
1:A:444:GLY:HA2	1:A:552:VAL:HG11	1.81	0.63
1:A:500:GLN:HE21	1:A:500:GLN:HA	1.64	0.63
2:B:215:THR:O	2:B:217:PRO:HD3	1.98	0.62
2:B:242:GLN:HE22	2:B:429:LEU:CD1	2.12	0.61
2:B:66:LYS:HG3	2:B:67:ASP:OD1	2.01	0.61
2:B:24:TRP:NE1	2:B:59:PRO:HB3	2.16	0.61
2:B:206:ARG:HD2	2:B:216:THR:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:VAL:HG21	3:A:1558:ZZE:H152	1.83	0.60
2:B:365:VAL:O	2:B:369:THR:HG23	2.00	0.60
1:A:23:GLN:HE22	1:A:60:VAL:N	1.86	0.60
1:A:27:THR:O	1:A:31:ILE:HG13	2.02	0.60
1:A:286:THR:O	1:A:287:LYS:HG2	2.01	0.60
1:A:548:VAL:HA	1:A:551:LEU:HD21	1.84	0.60
1:A:27:THR:HG21	1:A:29:GLU:HG2	1.82	0.60
1:A:73:LYS:NZ	1:A:146:TYR:OH	2.35	0.60
1:A:399:GLU:HA	1:A:402:TRP:CD1	2.37	0.59
1:A:261:VAL:HG13	1:A:276:VAL:HG11	1.82	0.59
1:A:254:VAL:HG22	1:A:293:ILE:HD11	1.84	0.59
1:A:23:GLN:NE2	1:A:60:VAL:N	2.49	0.59
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.85	0.59
2:B:360:ALA:CB	2:B:366:LYS:HD2	2.34	0.58
1:A:122:GLU:CD	1:A:122:GLU:H	2.07	0.58
1:A:412:PRO:HG3	2:B:401:TRP:CZ2	2.40	0.57
1:A:64:LYS:NZ	1:A:69:THR:HG23	2.20	0.57
2:B:172:ARG:HH21	2:B:180:ILE:HB	1.68	0.57
1:A:111:VAL:HG21	1:A:164:MET:CE	2.34	0.57
2:B:156:SER:HB2	2:B:157:PRO:HD3	1.86	0.57
1:A:194:GLU:H	1:A:194:GLU:CD	2.07	0.57
2:B:13:LYS:HD2	2:B:16:MET:CE	2.34	0.56
2:B:110:ASP:O	2:B:216:THR:HG23	2.05	0.56
1:A:206:ARG:HG3	1:A:216:THR:OG1	2.06	0.56
2:B:303:LEU:HD22	2:B:307:ARG:HH21	1.71	0.55
1:A:268:SER:O	1:A:351:THR:HG22	2.05	0.55
2:B:5:ILE:HG22	2:B:6:GLU:N	2.19	0.55
1:A:556:ILE:O	1:A:556:ILE:HG22	2.07	0.55
2:B:175:ASN:HD21	2:B:201:LYS:NZ	2.04	0.55
1:A:454:LYS:HG3	1:A:556:ILE:CD1	2.36	0.55
1:A:195:ILE:HB	1:A:199:ARG:NH2	2.21	0.54
1:A:454:LYS:HG3	1:A:556:ILE:HD11	1.89	0.54
1:A:454:LYS:O	1:A:552:VAL:HG13	2.08	0.54
1:A:441:TYR:CD2	1:A:544:GLY:HA3	2.43	0.53
2:B:168:LEU:HD13	2:B:180:ILE:HG21	1.91	0.53
1:A:288:ALA:HB3	1:A:291:GLU:HG2	1.89	0.53
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.43	0.53
2:B:242:GLN:HE22	2:B:429:LEU:HD13	1.73	0.53
1:A:285:GLY:O	1:A:287:LYS:N	2.42	0.52
1:A:198:HIS:O	1:A:202:ILE:HG12	2.09	0.52
1:A:17:ASP:O	1:A:83:ARG:HD3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:314:VAL:HG13	2:B:317:VAL:HG22	1.92	0.52
1:A:228:LEU:HD22	1:A:242:GLN:OE1	2.09	0.52
2:B:157:PRO:HG2	2:B:184:MET:HA	1.90	0.52
2:B:266:TRP:HH2	2:B:427:TYR:CE1	2.27	0.52
1:A:23:GLN:NE2	1:A:59:PRO:HA	2.24	0.52
1:A:173:LYS:NZ	1:A:173:LYS:HB3	2.24	0.52
2:B:163:SER:O	2:B:167:ILE:HG13	2.10	0.52
1:A:362:THR:CG2	1:A:363:ASN:N	2.73	0.52
1:A:362:THR:HG22	1:A:363:ASN:H	1.75	0.52
2:B:266:TRP:HH2	2:B:427:TYR:CZ	2.27	0.52
2:B:358:ARG:HD3	2:B:358:ARG:H	1.75	0.52
1:A:466:VAL:HB	1:A:551:LEU:HD12	1.92	0.51
2:B:65:LYS:O	2:B:68:SER:HB3	2.11	0.51
2:B:60:VAL:HG21	2:B:130:PHE:CD2	2.46	0.51
1:A:79:GLU:HG3	1:A:83:ARG:NH1	2.24	0.51
