Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:10 AM GMT

PDB ID	:	3DMJ
Title	:	CRYSTAL STRUCTURE OF HIV-1 V106A and Y181C MUTANT REVERSE TRANSCRIPTASE IN COMPLEX WITH GW564511.
Authors	:	Ren, J.; Chamberlain, P.P.; Stammers, D.K.
Deposited on	:	2008-07-01
Resolution	:	2.60 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 (i) symbol.

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

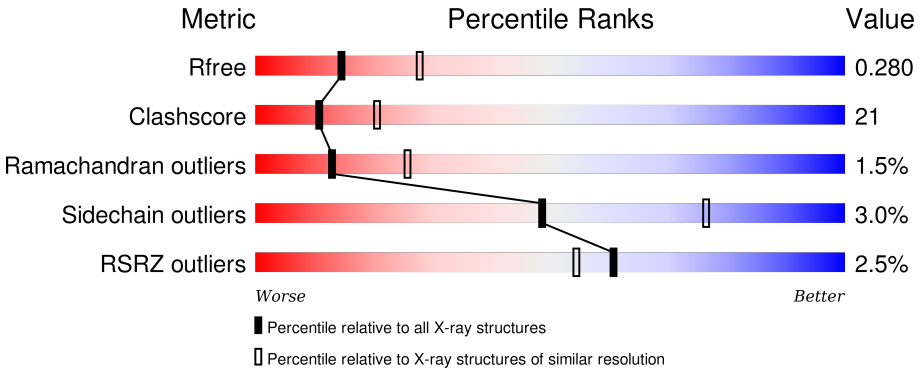
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	% 59% 33% • 5%
2	B	440	3% 56% 34% • 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7765 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	532	Total	C	N	O	S	0	0	0
			4347	2814	723	801	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	106	ALA	VAL	ENGINEERED	UNP P04585
A	181	CYS	TYR	ENGINEERED	UNP P04585

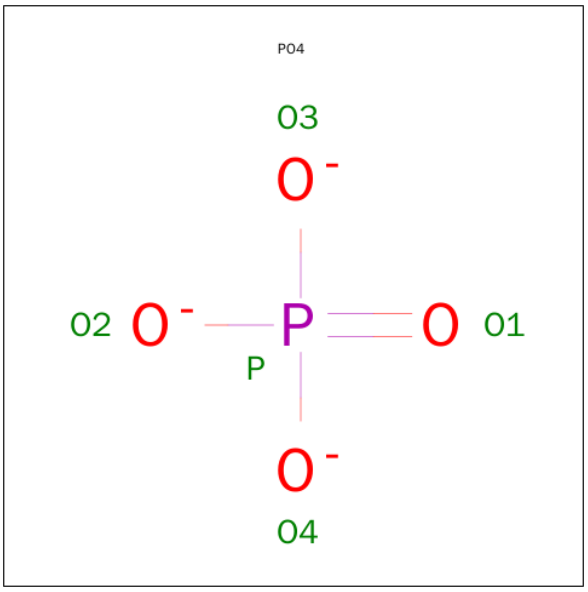
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	401	Total	C	N	O	S	0	0	0
			3309	2151	552	598	8			

There are 2 discrepancies between the modelled and reference sequences:

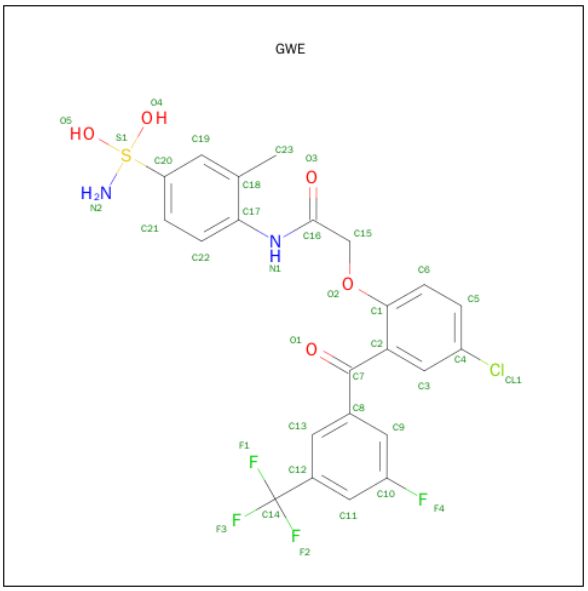
Chain	Residue	Modelled	Actual	Comment	Reference
B	106	ALA	VAL	ENGINEERED	UNP P04585
B	181	CYS	TYR	ENGINEERED	UNP P04585

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0

- Molecule 4 is N-{4-[AMINO(DIHYDROXY)-LAMBDA 4 -SULFANYL]-2-METHYLPHENYL}-2-(4-CHLORO-2-{[3-FLUORO-5-(TRIFLUOROMETHYL)PHENYL]CARBONYL}PHENOXY)ACETAMIDE (three-letter code: GWE) (formula: $C_{23}H_{19}ClF_4N_2O_5S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C Cl F N O S 36 23 1 4 2 5 1	0	0

- Molecule 5 is water.

