Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:25 PM GMT

PDB ID	:	1TKX
Title	:	CRYSTAL STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE IN COMPLEX WITH GW490745
Authors	:	Ren, J.; Hopkins, A.L.; Stuart, D.I.; Stammers, D.K.
Deposited on	:	2004-06-09
Resolution	:	2.85 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
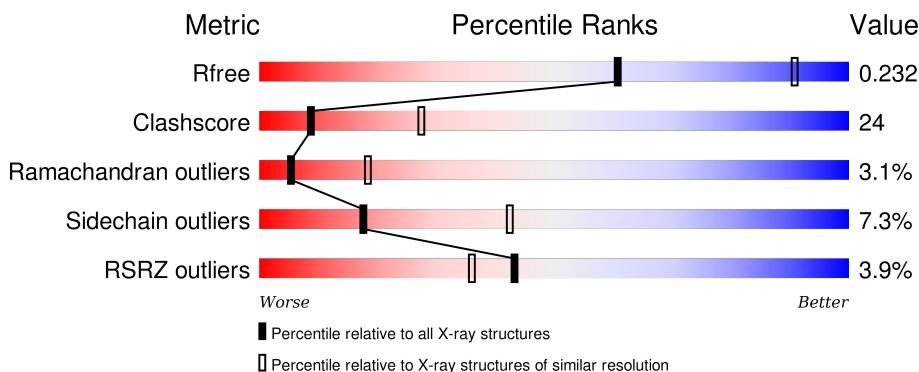
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.85 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		0.232
Clashscore		24
Ramachandran outliers		3.1%
Sidechain outliers		7.3%
RSRZ outliers		3.9%

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	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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	4% — 45% / 43% / 7% / •
2	B	440	4% — 54% / 35% / • / 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7745 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 Pol polyprotein, Reverse transcriptase, Chain A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	535	4381	2835	730	808	8	0	0	0
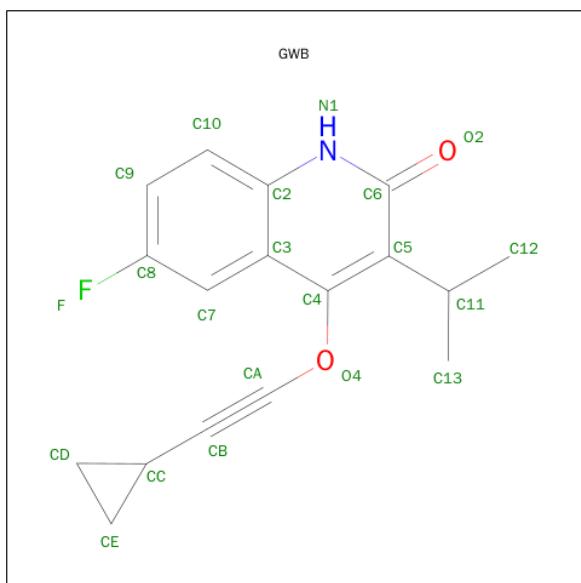
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	CSD	CYS	OXIDIZED CYS	UNP P04585

- Molecule 2 is a protein called Pol polyprotein, Reverse transcriptase, Chain B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	404	3343	2174	555	607	7	0	0	0

- Molecule 3 is 4-[(CYCLOPROPYLETHYNYL)OXY]-6-FLUORO-3-ISOPROPYLQUINOLIN-2(1H)-ONE (three-letter code: GWB) (formula: $C_{17}H_{16}FNO_2$).
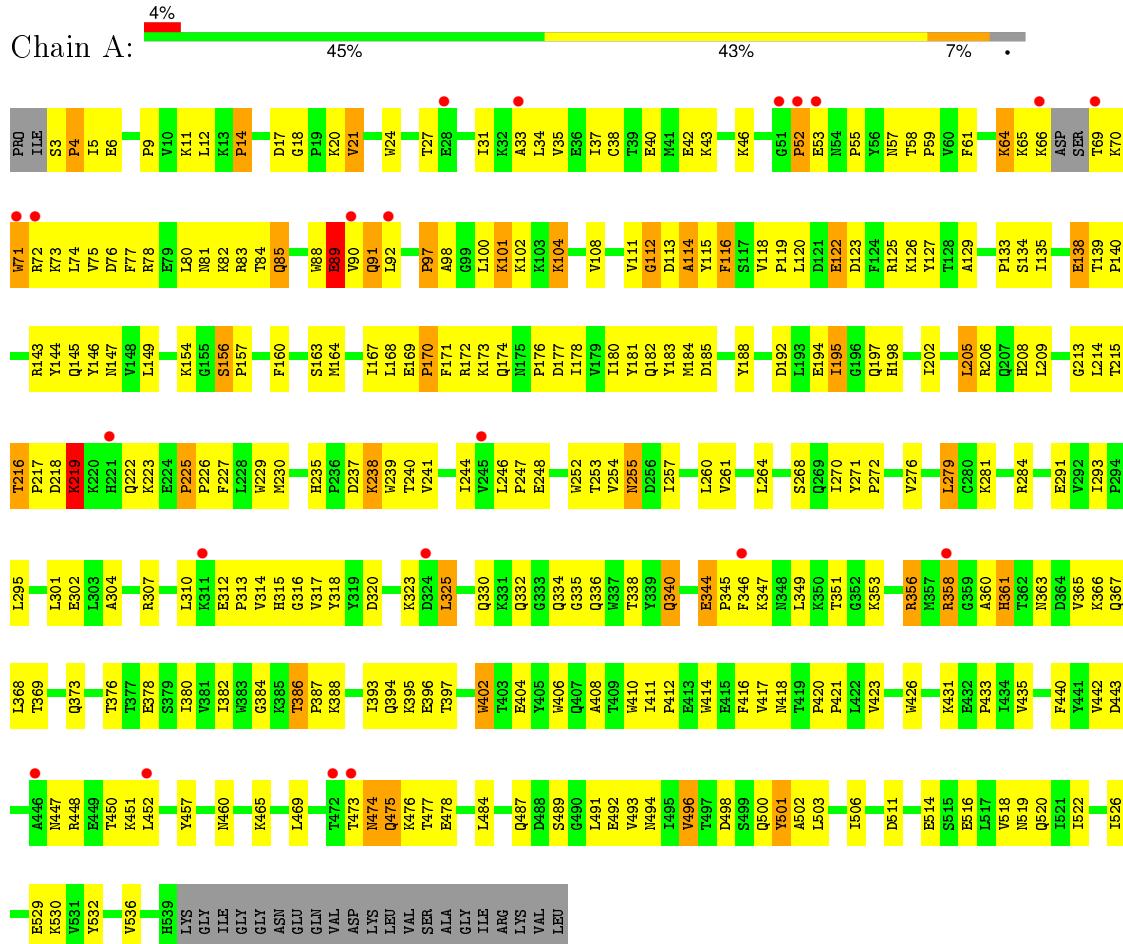
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
3	A	1	21	17	1	1	2	0	0