2:B:266:TRP:CH2	2:B:427:TYR:CZ	2.98	0.51
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.45	0.51
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.93	0.51
1:A:183:TYR:CE1	1:A:184:MET:HG3	2.45	0.51
1:A:162:SER:OG	2:B:52:PRO:HD3	2.10	0.50
1:A:111:VAL:HG21	1:A:164:MET:HE1	1.93	0.50
1:A:438:GLU:CG	1:A:461:ARG:HD2	2.41	0.50
2:B:24:TRP:NE1	2:B:61:PHE:CZ	2.80	0.50
1:A:417:VAL:HG13	1:A:419:THR:HG22	1.93	0.50
1:A:106:VAL:HG11	3:A:1558:ZZE:C1	2.41	0.50
2:B:194:GLU:HG3	2:B:196:GLY:H	1.75	0.50
1:A:27:THR:HG22	1:A:29:GLU:HG2	1.94	0.50
1:A:434:ILE:HD13	1:A:530:LYS:HB3	1.94	0.50
2:B:242:GLN:HG3	2:B:242:GLN:O	2.10	0.50
1:A:332:GLN:HG3	1:A:338:THR:HG23	1.94	0.49
1:A:458:VAL:CG1	1:A:548:VAL:HG22	2.42	0.49
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.95	0.49
1:A:357:MET:O	1:A:359:GLY:N	2.32	0.49
1:A:335:GLY:HA2	1:A:367:GLN:OE1	2.13	0.49
1:A:467:VAL:HG23	1:A:484:LEU:HD11	1.94	0.49
1:A:511:ASP:OD1	1:A:512:GLN:HG3	2.12	0.49
2:B:112:GLY:HA3	2:B:151:GLN:HE21	1.77	0.49
1:A:402:TRP:CZ2	1:A:403:THR:HG22	2.48	0.49
1:A:60:VAL:HG22	1:A:130:PHE:HB2	1.95	0.48
1:A:246:LEU:HD11	1:A:310:LEU:HD12	1.95	0.48
2:B:266:TRP:CZ3	2:B:426:TRP:HB3	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:122:GLU:H	2:B:122:GLU:CD	2.17	0.48
2:B:109:LEU:HG	2:B:216:THR:HG22	1.94	0.48
2:B:395:LYS:HG3	2:B:416:PHE:CE2	2.48	0.48
1:A:96:HIS:HD1	1:A:98:ALA:H	1.61	0.48
1:A:27:THR:HG22	1:A:29:GLU:H	1.77	0.48
2:B:200:THR:O	2:B:204:GLU:HG3	2.14	0.48
1:A:139:THR:CB	1:A:140:PRO:HD2	2.27	0.47
1:A:457:TYR:HA	1:A:548:VAL:HG11	1.95	0.47
2:B:253:THR:O	2:B:257:ILE:HG13	2.14	0.47
1:A:78:ARG:O	1:A:82:LYS:HG3	2.14	0.47
1:A:361:HIS:HD2	1:A:513:SER:OG	1.97	0.47
2:B:275:LYS:HB2	2:B:302:GLU:HG3	1.97	0.47
2:B:254:VAL:O	2:B:258:GLN:HG3	2.15	0.47
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.97	0.46
2:B:276:VAL:HA	2:B:302:GLU:OE2	2.16	0.46
2:B:13:LYS:NZ	2:B:85:GLN:HG2	2.29	0.46
2:B:234:LEU:HD21	2:B:377:THR:CG2	2.45	0.46
1:A:438:GLU:HG3	1:A:461:ARG:HD2	1.96	0.46
2:B:266:TRP:HE1	2:B:346:PHE:HE1	1.63	0.46
1:A:30:LYS:HE2	1:A:62:ALA:O	2.16	0.46
1:A:438:GLU:OE1	1:A:463:ARG:NH2	2.46	0.45
2:B:266:TRP:CE3	2:B:426:TRP:HB3	2.51	0.45
2:B:393:ILE:HG12	2:B:394:GLN:N	2.32	0.45
1:A:66:LYS:NZ	1:A:67:ASP:H	2.15	0.45
1:A:362:THR:CG2	1:A:363:ASN:H	2.29	0.45
1:A:195:ILE:HB	1:A:199:ARG:HH22	1.81	0.45
2:B:305:GLU:O	2:B:309:ILE:HG13	2.16	0.45
1:A:218:ASP:O	1:A:220:LYS:N	2.50	0.45
2:B:13:LYS:HB2	2:B:16:MET:CG	2.39	0.45
1:A:461:ARG:HH11	1:A:461:ARG:CG	2.28	0.45
1:A:359:GLY:C	1:A:361:HIS:H	2.19	0.44
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.99	0.44
1:A:278:GLN:NE2	1:A:281:LYS:HD2	2.32	0.44
2:B:358:ARG:HD3	2:B:358:ARG:N	2.32	0.44
2:B:103:LYS:HE3	2:B:179:VAL:HG23	1.98	0.44
1:A:283:LEU:O	1:A:286:THR:HG23	2.17	0.44