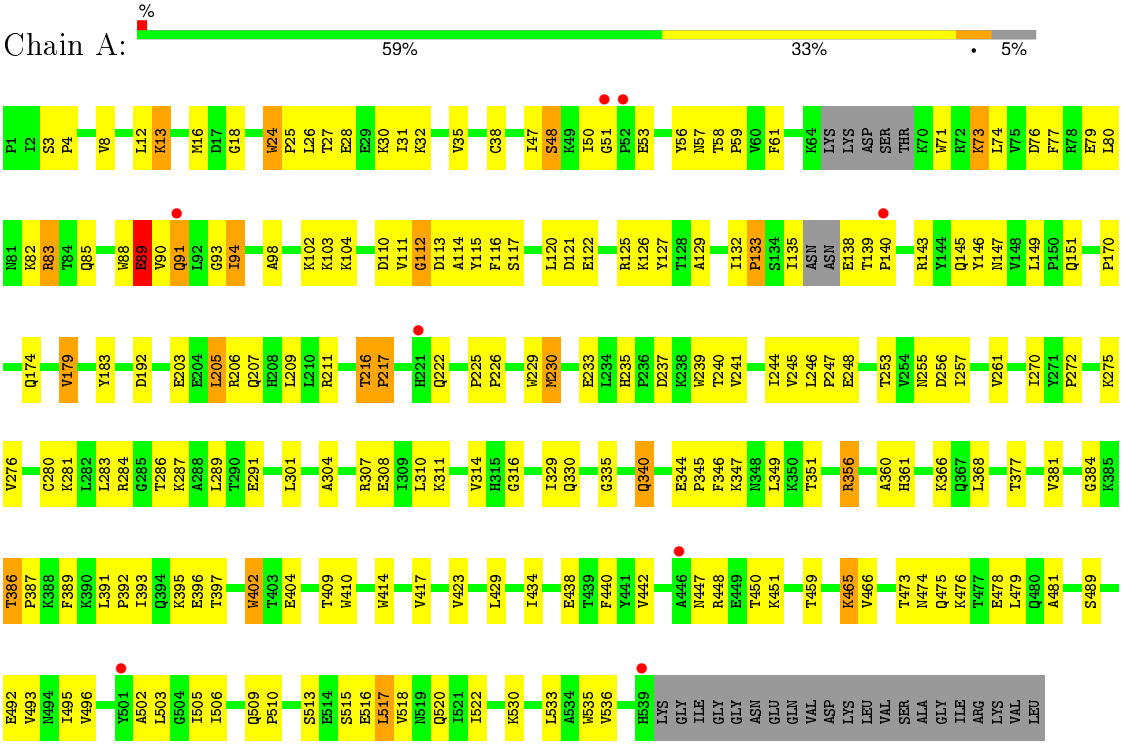
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	32	Total O 32 32	0	0
5	B	31	Total O 31 31	0	0

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.

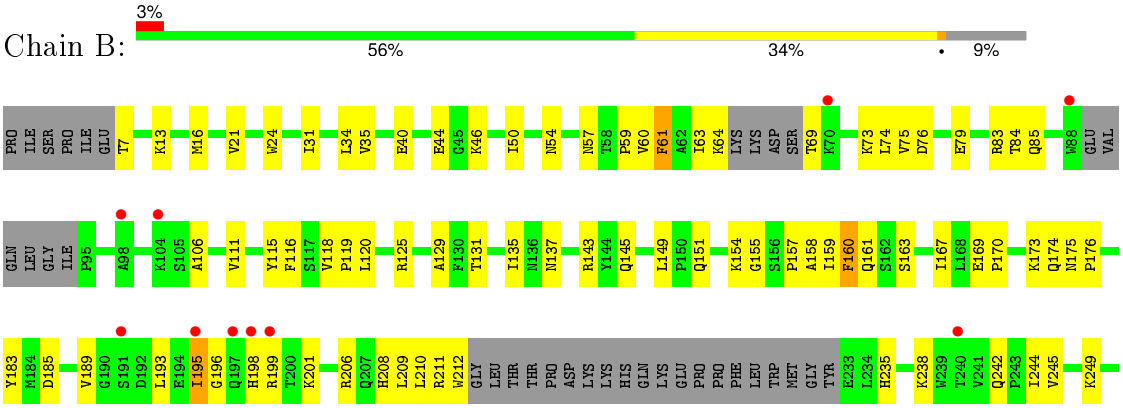
- Molecule 1: Reverse transcriptase/ribonuclease H

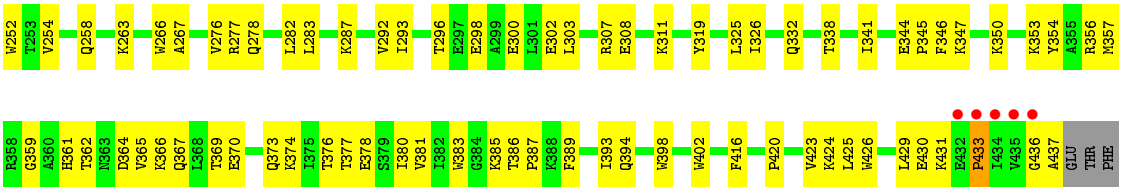
Chain A:



- Molecule 2: p51 RT

Chain B:




W252 T253 V254 Q258 K263 W266 A267 V276 R277 Q278 L282 L283 K287 V292 I293 T296 E297 E298 A299 E300 L301 E302 L303 R307 E308 K311 Y319 L325 I326 Q332 T338 I341 E344 P345 F346 K347 K350 K353 Y354 A355 R356 M357
R358 G359 A360 H361 T362 N363 D364 V365 K366 Q367 L368 T369 E370 Q373 K374 I375 T376 T377 E378 S379 I380 V381 I382 W383 G384 K385 T386 P387 K388 F389 I393 Q394 W398 W402 F416 P420 V423 K424 L425 W426 L429 E430 K431 E432 P433 I434 V435 G436 A437 GLU THR PHE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	137.19Å 108.99Å 71.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.78 – 2.60 29.78 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.78-2.60) 99.9 (29.78-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.197 , 0.284 0.199 , 0.280	Depositor DCC
R_{free} test set	1679 reflections (5.22%)	DCC
Wilson B-factor (Å^2)	55.5	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 59.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	1 of 33834 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7765	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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: GWE, CSD, PO4

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	0.39	0/4453	0.64	0/6051
2	B	0.39	0/3401	0.63	0/4618
All	All	0.39	0/7854	0.63	0/10669

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	183	TYR	Sidechain

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	4347	0	4390	189	0
2	B	3309	0	3340	148	0
3	A	5	0	0	0	0
3	B	5	0	0	1	0
4	A	36	0	17	0	0
5	A	32	0	0	1	0
5	B	31	0	0	3	0
All	All	7765	0	7747	326	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 21.