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: Pol polyprotein, Reverse transcriptase, Chain A

- Molecule 2: Pol polyprotein, Reverse transcriptase, Chain B

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	138.20Å 109.70Å 72.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.63 – 2.85 29.62 – 2.85	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.63-2.85) 98.4 (29.62-2.85)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 2.85Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.216 , 0.287 0.212 , 0.232	Depositor DCC
R_{free} test set	1260 reflections (5.08%)	DCC
Wilson B-factor (Å^2)	63.7	Xtriage
Anisotropy	0.437	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 81.3	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 26084 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7745	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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.

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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: CSD, GWB

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	0.40	0/4488	0.67	1/6099 (0.0%)
2	B	0.41	0/3436	0.67	0/4667
All	All	0.40	0/7924	0.67	1/10766 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	388	LYS	N-CA-C	-5.90	95.07	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	4381	0	4423	240	0
2	B	3343	0	3368	137	0
3	A	21	0	16	3	0
All	All	7745	0	7807	367	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 24.

All (367) 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:169:GLU:HB2	2:B:170:PRO:HD3	1.45	0.96
1:A:64:LYS:O	1:A:64:LYS:HD3	1.64	0.96
1:A:448:ARG:HE	1:A:474:ASN:H	1.01	0.92
1:A:516:GLU:O	1:A:520:GLN:HG3	1.73	0.89
2:B:56:TYR:HE2	2:B:126:LYS:HE2	1.40	0.87
2:B:175:ASN:HD21	2:B:201:LYS:HD2	1.37	0.87
1:A:101:LYS:N	1:A:101:LYS:HE3	1.91	0.86
1:A:344:GLU:HG3	1:A:347:LYS:HD2	1.55	0.86
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.61	0.83
1:A:11:LYS:O	1:A:85:GLN:HB3	1.78	0.83
1:A:393:ILE:HB	1:A:423:VAL:HG22	1.61	0.82
1:A:503:LEU:HA	1:A:506:ILE:HD12	1.62	0.82
2:B:163:SER:O	2:B:167:ILE:HG23	1.80	0.82
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.62	0.81
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.62	0.80
1:A:240:THR:HG22	1:A:315:HIS:HB3	1.63	0.80
2:B:175:ASN:ND2	2:B:201:LYS:HD2	1.97	0.79
1:A:31:ILE:O	1:A:35:VAL:HG23	1.83	0.79
1:A:34:LEU:CD2	1:A:73:LYS:HB2	2.13	0.78
1:A:239:TRP:CZ2	1:A:316:GLY:HA3	2.19	0.78
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.65	0.77
2:B:122:GLU:CG	2:B:125:ARG:NH1	2.48	0.76
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.67	0.76
2:B:31:ILE:O	2:B:35:VAL:HG23	1.86	0.76
2:B:366:LYS:O	2:B:370:GLU:HG3	1.86	0.75
1:A:516:GLU:O	1:A:519:ASN:HB2	1.86	0.75
2:B:170:PRO:O	2:B:174:GLN:HG3	1.87	0.74
2:B:122:GLU:HG2	2:B:125:ARG:NH1	2.04	0.73
1:A:448:ARG:HH21	1:A:475:GLN:H	1.33	0.73
1:A:448:ARG:HE	1:A:474:ASN:N	1.83	0.73
1:A:264:LEU:HD13	1:A:276:VAL:HG12	1.71	0.72
1:A:448:ARG:NE	1:A:474:ASN:H	1.84	0.72
2:B:420:PRO:HB2	2:B:423:VAL:HG23	1.72	0.70
1:A:244:ILE:HG23	1:A:310:LEU:HD13	1.74	0.69
1:A:116:PHE:HE1	1:A:146:TYR:HE1	1.39	0.69
1:A:170:PRO:O	1:A:174:GLN:HG3	1.93	0.69
1:A:239:TRP:CE2	1:A:316:GLY:HA3	2.27	0.69
2:B:27:THR:OG1	2:B:30:LYS:HG3	1.93	0.69
1:A:129:ALA:HB1	1:A:143:ARG:HH12	1.57	0.69
2:B:103:LYS:HE2	2:B:179:VAL:HG23	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:122:GLU:HG3	2:B:125:ARG:NH1	2.08	0.68
1:A:366:LYS:O	1:A:369:THR:HB	1.93	0.67
1:A:226:PRO:HB3	1:A:235:HIS:CE1	2.29	0.67