1:A:491:LEU:H	1:A:491:LEU:HD23	1.82	0.44
2:B:28:GLU:HB2	2:B:135:ILE:HD11	1.99	0.44
1:A:206:ARG:HD3	1:A:218:ASP:OD1	2.18	0.44
1:A:548:VAL:HA	1:A:551:LEU:CD2	2.47	0.44
1:A:194:GLU:O	1:A:195:ILE:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:332:GLN:HA	2:B:424:LYS:HE3	2.00	0.44
1:A:460:ASN:HA	2:B:286:THR:O	2.17	0.44
1:A:23:GLN:NE2	1:A:60:VAL:HG23	2.33	0.43
2:B:194:GLU:HB3	2:B:197:GLN:NE2	2.33	0.43
1:A:406:TRP:HE3	1:A:407:GLN:NE2	2.16	0.43
2:B:65:LYS:HE2	2:B:72:ARG:HD2	1.99	0.43
2:B:270:ILE:HG12	2:B:346:PHE:HB3	2.00	0.43
1:A:339:TYR:CZ	1:A:352:GLY:HA3	2.54	0.43
1:A:255:ASN:HB2	1:A:289:LEU:HG	2.01	0.43
2:B:24:TRP:HE1	2:B:59:PRO:CB	2.29	0.43
2:B:105:SER:O	2:B:190:GLY:HA2	2.19	0.43
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.59	0.43
1:A:396:GLU:CD	1:A:396:GLU:H	2.22	0.42
1:A:454:LYS:HB2	1:A:552:VAL:O	2.19	0.42
2:B:276:VAL:HG22	2:B:276:VAL:O	2.19	0.42
2:B:395:LYS:HG2	2:B:399:GLU:CG	2.50	0.42
1:A:181:TYR:CE1	2:B:138:GLU:HB3	2.54	0.42
2:B:241:VAL:HG13	2:B:351:THR:OG1	2.20	0.42
1:A:216:THR:HB	1:A:217:PRO:HD2	2.01	0.42
2:B:103:LYS:O	2:B:236:PRO:HG2	2.20	0.42
2:B:5:ILE:H	2:B:119:PRO:HG3	1.83	0.42
1:A:31:ILE:O	1:A:35:VAL:HG23	2.20	0.42
2:B:358:ARG:CD	2:B:358:ARG:H	2.32	0.42
2:B:340:GLN:HG2	2:B:427:TYR:CZ	2.55	0.41
1:A:486:LEU:HB3	1:A:524:GLN:CG	2.49	0.41
1:A:311:LYS:HA	1:A:311:LYS:CE	2.45	0.41
2:B:314:VAL:HG13	2:B:317:VAL:CG2	2.50	0.41
1:A:459:THR:O	2:B:286:THR:HG21	2.21	0.41
1:A:379:SER:CB	1:A:387:PRO:HD3	2.50	0.41
2:B:16:MET:HE3	2:B:83:ARG:HA	2.02	0.41
2:B:303:LEU:HD22	2:B:307:ARG:NH2	2.36	0.41
2:B:313:PRO:HB2	2:B:314:VAL:H	1.64	0.41
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.56	0.41
2:B:94:ILE:HA	2:B:95:PRO:HD3	1.93	0.41
2:B:115:TYR:HB3	2:B:149:LEU:HB2	2.02	0.41
1:A:175:ASN:N	1:A:176:PRO:HD3	2.35	0.41
1:A:362:THR:HG22	1:A:363:ASN:O	2.20	0.41
1:A:429:LEU:HD11	1:A:506:ILE:HG22	2.01	0.41
1:A:242:GLN:NE2	1:A:243:PRO:HD2	2.35	0.41
2:B:167:ILE:HG12	2:B:212:TRP:CD2	2.55	0.41
1:A:408:ALA:HB1	2:B:364:ASP:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:THR:CG2	1:A:352:GLY:N	2.84	0.41
1:A:483:TYR:CE1	1:A:520:GLN:HB3	2.56	0.41
1:A:253:THR:HA	1:A:292:VAL:HA	2.02	0.41
2:B:201:LYS:HD3	2:B:201:LYS:HA	1.96	0.41
2:B:28:GLU:CB	2:B:135:ILE:HD11	2.50	0.41
2:B:395:LYS:O	2:B:399:GLU:HG2	2.21	0.41
1:A:28:GLU:HG2	1:A:32:LYS:HE3	2.03	0.40
1:A:540:LYS:HB2	1:A:542:ILE:HG13	2.03	0.40
2:B:368:LEU:O	2:B:372:VAL:HG23	2.20	0.40
1:A:454:LYS:C	1:A:552:VAL:HG13	2.41	0.40
1:A:396:GLU:HA	1:A:399:GLU:HG2	2.03	0.40
2:B:345:PRO:O	2:B:346:PHE:HB2	2.22	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	556/560 (99%)	505 (91%)	31 (6%)	20 (4%)	4	14
2	B	407/440 (92%)	381 (94%)	19 (5%)	7 (2%)	11	36
All	All	963/1000 (96%)	886 (92%)	50 (5%)	27 (3%)	6	21