All (326) 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:353:LYS:HE3	2:B:430:GLU:HB3	1.31	1.12
2:B:235:HIS:HB2	2:B:238:LYS:HD2	1.47	0.94
1:A:448:ARG:NH2	1:A:475:GLN:H	1.67	0.93
1:A:115:TYR:HB2	1:A:151:GLN:HE21	1.37	0.89
1:A:217:PRO:HB2	1:A:222:GLN:HE21	1.42	0.84
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.62	0.82
2:B:79:GLU:O	2:B:83:ARG:HG3	1.78	0.82
1:A:79:GLU:O	1:A:83:ARG:HD2	1.80	0.81
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.63	0.81
1:A:270:ILE:HG22	1:A:314:VAL:HG11	1.62	0.80
1:A:115:TYR:HB2	1:A:151:GLN:NE2	1.98	0.79
2:B:59:PRO:HG2	2:B:76:ASP:HB3	1.63	0.79
2:B:332:GLN:NE2	2:B:424:LYS:HE2	1.98	0.79
1:A:112:GLY:C	1:A:114:ALA:H	1.85	0.78
2:B:161:GLN:HA	2:B:161:GLN:NE2	2.02	0.73
2:B:195:ILE:HG13	2:B:196:GLY:H	1.54	0.72
1:A:518:VAL:O	1:A:522:ILE:HG13	1.90	0.72
2:B:63:ILE:HD13	2:B:74:LEU:HD22	1.72	0.72
2:B:73:LYS:HB3	2:B:73:LYS:NZ	2.05	0.71
1:A:393:ILE:HB	1:A:423:VAL:HG13	1.69	0.71
2:B:278:GLN:HG3	2:B:298:GLU:HB3	1.73	0.71
1:A:244:ILE:HB	1:A:310:LEU:HD13	1.73	0.71
1:A:206:ARG:HG2	1:A:216:THR:HG21	1.72	0.71
1:A:112:GLY:O	1:A:114:ALA:N	2.24	0.71
1:A:492:GLU:HG2	1:A:530:LYS:HB2	1.71	0.71
1:A:393:ILE:HB	1:A:423:VAL:CG1	2.19	0.70
1:A:217:PRO:HB2	1:A:222:GLN:NE2	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:ILE:HB	2:B:199:ARG:HH12	1.56	0.70
2:B:46:LYS:HD3	2:B:116:PHE:HD2	1.56	0.69
1:A:448:ARG:NE	1:A:474:ASN:H	1.89	0.69
1:A:465:LYS:HG3	1:A:466:VAL:N	2.06	0.69
1:A:24:TRP:HD1	1:A:25:PRO:HD2	1.57	0.68
1:A:73:LYS:HB2	1:A:73:LYS:NZ	2.08	0.68
2:B:158:ALA:O	2:B:161:GLN:HB2	1.93	0.68
1:A:89:GLU:O	1:A:91:GLN:N	2.27	0.67
1:A:366:LYS:NZ	2:B:394:GLN:NE2	2.41	0.67
2:B:155:GLY:O	2:B:159:ILE:HG12	1.95	0.67
2:B:195:ILE:HB	2:B:199:ARG:NH1	2.10	0.66
2:B:151:GLN:HG3	5:B:1004:HOH:O	1.96	0.66
1:A:239:TRP:CZ2	1:A:316:GLY:HA3	2.30	0.66
1:A:114:ALA:HA	1:A:117:SER:OG	1.96	0.66
2:B:54:ASN:O	2:B:143:ARG:NH2	2.29	0.65
1:A:448:ARG:HE	1:A:473:THR:HB	1.62	0.64
2:B:175:ASN:ND2	2:B:201:LYS:NZ	2.44	0.64
2:B:308:GLU:OE1	2:B:311:LYS:HD2	1.98	0.64
1:A:272:PRO:HA	5:A:1038:HOH:O	1.98	0.64
2:B:175:ASN:HD22	2:B:201:LYS:NZ	1.96	0.63
1:A:409:THR:O	2:B:364:ASP:HB2	1.99	0.63
1:A:31:ILE:O	1:A:35:VAL:HG23	1.98	0.63
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.34	0.63
1:A:103:LYS:HE3	1:A:179:VAL:HG11	1.81	0.63
1:A:88:TRP:CE3	1:A:88:TRP:HA	2.34	0.62
1:A:366:LYS:HZ1	2:B:394:GLN:HE21	1.48	0.62
1:A:392:PRO:O	1:A:423:VAL:HG12	2.00	0.62
2:B:356:ARG:HH11	2:B:356:ARG:HG3	1.65	0.61
1:A:112:GLY:C	1:A:114:ALA:N	2.54	0.61
2:B:420:PRO:HB2	2:B:423:VAL:HG23	1.81	0.61
2:B:13:LYS:HB2	2:B:16:MET:HG3	1.83	0.61
2:B:356:ARG:HB2	2:B:367:GLN:HG2	1.82	0.61
2:B:376:THR:O	2:B:380:ILE:HG13	2.01	0.61
1:A:206:ARG:HH11	1:A:216:THR:CG2	2.13	0.60
1:A:448:ARG:HH21	1:A:475:GLN:H	1.44	0.60
2:B:111:VAL:HG22	2:B:185:ASP:O	2.00	0.60
2:B:249:LYS:HB2	2:B:252:TRP:CE2	2.36	0.60
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.37	0.60