2:B:235:HIS:O	2:B:238:LYS:HG2	1.95	0.67
2:B:426:TRP:O	2:B:429:LEU:HB2	1.94	0.67
1:A:344:GLU:CG	1:A:347:LYS:HD2	2.25	0.67
2:B:161:GLN:HA	2:B:161:GLN:NE2	2.10	0.67
1:A:238:LYS:HB2	1:A:316:GLY:O	1.94	0.66
1:A:65:LYS:HB2	1:A:72:ARG:HD2	1.77	0.66
1:A:65:LYS:HG2	1:A:66:LYS:H	1.59	0.66
2:B:338:THR:HG22	2:B:353:LYS:HG3	1.78	0.66
1:A:114:ALA:HB1	1:A:160:PHE:CE2	2.31	0.66
1:A:268:SER:HB3	1:A:353:LYS:HE2	1.77	0.65
1:A:317:VAL:HG21	1:A:347:LYS:HB3	1.78	0.65
1:A:164:MET:O	1:A:168:LEU:HG	1.97	0.65
1:A:3:SER:OG	1:A:5:ILE:HG13	1.97	0.64
2:B:56:TYR:CE2	2:B:126:LYS:HE2	2.29	0.64
1:A:218:ASP:HA	1:A:222:GLN:HG2	1.79	0.64
1:A:116:PHE:CE1	1:A:146:TYR:HE1	2.16	0.63
1:A:122:GLU:CD	1:A:122:GLU:H	2.00	0.63
1:A:475:GLN:HG3	1:A:476:LYS:N	2.14	0.63
1:A:225:PRO:HA	1:A:226:PRO:C	2.17	0.63
1:A:335:GLY:O	1:A:356:ARG:HA	1.99	0.62
1:A:135:ILE:O	1:A:138:GLU:HG3	1.99	0.62
1:A:18:GLY:HA3	1:A:127:TYR:HD1	1.64	0.62
1:A:344:GLU:HG2	1:A:347:LYS:HB2	1.82	0.62
1:A:64:LYS:C	1:A:64:LYS:HD3	2.20	0.62
1:A:73:LYS:HE3	1:A:75:VAL:CG2	2.28	0.62
2:B:171:PHE:CD2	2:B:205:LEU:HD13	2.35	0.61
1:A:241:VAL:HG21	1:A:270:ILE:HG21	1.82	0.61
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.34	0.61
1:A:253:THR:O	1:A:257:ILE:HG13	2.00	0.61
2:B:122:GLU:CG	2:B:125:ARG:HH12	2.14	0.61
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.35	0.61
1:A:475:GLN:HG3	1:A:476:LYS:H	1.65	0.61
1:A:317:VAL:HG12	1:A:318:TYR:N	2.16	0.61
2:B:169:GLU:HB2	2:B:170:PRO:CD	2.24	0.60
1:A:34:LEU:HD23	1:A:73:LYS:HB2	1.83	0.60
1:A:244:ILE:CG2	1:A:310:LEU:HD13	2.30	0.60
1:A:257:ILE:O	1:A:261:VAL:HG23	2.01	0.60
1:A:170:PRO:HG2	1:A:171:PHE:H	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:LYS:HE2	1:A:116:PHE:HB3	1.83	0.59
2:B:61:PHE:CE1	2:B:74:LEU:HD23	2.37	0.59
1:A:340:GLN:CB	1:A:351:THR:HG22	2.32	0.59
2:B:111:VAL:CG1	2:B:187:LEU:HD22	2.30	0.59
2:B:379:SER:OG	2:B:387:PRO:HD3	2.02	0.59
1:A:240:THR:HG22	1:A:315:HIS:CB	2.32	0.59
2:B:84:THR:HB	2:B:154:LYS:HE2	1.84	0.59
1:A:330:GLN:HB2	1:A:338:THR:OG1	2.02	0.59
2:B:125:ARG:NE	2:B:147:ASN:HA	2.18	0.59
1:A:206:ARG:HG2	1:A:206:ARG:HH11	1.68	0.59
2:B:365:VAL:O	2:B:369:THR:HG23	2.03	0.59
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.83	0.58
1:A:58:THR:HG23	1:A:59:PRO:HD2	1.84	0.58
1:A:312:GLU:HG2	1:A:313:PRO:HD2	1.84	0.58
1:A:360:ALA:HA	1:A:514:GLU:HB3	1.86	0.57
1:A:65:LYS:CB	1:A:72:ARG:HD2	2.35	0.57
2:B:308:GLU:O	2:B:311:LYS:HB2	2.03	0.57
1:A:218:ASP:O	1:A:219:LYS:CB	2.53	0.57
1:A:18:GLY:HA3	1:A:127:TYR:CD1	2.40	0.57
1:A:194:GLU:O	1:A:197:GLN:N	2.38	0.57
2:B:125:ARG:HE	2:B:147:ASN:HA	1.70	0.56
1:A:335:GLY:HA2	1:A:367:GLN:OE1	2.05	0.56
1:A:58:THR:HG23	1:A:76:ASP:O	2.05	0.56
1:A:408:ALA:HB3	2:B:393:ILE:HG13	1.88	0.56
1:A:225:PRO:HG3	1:A:227:PHE:CE2	2.41	0.56
2:B:376:THR:CG2	2:B:386:THR:HG22	2.35	0.56
1:A:501:TYR:HD2	1:A:501:TYR:O	1.87	0.56
1:A:301:LEU:O	1:A:304:ALA:HB3	2.05	0.56
1:A:440:PHE:CZ	1:A:489:SER:HB3	2.41	0.56
2:B:46:LYS:HE2	2:B:116:PHE:CD1	2.41	0.55
2:B:53:GLU:CD	2:B:53:GLU:H	2.09	0.55
1:A:246:LEU:O	1:A:307:ARG:NH1	2.35	0.55
1:A:5:ILE:HD13	1:A:167:ILE:HD11	1.89	0.55
2:B:366:LYS:HG3	2:B:405:TYR:CD2	2.42	0.55
2:B:165:THR:HG23	2:B:166:LYS:H	1.72	0.55
2:B:64:LYS:HE2	2:B:71:TRP:CE2	2.40	0.55
1:A:92:LEU:O	1:A:92:LEU:HD23	2.05	0.55
1:A:475:GLN:HA	1:A:478:GLU:OE2	2.07	0.55
2:B:266:TRP:HZ3	2:B:426:TRP:CD1	2.25	0.55
1:A:65:LYS:HG2	1:A:66:LYS:N	2.22	0.54
1:A:112:GLY:O	1:A:114:ALA:N	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:VAL:HG21	1:A:270:ILE:HD13	1.88	0.54
2:B:139:THR:HG22	2:B:140:PRO:O	2.07	0.54
2:B:167:ILE:O	2:B:208:HIS:CE1	2.60	0.54