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	GLU
1	A	135	ILE
1	A	195	ILE
1	A	219	LYS
1	A	286	THR
1	A	358	ARG

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Mol	Chain	Res	Type
1	A	491	LEU
2	B	85	GLN
2	B	313	PRO
2	B	314	VAL
1	A	111	VAL
1	A	114	ALA
1	A	196	GLY
1	A	357	MET
2	B	86	ASP
2	B	361	HIS
1	A	14	PRO
1	A	88	TRP
1	A	345	PRO
1	A	360	ALA
1	A	361	HIS
1	A	138	GLU
1	A	287	LYS
1	A	356	ARG
2	B	245	VAL
2	B	358	ARG
1	A	139	THR

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	497/500 (99%)	469 (94%)	28 (6%)	26	59
2	B	372/400 (93%)	356 (96%)	16 (4%)	35	70
All	All	869/900 (97%)	825 (95%)	44 (5%)	29	63

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	23	GLN

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Mol	Chain	Res	Type
1	A	37	ILE
1	A	60	VAL
1	A	89	GLU
1	A	91	GLN
1	A	102	LYS
1	A	104	LYS
1	A	107	THR
1	A	136	ASN
1	A	145	GLN
1	A	215	THR
1	A	219	LYS
1	A	230	MET
1	A	311	LYS
1	A	334	GLN
1	A	340	GLN
1	A	356	ARG
1	A	357	MET
1	A	402	TRP
1	A	406	TRP
1	A	448	ARG
1	A	463	ARG
1	A	474	ASN
1	A	496	VAL
1	A	500	GLN
1	A	517	LEU
1	A	548	VAL
2	B	6	GLU
2	B	11	LYS
2	B	24	TRP
2	B	65	LYS
2	B	87	PHE
2	B	109	LEU
2	B	139	THR
2	B	174	GLN
2	B	194	GLU
2	B	214	LEU
2	B	237	ASP
2	B	242	GLN
2	B	250	ASP
2	B	325	LEU
2	B	358	ARG
2	B	399	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	137	ASN
1	A	174	GLN
1	A	207	GLN
1	A	269	GLN
1	A	278	GLN
1	A	334	GLN
1	A	361	HIS
1	A	373	GLN
1	A	407	GLN
1	A	428	GLN
1	A	480	GLN
1	A	500	GLN
1	A	512	GLN
1	A	519	ASN
1	A	545	ASN
1	A	547	GLN
2	B	147	ASN
2	B	151	GLN
2	B	175	ASN
2	B	182	GLN
2	B	208	HIS
2	B	242	GLN
2	B	278	GLN
2	B	336	GLN
2	B	394	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	ZZE	A	1558	-	23,24,24	2.28	7 (30%)	26,32,32	4.14	9 (34%)