1:A:50:ILE:CG2	1:A:145:GLN:HG2	2.31	0.60
1:A:28:GLU:HA	1:A:135:ILE:HD11	1.84	0.60
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:LYS:HB2	1:A:82:LYS:NZ	2.17	0.60
2:B:157:PRO:HD3	5:B:1016:HOH:O	2.00	0.59
1:A:442:VAL:HG22	1:A:496:VAL:O	2.03	0.59
1:A:479:LEU:HB2	1:A:517:LEU:HD13	1.83	0.59
1:A:126:LYS:HE2	1:A:127:TYR:CZ	2.38	0.59
2:B:254:VAL:O	2:B:258:GLN:HG3	2.01	0.59
2:B:167:ILE:HG22	2:B:212:TRP:CZ2	2.37	0.59
1:A:30:LYS:HE2	1:A:71:TRP:CZ3	2.38	0.58
1:A:116:PHE:HE2	1:A:146:TYR:HE1	1.52	0.58
1:A:50:ILE:HG21	1:A:145:GLN:HG2	1.85	0.58
1:A:344:GLU:HB2	1:A:347:LYS:HD2	1.84	0.58
1:A:206:ARG:HH11	1:A:216:THR:HG23	1.69	0.58
1:A:28:GLU:O	1:A:32:LYS:HB2	2.04	0.58
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.04	0.58
2:B:263:LYS:HD3	2:B:429:LEU:HD21	1.86	0.58
1:A:27:THR:O	1:A:31:ILE:HG13	2.03	0.58
2:B:106:ALA:HA	2:B:189:VAL:O	2.03	0.58
1:A:335:GLY:HA3	1:A:356:ARG:HD3	1.85	0.58
2:B:173:LYS:O	2:B:176:PRO:HD3	2.03	0.57
2:B:175:ASN:HD22	2:B:201:LYS:HZ2	1.53	0.57
1:A:26:LEU:HD12	1:A:133:PRO:HG2	1.85	0.57
2:B:57:ASN:HA	2:B:129:ALA:O	2.05	0.57
2:B:235:HIS:CB	2:B:238:LYS:HD2	2.27	0.57
1:A:366:LYS:HZ1	2:B:394:GLN:NE2	2.02	0.57
1:A:24:TRP:CD1	1:A:25:PRO:HD2	2.39	0.56
1:A:502:ALA:HA	1:A:505:ILE:HD12	1.88	0.56
2:B:169:GLU:HB2	2:B:170:PRO:HD3	1.87	0.56
2:B:235:HIS:HB2	2:B:238:LYS:CD	2.27	0.56
2:B:361:HIS:HB3	5:B:1013:HOH:O	2.06	0.56
2:B:120:LEU:HD23	2:B:125:ARG:HG2	1.87	0.56
1:A:503:LEU:HD13	1:A:535:TRP:CG	2.41	0.56
1:A:402:TRP:CZ2	2:B:362:THR:HA	2.40	0.56
1:A:448:ARG:CZ	1:A:474:ASN:H	2.19	0.56
1:A:335:GLY:HA3	1:A:356:ARG:CD	2.35	0.56
1:A:206:ARG:HH12	1:A:222:GLN:NE2	2.03	0.56
1:A:434:ILE:HD13	1:A:530:LYS:HB3	1.88	0.55
1:A:16:MET:HE2	1:A:83:ARG:HG3	1.89	0.55
2:B:161:GLN:HA	2:B:161:GLN:HE21	1.68	0.55
1:A:31:ILE:HD12	1:A:135:ILE:HD13	1.88	0.55
1:A:138:GLU:HG2	1:A:139:THR:N	2.21	0.55
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.47	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:ILE:O	2:B:35:VAL:HG23	2.07	0.54
2:B:353:LYS:CE	2:B:430:GLU:HB3	2.21	0.54
1:A:384:GLY:HA3	2:B:135:ILE:HD12	1.89	0.54
1:A:53:GLU:CD	1:A:53:GLU:H	2.10	0.54
1:A:366:LYS:HZ2	2:B:394:GLN:HE22	1.55	0.54
1:A:346:PHE:N	1:A:346:PHE:CD2	2.75	0.54
2:B:425:LEU:O	2:B:429:LEU:HD13	2.07	0.54
1:A:366:LYS:HZ2	2:B:394:GLN:NE2	2.06	0.53
2:B:376:THR:CG2	2:B:386:THR:HG22	2.38	0.53
1:A:402:TRP:CH2	2:B:362:THR:HA	2.42	0.53
2:B:356:ARG:NH1	2:B:357:MET:O	2.41	0.53
2:B:57:ASN:HD22	2:B:143:ARG:NH1	2.06	0.53
2:B:195:ILE:CB	2:B:199:ARG:HH12	2.20	0.53
2:B:73:LYS:HB3	2:B:73:LYS:HZ3	1.73	0.53
2:B:57:ASN:HD22	2:B:143:ARG:HH11	1.57	0.53
2:B:60:VAL:HG23	2:B:75:VAL:HG22	1.89	0.53
2:B:350:LYS:HE3	2:B:378:GLU:OE1	2.09	0.53
1:A:74:LEU:C	1:A:74:LEU:HD23	2.28	0.53
1:A:308:GLU:HA	1:A:311:LYS:CE	2.39	0.53
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.91	0.52
2:B:159:ILE:C	2:B:161:GLN:H	2.13	0.52
2:B:245:VAL:HG23	2:B:431:LYS:HB2	1.90	0.52
1:A:73:LYS:HB2	1:A:73:LYS:HZ2	1.74	0.52