1:A:206:ARG:HH21	1:A:217:PRO:HA	1.70	0.54
1:A:492:GLU:HA	1:A:530:LYS:O	2.07	0.54
2:B:320:ASP:OD2	2:B:323:LYS:HD3	2.07	0.54
2:B:195:ILE:HG23	2:B:196:GLY:N	2.21	0.54
1:A:181:TYR:HB3	1:A:188:TYR:HB2	1.90	0.54
2:B:154:LYS:O	2:B:157:PRO:HD2	2.08	0.54
1:A:498:ASP:HA	1:A:536:VAL:O	2.07	0.54
2:B:160:PHE:CD1	2:B:160:PHE:O	2.61	0.54
1:A:108:VAL:O	1:A:108:VAL:HG13	2.08	0.54
2:B:165:THR:HG23	2:B:166:LYS:N	2.22	0.53
1:A:173:LYS:O	1:A:176:PRO:HD3	2.09	0.53
1:A:197:GLN:HA	1:A:197:GLN:OE1	2.08	0.53
2:B:23:GLN:HG2	2:B:133:PRO:HD3	1.89	0.53
1:A:253:THR:HA	1:A:291:GLU:O	2.08	0.53
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.44	0.53
1:A:139:THR:HB	1:A:140:PRO:HD2	1.91	0.53
1:A:237:ASP:N	1:A:237:ASP:OD2	2.42	0.53
2:B:344:GLU:HB3	2:B:347:LYS:HE3	1.89	0.53
2:B:61:PHE:CZ	2:B:74:LEU:HD23	2.44	0.53
1:A:420:PRO:HA	1:A:421:PRO:C	2.29	0.53
2:B:39:THR:O	2:B:43:LYS:HG2	2.08	0.53
2:B:424:LYS:HD2	2:B:425:LEU:HD13	1.90	0.52
1:A:376:THR:O	1:A:380:ILE:HG12	2.09	0.52
1:A:169:GLU:N	1:A:170:PRO:HD2	2.25	0.52
1:A:34:LEU:HD21	1:A:73:LYS:HB2	1.91	0.52
2:B:113:ASP:O	2:B:116:PHE:HD2	1.92	0.52
1:A:108:VAL:CG1	1:A:223:LYS:HB2	2.39	0.52
2:B:195:ILE:HD11	2:B:199:ARG:CZ	2.40	0.52
2:B:183:TYR:CE1	2:B:184:MET:HG2	2.43	0.52
2:B:33:ALA:O	2:B:37:ILE:HG13	2.09	0.52
2:B:19:PRO:O	2:B:20:LYS:HG2	2.09	0.52
1:A:134:SER:OG	1:A:138:GLU:HB2	2.10	0.52
1:A:448:ARG:CZ	1:A:473:THR:HB	2.40	0.52
2:B:238:LYS:HZ2	2:B:239:TRP:HD1	1.56	0.52
1:A:225:PRO:HA	1:A:226:PRO:O	2.10	0.52
1:A:402:TRP:C	1:A:402:TRP:CD1	2.83	0.52
1:A:115:TYR:HD1	1:A:115:TYR:H	1.55	0.52
2:B:11:LYS:N	2:B:85:GLN:OE1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:GLU:O	1:A:197:GLN:HB2	2.11	0.51
1:A:293:ILE:HD12	1:A:293:ILE:N	2.25	0.51
1:A:100:LEU:C	1:A:101:LYS:HE3	2.31	0.51
1:A:163:SER:O	1:A:167:ILE:HG13	2.10	0.51
1:A:206:ARG:NH1	1:A:206:ARG:HG2	2.25	0.51
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.91	0.51
1:A:518:VAL:O	1:A:522:ILE:HG13	2.11	0.51
1:A:378:GLU:O	1:A:382:ILE:HG12	2.11	0.51
1:A:235:HIS:HB2	1:A:238:LYS:O	2.11	0.51
2:B:122:GLU:HG3	2:B:125:ARG:HH12	1.73	0.51
1:A:64:LYS:HE2	1:A:69:THR:HG23	1.93	0.50
1:A:21:VAL:CG1	1:A:59:PRO:HD3	2.42	0.50
2:B:276:VAL:O	2:B:280:CYS:HB2	2.11	0.50
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.91	0.50
1:A:33:ALA:HB1	1:A:71:TRP:HB3	1.94	0.50
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.12	0.50
1:A:129:ALA:HB1	1:A:143:ARG:NH1	2.26	0.50
1:A:215:THR:O	1:A:216:THR:C	2.48	0.50
1:A:474:ASN:O	1:A:478:GLU:HG3	2.11	0.50
1:A:85:GLN:O	1:A:154:LYS:NZ	2.42	0.50
1:A:393:ILE:HB	1:A:423:VAL:CG2	2.38	0.50
1:A:90:VAL:O	1:A:91:GLN:C	2.50	0.50
1:A:433:PRO:HG3	1:A:532:TYR:CE2	2.47	0.50
2:B:161:GLN:O	2:B:165:THR:HG22	2.12	0.49
1:A:360:ALA:O	1:A:361:HIS:HB3	2.12	0.49
1:A:229:TRP:CD2	3:A:999:GWB:HE1	2.47	0.49
2:B:78:ARG:O	2:B:82:LYS:HG3	2.11	0.49
1:A:363:ASN:HB2	1:A:511:ASP:OD2	2.12	0.49
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.47	0.49
2:B:421:PRO:O	2:B:425:LEU:HD22	2.12	0.49
1:A:406:TRP:CZ3	2:B:418:ASN:HA	2.46	0.49
1:A:225:PRO:HG3	1:A:227:PHE:CZ	2.48	0.49
2:B:379:SER:CB	2:B:387:PRO:HD3	2.42	0.49
1:A:229:TRP:CD1	1:A:230:MET:HG2	2.47	0.48
1:A:460:ASN:HA	2:B:286:THR:O	2.12	0.48
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.95	0.48
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.94	0.48
1:A:442:VAL:HG22	1:A:496:VAL:O	2.13	0.48
2:B:287:LYS:HE2	2:B:293:ILE:HD11	1.94	0.48
2:B:266:TRP:CZ3	2:B:426:TRP:CG	3.01	0.48
1:A:501:TYR:O	1:A:501:TYR:CD2	2.65	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:ILE:HD11	2:B:199:ARG:NE	2.28	0.48