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	ZZE	A	1558	-	-	0/13/15/15	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1558	ZZE	C10-N5	-3.14	1.41	1.47
3	A	1558	ZZE	C21-N23	2.40	1.20	1.14
3	A	1558	ZZE	C19-C16	2.66	1.44	1.39
3	A	1558	ZZE	C10-C15	2.71	1.58	1.50
3	A	1558	ZZE	C13-C16	3.28	1.45	1.39
3	A	1558	ZZE	C19-C17	4.53	1.48	1.39
3	A	1558	ZZE	C13-C9	5.99	1.49	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1558	ZZE	C14-C17-C21	-11.91	104.46	119.51
3	A	1558	ZZE	C16-C13-C9	-2.45	116.12	119.47
3	A	1558	ZZE	C15-C10-N5	-2.40	105.95	110.85
3	A	1558	ZZE	C19-C17-C14	2.39	124.14	119.72
3	A	1558	ZZE	C6-C2-N5	4.18	129.77	120.20
3	A	1558	ZZE	C2-C1-C3	5.26	111.64	104.05
3	A	1558	ZZE	C3-N7-N5	7.72	111.08	104.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1558	ZZE	C9-O4-C1	8.70	133.61	118.46
3	A	1558	ZZE	C19-C17-C21	9.40	131.40	119.51

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1558	ZZE	2	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(Å²)	Q<0.9
1	A	558/560 (99%)	0.18	37 (6%)	22	13	31, 58, 105, 194	0
2	B	413/440 (93%)	0.18	31 (7%)	17	9	29, 57, 108, 128	0
All	All	971/1000 (97%)	0.18	68 (7%)	19	11	29, 57, 107, 194	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	3	SER	9.8
1	A	549	ASP	9.2
2	B	4	PRO	8.9
2	B	357	MET	8.6
1	A	553	SER	8.2
1	A	548	VAL	7.8
2	B	216	THR	7.1
2	B	230	MET	7.0
2	B	231	GLY	6.6
2	B	13	LYS	6.3
1	A	556	ILE	6.2
1	A	359	GLY	6.2
1	A	550	LYS	6.2
2	B	358	ARG	5.7
1	A	547	GLN	5.7
1	A	546	GLU	5.1
1	A	539	HIS	5.0
1	A	552	VAL	4.9
1	A	358	ARG	4.7
2	B	297	GLU	4.7
1	A	541	GLY	4.5
1	A	551	LEU	4.5
1	A	24	TRP	4.4
1	A	555	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
2	B	359	GLY	4.3
1	A	557	ARG	4.3
2	B	67	ASP	4.3
2	B	66	LYS	4.3
1	A	67	ASP	4.1
1	A	544	GLY	4.1
1	A	554	ALA	4.0
2	B	360	ALA	4.0
2	B	69	THR	3.9
2	B	65	LYS	3.9
2	B	361	HIS	3.9
2	B	5	ILE	3.8
2	B	14	PRO	3.7
1	A	286	THR	3.6
2	B	6	GLU	3.5
2	B	232	TYR	3.3
1	A	65	LYS	3.2
1	A	70	LYS	3.2
1	A	284	ARG	2.9
1	A	287	LYS	2.9
1	A	53	GLU	2.8
2	B	243	PRO	2.7
2	B	362	THR	2.7
2	B	16	MET	2.7
1	A	66	LYS	2.6
2	B	68	SER	2.6
1	A	558	LYS	2.6
1	A	221	HIS	2.6
1	A	514	GLU	2.6
2	B	213	GLY	2.6
1	A	15	GLY	2.5
2	B	217	PRO	2.4
1	A	360	ALA	2.4
1	A	68	SER	2.4
2	B	15	GLY	2.4
2	B	308	GLU	2.3
1	A	69	THR	2.3
1	A	545	ASN	2.3
2	B	298	GLU	2.3
2	B	250	ASP	2.2
1	A	311	LYS	2.2
1	A	288	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	429	LEU	2.1
1	A	206	ARG	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($Å^2$)	Q<0.9
3	ZZE	A	1558	23/23	0.93	0.24	0.62	46,50,55,59	0

6.5 Other polymers (i)

There are no such residues in this entry.