2:B:356:ARG:HG3	2:B:356:ARG:NH1	2.22	0.52
2:B:433:PRO:HB3	2:B:436:GLY:O	2.10	0.52
1:A:473:THR:OG1	1:A:476:LYS:HG3	2.10	0.52
1:A:479:LEU:CB	1:A:517:LEU:HD13	2.40	0.52
1:A:255:ASN:HD22	1:A:289:LEU:HB3	1.74	0.52
2:B:208:HIS:O	2:B:211:ARG:HG2	2.10	0.52
2:B:206:ARG:O	2:B:210:LEU:N	2.41	0.52
2:B:359:GLY:H	3:B:1300:PO4:P	2.31	0.52
2:B:34:LEU:CD2	2:B:73:LYS:HG3	2.40	0.52
2:B:73:LYS:HZ2	2:B:73:LYS:HB3	1.74	0.51
1:A:58:THR:HG23	1:A:59:PRO:HD2	1.91	0.51
2:B:277:ARG:HB3	2:B:277:ARG:CZ	2.39	0.51
1:A:115:TYR:O	1:A:149:LEU:HB2	2.10	0.51
2:B:278:GLN:NE2	2:B:278:GLN:HA	2.25	0.51
2:B:46:LYS:HD3	2:B:116:PHE:CD2	2.43	0.51
2:B:366:LYS:O	2:B:370:GLU:HG3	2.11	0.51
2:B:369:THR:O	2:B:373:GLN:HG3	2.10	0.51
1:A:356:ARG:HG2	1:A:356:ARG:HH11	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:THR:HB	1:A:140:PRO:CD	2.40	0.51
2:B:266:TRP:HZ3	2:B:426:TRP:CD1	2.29	0.51
1:A:206:ARG:HH22	1:A:222:GLN:NE2	2.09	0.51
1:A:51:GLY:HA3	1:A:53:GLU:OE1	2.10	0.51
2:B:245:VAL:CG2	2:B:431:LYS:HB2	2.40	0.51
1:A:516:GLU:O	1:A:520:GLN:HG3	2.11	0.51
1:A:257:ILE:O	1:A:261:VAL:HG23	2.11	0.51
1:A:206:ARG:CG	1:A:216:THR:HG21	2.41	0.50
2:B:211:ARG:HG3	2:B:212:TRP:CD1	2.46	0.50
1:A:116:PHE:CE2	1:A:146:TYR:HE1	2.28	0.50
1:A:308:GLU:HA	1:A:311:LYS:HE2	1.93	0.50
1:A:206:ARG:NH1	1:A:216:THR:HG23	2.26	0.50
2:B:244:ILE:HG13	2:B:426:TRP:CZ2	2.45	0.50
1:A:270:ILE:HG22	1:A:314:VAL:CG1	2.39	0.50
2:B:292:VAL:O	2:B:293:ILE:HD13	2.12	0.50
1:A:225:PRO:HA	1:A:226:PRO:C	2.32	0.50
1:A:377:THR:O	1:A:381:VAL:HG23	2.12	0.50
1:A:38:CYS:O	1:A:47:ILE:HD11	2.12	0.50
2:B:34:LEU:HD22	2:B:73:LYS:HG3	1.94	0.50
1:A:183:TYR:CD1	1:A:229:TRP:HH2	2.29	0.50
1:A:58:THR:HG23	1:A:76:ASP:O	2.12	0.50
1:A:205:LEU:HD22	1:A:209:LEU:HG	1.93	0.50
2:B:115:TYR:HB3	2:B:149:LEU:CB	2.40	0.49
2:B:354:TYR:OH	2:B:357:MET:HG2	2.12	0.49
2:B:365:VAL:O	2:B:369:THR:HG23	2.11	0.49
1:A:104:LYS:HD2	1:A:192:ASP:O	2.12	0.49
1:A:515:SER:HB3	1:A:518:VAL:HG23	1.94	0.49
1:A:122:GLU:CD	1:A:122:GLU:H	2.16	0.49
2:B:332:GLN:HG3	2:B:338:THR:HG23	1.94	0.49
1:A:88:TRP:HE3	1:A:88:TRP:HA	1.74	0.49
2:B:266:TRP:CZ3	2:B:426:TRP:CG	3.00	0.49
1:A:489:SER:HB2	1:A:493:VAL:HB	1.93	0.49
1:A:448:ARG:NE	1:A:473:THR:HB	2.27	0.49
2:B:356:ARG:CB	2:B:367:GLN:HG2	2.42	0.49
1:A:417:VAL:O	1:A:417:VAL:HG13	2.12	0.49
1:A:248:GLU:OE2	1:A:248:GLU:HA	2.12	0.49
1:A:83:ARG:HH11	1:A:83:ARG:HG2	1.77	0.49
1:A:402:TRP:CD1	1:A:402:TRP:C	2.85	0.49
1:A:57:ASN:HA	1:A:129:ALA:O	2.13	0.48
1:A:438:GLU:HG2	1:A:459:THR:HB	1.94	0.48
1:A:239:TRP:CE2	1:A:316:GLY:HA3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:GLU:HB2	1:A:240:THR:OG1	2.12	0.48
1:A:448:ARG:HH11	1:A:448:ARG:HG3	1.79	0.48
1:A:73:LYS:HB2	1:A:73:LYS:HZ3	1.79	0.48
1:A:335:GLY:O	1:A:356:ARG:HA	2.12	0.48
2:B:64:LYS:HD2	2:B:69:THR:HG22	1.95	0.48
2:B:326:ILE:O	2:B:341:ILE:HA	2.12	0.48
2:B:151:GLN:HB3	2:B:185:ASP:OD1	2.14	0.48
2:B:436:GLY:O	2:B:437:ALA:HB2	2.12	0.48
1:A:253:THR:HG23	1:A:256:ASP:OD2	2.14	0.48