1:A:271:TYR:HA	1:A:272:PRO:HD3	1.64	0.48
1:A:69:THR:HG22	1:A:69:THR:O	2.13	0.48
1:A:46:LYS:HE2	1:A:116:PHE:CB	2.42	0.48
2:B:332:GLN:HE22	2:B:424:LYS:HD3	1.78	0.48
1:A:24:TRP:CG	1:A:61:PHE:HE1	2.31	0.48
1:A:469:LEU:HD12	1:A:477:THR:HG22	1.96	0.48
1:A:246:LEU:HD22	1:A:260:LEU:HD11	1.94	0.48
2:B:388:LYS:HE2	2:B:415:GLU:HB3	1.95	0.48
1:A:77:PHE:CD2	1:A:80:LEU:HD23	2.48	0.48
1:A:101:LYS:NZ	2:B:138:GLU:OE1	2.46	0.47
2:B:202:ILE:O	2:B:205:LEU:HB3	2.14	0.47
1:A:215:THR:O	1:A:216:THR:O	2.32	0.47
1:A:447:ASN:O	1:A:451:LYS:N	2.48	0.47
1:A:98:ALA:HB2	1:A:349:LEU:O	2.14	0.47
1:A:180:ILE:HG22	1:A:181:TYR:N	2.28	0.47
1:A:17:ASP:O	1:A:83:ARG:HD3	2.13	0.47
1:A:122:GLU:N	1:A:122:GLU:OE1	2.42	0.47
1:A:139:THR:HB	1:A:140:PRO:CD	2.43	0.47
1:A:20:LYS:NZ	1:A:55:PRO:HB2	2.28	0.47
2:B:167:ILE:HD12	2:B:209:LEU:HD12	1.97	0.47
2:B:118:VAL:HG13	2:B:119:PRO:HD2	1.97	0.47
1:A:57:ASN:HA	1:A:129:ALA:O	2.14	0.47
1:A:519:ASN:O	1:A:522:ILE:HB	2.14	0.47
1:A:38:CYS:HB3	1:A:144:TYR:CE1	2.50	0.47
2:B:210:LEU:C	2:B:212:TRP:H	2.19	0.47
1:A:209:LEU:HB3	1:A:214:LEU:HB2	1.97	0.46
2:B:279:LEU:HA	2:B:282:LEU:HD12	1.98	0.46
2:B:278:GLN:HG3	2:B:298:GLU:HB3	1.97	0.46
2:B:332:GLN:NE2	2:B:424:LYS:HE2	2.30	0.46
1:A:184:MET:HB3	1:A:185:ASP:H	1.58	0.46
1:A:31:ILE:HG12	1:A:133:PRO:HG2	1.97	0.46
2:B:52:PRO:HD2	2:B:53:GLU:OE1	2.15	0.46
2:B:332:GLN:NE2	2:B:428:GLN:HB2	2.31	0.46
1:A:241:VAL:HB	1:A:314:VAL:HG23	1.96	0.46
1:A:81:ASN:C	1:A:83:ARG:H	2.19	0.46
1:A:104:LYS:HD3	1:A:192:ASP:O	2.16	0.46
2:B:209:LEU:HA	2:B:209:LEU:HD12	1.84	0.45
1:A:241:VAL:HB	1:A:314:VAL:CG2	2.46	0.45
1:A:58:THR:CG2	1:A:76:ASP:O	2.64	0.45
1:A:108:VAL:HG13	1:A:223:LYS:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:LYS:O	1:A:284:ARG:HG3	2.16	0.45
1:A:198:HIS:NE2	1:A:202:ILE:HD11	2.30	0.45
1:A:246:LEU:HD22	1:A:260:LEU:CD1	2.47	0.45
2:B:267:ALA:HB2	2:B:426:TRP:CZ3	2.52	0.45
1:A:125:ARG:NE	1:A:147:ASN:HA	2.32	0.45
1:A:206:ARG:NH2	1:A:216:THR:O	2.50	0.45
1:A:58:THR:CG2	1:A:59:PRO:HD2	2.46	0.45
2:B:94:ILE:HD11	2:B:182:GLN:H	1.80	0.45
1:A:218:ASP:HA	1:A:222:GLN:CG	2.46	0.45
1:A:440:PHE:CE1	1:A:489:SER:HB3	2.52	0.45
2:B:46:LYS:HE2	2:B:116:PHE:HD1	1.81	0.45
1:A:457:TYR:CE2	1:A:465:LYS:HB3	2.52	0.45
1:A:219:LYS:H	1:A:222:GLN:HG3	1.82	0.45
1:A:43:LYS:HA	1:A:43:LYS:HD3	1.60	0.45
1:A:73:LYS:HG3	1:A:74:LEU:N	2.32	0.44
2:B:64:LYS:HE2	2:B:71:TRP:CZ2	2.52	0.44
1:A:402:TRP:CZ2	2:B:362:THR:HA	2.52	0.44
1:A:344:GLU:O	1:A:344:GLU:HG2	2.17	0.44
1:A:502:ALA:O	1:A:506:ILE:HG13	2.17	0.44
1:A:408:ALA:HB3	2:B:393:ILE:CG1	2.47	0.44
2:B:17:ASP:OD1	2:B:18:GLY:N	2.51	0.44
1:A:27:THR:O	1:A:31:ILE:HG13	2.17	0.44
2:B:98:ALA:O	2:B:101:LYS:HE2	2.17	0.44
2:B:118:VAL:CG1	2:B:119:PRO:HD2	2.47	0.44
1:A:402:TRP:CH2	2:B:362:THR:HA	2.52	0.44
2:B:244:ILE:HG21	2:B:426:TRP:CZ2	2.52	0.44
1:A:448:ARG:NH2	1:A:475:GLN:H	2.08	0.44
1:A:380:ILE:O	1:A:384:GLY:HA2	2.18	0.44
1:A:183:TYR:CD1	1:A:184:MET:HB2	2.53	0.44
2:B:270:ILE:O	2:B:272:PRO:HD3	2.18	0.44
2:B:13:LYS:HB2	2:B:16:MET:HG3	1.99	0.44
2:B:325:LEU:HD22	2:B:385:LYS:HD3	1.99	0.43
1:A:279:LEU:HD12	1:A:302:GLU:OE1	2.17	0.43
1:A:241:VAL:CG2	1:A:270:ILE:HD13	2.48	0.43
1:A:9:PRO:HG2	2:B:53:GLU:HG3	1.99	0.43
1:A:317:VAL:CG2	1:A:347:LYS:HB3	2.45	0.43
1:A:205:LEU:O	1:A:208:HIS:HB3	2.19	0.43
1:A:314:VAL:HG23	1:A:314:VAL:O	2.19	0.43
1:A:340:GLN:HB2	1:A:351:THR:HG22	2.01	0.43
1:A:71:TRP:HA	1:A:71:TRP:CE3	2.54	0.43
1:A:484:LEU:HD23	1:A:487:GLN:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:VAL:HG13	1:A:59:PRO:HD3	2.00	0.43