1:A:30:LYS:HE2	1:A:71:TRP:CH2	2.48	0.48
2:B:319:TYR:HE2	2:B:325:LEU:HD13	1.79	0.48
1:A:448:ARG:HE	1:A:473:THR:CB	2.25	0.48
1:A:515:SER:HB3	1:A:518:VAL:CG2	2.44	0.48
1:A:170:PRO:O	1:A:174:GLN:HG3	2.14	0.48
2:B:235:HIS:O	2:B:238:LYS:HG2	2.14	0.47
1:A:536:VAL:HG12	2:B:258:GLN:HB3	1.96	0.47
1:A:48:SER:O	1:A:50:ILE:HG23	2.14	0.47
1:A:211:ARG:HG2	1:A:211:ARG:HH11	1.79	0.47
2:B:332:GLN:HE22	2:B:424:LYS:HE2	1.79	0.47
2:B:325:LEU:HD22	2:B:385:LYS:HD2	1.95	0.47
1:A:98:ALA:HB2	1:A:349:LEU:O	2.14	0.47
2:B:345:PRO:O	2:B:346:PHE:HB2	2.15	0.47
1:A:478:GLU:O	1:A:481:ALA:HB3	2.15	0.47
2:B:170:PRO:O	2:B:174:GLN:HG3	2.15	0.47
2:B:160:PHE:CD1	2:B:160:PHE:O	2.68	0.47
1:A:110:ASP:O	1:A:217:PRO:HD3	2.15	0.46
2:B:282:LEU:HD21	2:B:296:THR:HG23	1.98	0.46
1:A:94:ILE:CD1	1:A:230:MET:HG2	2.45	0.46
2:B:319:TYR:OH	2:B:385:LYS:HE3	2.16	0.46
1:A:237:ASP:N	1:A:237:ASP:OD2	2.47	0.46
1:A:360:ALA:O	1:A:513:SER:HB2	2.16	0.46
1:A:393:ILE:CB	1:A:423:VAL:HG13	2.42	0.46
1:A:203:GLU:HG3	1:A:207:GLN:HE21	1.81	0.46
1:A:111:VAL:O	1:A:114:ALA:HB3	2.16	0.46
1:A:396:GLU:HG3	1:A:397:THR:N	2.29	0.46
1:A:356:ARG:HG2	1:A:356:ARG:NH1	2.30	0.46
1:A:98:ALA:HB1	1:A:349:LEU:HB3	1.97	0.46
1:A:102:LYS:HE2	1:A:237:ASP:HA	1.98	0.46
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.98	0.46
1:A:226:PRO:HB3	1:A:235:HIS:ND1	2.32	0.45
2:B:393:ILE:O	2:B:416:PHE:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:376:THR:HG23	2:B:386:THR:HG22	1.98	0.45
1:A:255:ASN:ND2	1:A:289:LEU:HD13	2.31	0.45
1:A:115:TYR:CB	1:A:151:GLN:NE2	2.75	0.45
1:A:58:THR:CG2	1:A:76:ASP:O	2.65	0.45
1:A:448:ARG:HE	1:A:473:THR:CA	2.29	0.45
2:B:199:ARG:HG3	2:B:199:ARG:HH11	1.82	0.45
2:B:344:GLU:HB2	2:B:347:LYS:HD2	1.97	0.45
2:B:175:ASN:HD21	2:B:201:LYS:CE	2.30	0.45
2:B:40:GLU:O	2:B:44:GLU:HG3	2.17	0.45
1:A:16:MET:HE2	1:A:83:ARG:CG	2.47	0.44
1:A:434:ILE:CD1	1:A:530:LYS:HB3	2.46	0.44
1:A:139:THR:HB	1:A:140:PRO:HD2	2.00	0.44
2:B:325:LEU:HD21	2:B:383:TRP:CE3	2.52	0.44
1:A:93:GLY:O	2:B:137:ASN:HB3	2.17	0.44
1:A:492:GLU:HA	1:A:530:LYS:O	2.18	0.44
1:A:301:LEU:O	1:A:304:ALA:HB3	2.18	0.44
2:B:266:TRP:HZ3	2:B:426:TRP:CG	2.36	0.44
2:B:201:LYS:HD3	2:B:201:LYS:HA	1.85	0.44
2:B:369:THR:HG22	2:B:398:TRP:CZ3	2.51	0.44
1:A:429:LEU:CD1	1:A:506:ILE:HA	2.48	0.44
2:B:195:ILE:O	2:B:198:HIS:HB3	2.17	0.44
2:B:161:GLN:CA	2:B:161:GLN:NE2	2.72	0.43
2:B:31:ILE:HD12	2:B:135:ILE:CD1	2.48	0.43
1:A:440:PHE:CD2	1:A:459:THR:HG22	2.53	0.43
1:A:3:SER:HA	1:A:4:PRO:HD3	1.80	0.43
1:A:56:TYR:O	1:A:143:ARG:NH2	2.52	0.43
1:A:276:VAL:O	1:A:280:CSD:HB3	2.17	0.43
1:A:346:PHE:N	1:A:346:PHE:HD2	2.16	0.43
1:A:329:ILE:HD12	1:A:391:LEU:CD2	2.48	0.43
2:B:118:VAL:HB	2:B:149:LEU:HG	2.00	0.43
2:B:116:PHE:H	2:B:116:PHE:HD1	1.67	0.43
1:A:58:THR:CG2	1:A:59:PRO:HD2	2.49	0.43
2:B:242:GLN:OE1	2:B:242:GLN:HA	2.18	0.43
1:A:110:ASP:HB3	1:A:217:PRO:HG3	2.00	0.43
2:B:61:PHE:CD2	2:B:61:PHE:N	2.85	0.43
1:A:287:LYS:HG2	1:A:291:GLU:OE2	2.19	0.43