1:A:332:GLN:HG2	1:A:332:GLN:O	2.17	0.43
1:A:84:THR:HB	1:A:154:LYS:HD3	2.01	0.43
2:B:254:VAL:HG21	2:B:287:LYS:HG3	2.01	0.43
2:B:195:ILE:HG23	2:B:196:GLY:H	1.82	0.43
1:A:181:TYR:CD1	3:A:999:GWB:HC	2.54	0.43
1:A:77:PHE:O	1:A:78:ARG:C	2.56	0.43
2:B:27:THR:OG1	2:B:30:LYS:CG	2.63	0.43
1:A:168:LEU:O	1:A:172:ARG:HG3	2.18	0.43
2:B:51:GLY:HA3	2:B:53:GLU:OE2	2.19	0.43
2:B:344:GLU:CB	2:B:347:LYS:HE3	2.48	0.43
2:B:323:LYS:HB3	2:B:343:GLN:NE2	2.34	0.43
2:B:106:VAL:HA	2:B:189:VAL:O	2.18	0.43
1:A:394:GLN:HB2	1:A:397:THR:OG1	2.19	0.43
2:B:79:GLU:O	2:B:83:ARG:HG3	2.18	0.43
1:A:125:ARG:HB3	1:A:145:GLN:NE2	2.33	0.43
1:A:448:ARG:HA	1:A:448:ARG:HD3	1.86	0.42
1:A:213:GLY:O	1:A:214:LEU:HD23	2.19	0.42
2:B:244:ILE:HD13	2:B:430:GLU:HG3	2.01	0.42
2:B:319:TYR:CE1	2:B:321:PRO:HG3	2.54	0.42
1:A:37:ILE:O	1:A:40:GLU:HB3	2.19	0.42
1:A:206:ARG:CZ	1:A:216:THR:O	2.68	0.42
1:A:493:VAL:HG12	1:A:494:ASN:N	2.34	0.42
1:A:65:LYS:O	1:A:69:THR:HA	2.19	0.42
2:B:206:ARG:O	2:B:207:GLN:C	2.58	0.42
1:A:325:LEU:HA	1:A:325:LEU:HD23	1.73	0.42
1:A:254:VAL:O	1:A:255:ASN:C	2.57	0.42
1:A:477:THR:O	1:A:478:GLU:C	2.57	0.42
1:A:91:GLN:HE22	1:A:181:TYR:HE2	1.67	0.42
1:A:346:PHE:N	1:A:346:PHE:CD2	2.85	0.42
2:B:283:LEU:HD12	2:B:283:LEU:HA	1.81	0.42
2:B:271:TYR:HB3	2:B:309:ILE:HG21	2.00	0.42
2:B:334:GLN:O	2:B:336:GLN:OE1	2.37	0.42
2:B:332:GLN:HE22	2:B:428:GLN:HB2	1.84	0.42
1:A:416:PHE:CD1	1:A:417:VAL:N	2.88	0.42
2:B:27:THR:HG1	2:B:30:LYS:HG3	1.83	0.42
1:A:418:ASN:OD1	1:A:420:PRO:HD3	2.20	0.42
1:A:138:GLU:HB3	1:A:139:THR:H	1.66	0.42
1:A:118:VAL:HA	1:A:119:PRO:HD3	1.81	0.42
2:B:239:TRP:CH2	2:B:378:GLU:HA	2.55	0.41
1:A:118:VAL:HB	1:A:149:LEU:HD22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:TYR:HB3	2:B:149:LEU:CB	2.39	0.41
1:A:334:GLN:O	1:A:356:ARG:HD2	2.19	0.41
1:A:336:GLN:HG3	1:A:356:ARG:HB2	2.02	0.41
1:A:216:THR:HG23	1:A:216:THR:O	2.20	0.41
1:A:247:PRO:C	1:A:307:ARG:HH22	2.23	0.41
2:B:94:ILE:CD1	2:B:182:GLN:H	2.33	0.41
1:A:386:THR:HA	1:A:387:PRO:HD3	1.92	0.41
1:A:491:LEU:O	1:A:529:GLU:N	2.46	0.41
2:B:139:THR:HG23	2:B:140:PRO:HD2	2.01	0.41
1:A:426:TRP:HB3	1:A:526:ILE:HG12	2.03	0.41
1:A:64:LYS:O	1:A:64:LYS:CD	2.52	0.41
1:A:176:PRO:C	1:A:178:ILE:H	2.23	0.41
1:A:88:TRP:O	1:A:89:GLU:O	2.37	0.41
2:B:120:LEU:O	2:B:121:ASP:C	2.58	0.41
1:A:317:VAL:CG1	1:A:318:TYR:N	2.82	0.41
1:A:356:ARG:HG2	1:A:358:ARG:NH1	2.36	0.41
2:B:202:ILE:O	2:B:205:LEU:N	2.53	0.41
1:A:270:ILE:HG21	1:A:314:VAL:HG21	2.03	0.41
2:B:161:GLN:CA	2:B:161:GLN:NE2	2.76	0.41
2:B:134:SER:CB	2:B:139:THR:HB	2.51	0.41
2:B:164:MET:O	2:B:167:ILE:HG12	2.21	0.41
2:B:118:VAL:HB	2:B:149:LEU:CD1	2.51	0.41
1:A:135:ILE:N	1:A:135:ILE:HD12	2.36	0.41
1:A:363:ASN:OD1	1:A:365:VAL:N	2.54	0.41
2:B:94:ILE:HG13	2:B:94:ILE:O	2.21	0.41
1:A:255:ASN:HD22	1:A:255:ASN:HA	1.53	0.41
1:A:320:ASP:OD1	1:A:323:LYS:HG3	2.20	0.41
1:A:410:TRP:CG	1:A:411:ILE:N	2.89	0.41
2:B:332:GLN:OE1	2:B:424:LYS:HG2	2.21	0.41
1:A:252:TRP:NE1	1:A:295:LEU:HD11	2.36	0.41
1:A:171:PHE:CE1	1:A:205:LEU:HA	2.56	0.40
1:A:181:TYR:CE1	3:A:999:GWB:HC	2.55	0.40
2:B:98:ALA:O	2:B:101:LYS:HG3	2.21	0.40
2:B:183:TYR:CD1	2:B:184:MET:HG2	2.56	0.40
1:A:493:VAL:HG12	1:A:494:ASN:H	1.86	0.40
2:B:149:LEU:HA	2:B:150:PRO:HD3	1.83	0.40
1:A:448:ARG:NE	1:A:473:THR:HB	2.37	0.40
2:B:201:LYS:O	2:B:204:GLU:HB3	2.22	0.40
2:B:158:ALA:O	2:B:161:GLN:HB2	2.21	0.40
1:A:42:GLU:HG2	1:A:43:LYS:HZ2	1.87	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	530/560 (95%)	462 (87%)	44 (8%)	24 (4%)	3	10
2	B	396/440 (90%)	356 (90%)	35 (9%)	5 (1%)	15	42
All	All	926/1000 (93%)	818 (88%)	79 (8%)	29 (3%)	5	18

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	GLU
1	A	112	GLY
1	A	216	THR
1	A	91	GLN
1	A	219	LYS
1	A	356	ARG
1	A	361	HIS
2	B	195	ILE
1	A	114	ALA
1	A	170	PRO
1	A	195	ILE
1	A	4	PRO
1	A	14	PRO
1	A	138	GLU
1	A	177	ASP
2	B	267	ALA
1	A	52	PRO
1	A	97	PRO
1	A	111	VAL
1	A	116	PHE
2	B	361	HIS
1	A	82	LYS
1	A	85	GLN
1	A	113	ASP
1	A	412	PRO

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Mol	Chain	Res	Type
2	B	169	GLU
1	A	225	PRO
1	A	156	SER
2	B	170	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	479/499 (96%)	434 (91%)	45 (9%)	11	29
2	B	368/400 (92%)	351 (95%)	17 (5%)	33	66
All	All	847/899 (94%)	785 (93%)	62 (7%)	17	42

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PRO
1	A	6	GLU
1	A	14	PRO
1	A	21	VAL
1	A	52	PRO
1	A	53	GLU
1	A	64	LYS
1	A	70	LYS
1	A	71	TRP
1	A	89	GLU
1	A	97	PRO
1	A	101	LYS
1	A	102	LYS
1	A	104	LYS
1	A	120	LEU
1	A	122	GLU
1	A	123	ASP
1	A	126	LYS
1	A	182	GLN

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Mol	Chain	Res	Type
1	A	195	ILE
1	A	205	LEU
1	A	219	LYS
1	A	238	LYS
1	A	248	GLU
1	A	255	ASN
1	A	279	LEU
1	A	325	LEU
1	A	340	GLN
1	A	344	GLU
1	A	345	PRO
1	A	358	ARG
1	A	368	LEU
1	A	373	GLN
1	A	386	THR
1	A	396	GLU
1	A	402	TRP
1	A	404	GLU
1	A	431	LYS
1	A	443	ASP
1	A	452	LEU
1	A	474	ASN
1	A	475	GLN
1	A	496	VAL
1	A	500	GLN
1	A	501	TYR
2	B	39	THR
2	B	40	GLU
2	B	68	SER
2	B	73	LYS
2	B	209	LEU
2	B	211	ARG
2	B	238	LYS
2	B	249	LYS
2	B	277	ARG
2	B	280	CYS
2	B	283	LEU
2	B	303	LEU
2	B	323	LYS
2	B	368	LEU
2	B	410	TRP
2	B	425	LEU

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Mol	Chain	Res	Type
2	B	429	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	182	GLN
1	A	255	ASN
1	A	278	GLN
1	A	334	GLN
1	A	336	GLN
1	A	361	HIS
1	A	475	GLN
1	A	500	GLN
2	B	57	ASN
2	B	161	GLN
2	B	175	ASN
2	B	182	GLN
2	B	197	GLN
2	B	208	HIS
2	B	332	GLN
2	B	336	GLN
2	B	361	HIS
2	B	394	GLN
2	B	428	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)

1 non-standard protein/DNA/RNA residue 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
1	CSD	A	280	1	3,7,8	0.73	0	3,8,10	3.05	1 (33%)

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
1	CSD	A	280	1	-	1/2/6/8	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	280	CSD	OD1-SG-CB	5.06	113.83	105.40

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	280	CSD	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

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).

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Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	GWB	A	999	-	19,23,23	2.24	6 (31%)	27,33,33	2.60	8 (29%)

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	GWB	A	999	-	-	0/6/12/12	0/2/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	GWB	C10-C9	2.67	1.42	1.36
3	A	999	GWB	C9-C8	2.90	1.42	1.37
3	A	999	GWB	C4-C5	2.94	1.40	1.36
3	A	999	GWB	C7-C8	3.46	1.42	1.35
3	A	999	GWB	C6-N1	4.12	1.40	1.33
3	A	999	GWB	CC-CB	5.75	1.68	1.45

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	999	GWB	CD-CC-CB	-4.42	103.97	119.38
3	A	999	GWB	C5-C6-N1	-4.29	118.32	125.18
3	A	999	GWB	CE-CC-CB	-4.13	104.98	119.38
3	A	999	GWB	C3-C2-N1	-4.09	119.72	123.45
3	A	999	GWB	C9-C8-C7	-2.65	120.44	123.51
3	A	999	GWB	O4-C4-C3	2.33	120.60	116.97
3	A	999	GWB	C8-C7-C3	2.52	120.77	118.64
3	A	999	GWB	C6-N1-C2	9.04	122.33	116.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	GWB	3	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	534/560 (95%)	-0.18	21 (3%)	43	36	26, 65, 110, 146	0
2	B	404/440 (91%)	-0.18	16 (3%)	42	34	27, 61, 111, 138	0
All	All	938/1000 (93%)	-0.18	37 (3%)	43	36	26, 63, 111, 146	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	240	THR	5.7
2	B	435	VAL	5.5
2	B	434	ILE	4.4
1	A	52	PRO	4.1
1	A	221	HIS	3.9
1	A	28	GLU	3.6
2	B	67	ASP	3.5
2	B	361	HIS	3.3
1	A	53	GLU	3.3
2	B	88	TRP	3.1
1	A	69	THR	3.0
2	B	195	ILE	3.0
1	A	472	THR	2.9
2	B	431	LYS	2.8
1	A	71	TRP	2.7
2	B	70	LYS	2.7
2	B	102	LYS	2.6
1	A	324	ASP	2.6
2	B	6	GLU	2.6
1	A	66	LYS	2.4
2	B	432	GLU	2.4
1	A	346	PHE	2.4
1	A	473	THR	2.4
1	A	311	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	284	ARG	2.3
1	A	358	ARG	2.3
1	A	92	LEU	2.3
1	A	90	VAL	2.2
2	B	104	LYS	2.1
1	A	452	LEU	2.1
1	A	72	ARG	2.1
1	A	245	VAL	2.1
1	A	446	ALA	2.0
1	A	51	GLY	2.0
2	B	177	ASP	2.0
1	A	33	ALA	2.0
2	B	87	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	CSD	A	280	8/9	0.96	0.15	-	52,60,64,66	0

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	GWB	A	999	21/21	0.95	0.20	1.09	39,45,52,56	0

6.5 Other polymers (i)

There are no such residues in this entry.