2:B:167:ILE:HG22	2:B:212:TRP:CH2	2.53	0.43
2:B:374:LYS:O	2:B:378:GLU:HG3	2.19	0.43
1:A:440:PHE:CG	1:A:459:THR:HG22	2.54	0.43
2:B:57:ASN:ND2	2:B:131:THR:OG1	2.52	0.43
1:A:31:ILE:HD12	1:A:135:ILE:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:398:TRP:O	2:B:402:TRP:HD1	2.02	0.43
2:B:426:TRP:O	2:B:429:LEU:HB2	2.19	0.43
1:A:12:LEU:O	1:A:13:LYS:O	2.37	0.43
2:B:50:ILE:CG2	2:B:145:GLN:HG2	2.49	0.42
1:A:448:ARG:NH2	1:A:475:GLN:N	2.50	0.42
1:A:502:ALA:O	1:A:506:ILE:HG13	2.19	0.42
1:A:283:LEU:O	1:A:286:THR:HG23	2.19	0.42
2:B:338:THR:HG22	2:B:353:LYS:HG2	2.01	0.42
2:B:154:LYS:O	2:B:157:PRO:HD2	2.19	0.42
1:A:77:PHE:CD2	1:A:80:LEU:HD23	2.54	0.42
1:A:246:LEU:O	1:A:307:ARG:NH1	2.47	0.42
1:A:18:GLY:HA3	1:A:56:TYR:CD1	2.54	0.42
1:A:245:VAL:HG23	1:A:245:VAL:O	2.20	0.42
1:A:329:ILE:HD12	1:A:391:LEU:HD22	2.01	0.42
1:A:116:PHE:HE2	1:A:146:TYR:CE1	2.35	0.42
2:B:287:LYS:HD3	2:B:293:ILE:HD11	2.01	0.42
1:A:211:ARG:HG2	1:A:211:ARG:NH1	2.34	0.42
2:B:116:PHE:CD1	2:B:116:PHE:N	2.87	0.42
2:B:267:ALA:HB2	2:B:426:TRP:CZ3	2.55	0.42
1:A:8:VAL:O	1:A:121:ASP:HB2	2.20	0.42
1:A:59:PRO:HG2	1:A:76:ASP:HB3	2.01	0.41
2:B:63:ILE:HD13	2:B:74:LEU:CD2	2.45	0.41
2:B:116:PHE:HZ	2:B:151:GLN:HE21	1.67	0.41
1:A:495:ILE:HB	1:A:533:LEU:HD23	2.02	0.41
2:B:276:VAL:HA	2:B:302:GLU:OE2	2.20	0.41
1:A:281:LYS:O	1:A:284:ARG:HG3	2.20	0.41
1:A:206:ARG:HH22	1:A:222:GLN:CD	2.23	0.41
2:B:377:THR:O	2:B:381:VAL:HG23	2.20	0.41
1:A:120:LEU:HD23	1:A:125:ARG:HG2	2.02	0.41
1:A:246:LEU:HA	1:A:247:PRO:HD2	1.85	0.41
2:B:303:LEU:O	2:B:307:ARG:HG3	2.19	0.41
1:A:24:TRP:HE3	1:A:61:PHE:CZ	2.38	0.41
2:B:84:THR:HB	2:B:154:LYS:HE2	2.02	0.41
2:B:163:SER:O	2:B:167:ILE:HG12	2.20	0.41
1:A:509:GLN:N	1:A:510:PRO:CD	2.84	0.41
1:A:340:GLN:CB	1:A:351:THR:HG22	2.48	0.41
1:A:329:ILE:HG22	1:A:330:GLN:N	2.36	0.41
2:B:175:ASN:ND2	2:B:201:LYS:CE	2.83	0.41
1:A:389:PHE:HB2	1:A:414:TRP:HB3	2.03	0.41
1:A:442:VAL:HB	1:A:481:ALA:HB1	2.03	0.41
1:A:345:PRO:O	1:A:346:PHE:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:TYR:CB	1:A:151:GLN:HE21	2.21	0.40
2:B:60:VAL:HG22	2:B:61:PHE:N	2.36	0.40
1:A:94:ILE:HD11	1:A:230:MET:HG2	2.04	0.40
1:A:409:THR:O	1:A:410:TRP:HB2	2.21	0.40
2:B:206:ARG:O	2:B:209:LEU:N	2.54	0.40
1:A:386:THR:HA	1:A:387:PRO:HD3	1.72	0.40
1:A:451:LYS:HE2	1:A:451:LYS:HB3	1.84	0.40
1:A:26:LEU:HD12	1:A:133:PRO:CG	2.51	0.40
2:B:135:ILE:H	2:B:135:ILE:HG12	1.73	0.40
2:B:287:LYS:HD3	2:B:293:ILE:CD1	2.51	0.40
2:B:344:GLU:CB	2:B:347:LYS:HD2	2.51	0.40
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.57	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	525/560 (94%)	486 (93%)	28 (5%)	11 (2%)	9 16
2	B	393/440 (89%)	364 (93%)	26 (7%)	3 (1%)	24 46
All	All	918/1000 (92%)	850 (93%)	54 (6%)	14 (2%)	13 26

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	VAL
1	A	113	ASP
2	B	195	ILE
1	A	91	GLN
1	A	133	PRO
1	A	85	GLN

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Mol	Chain	Res	Type
1	A	361	HIS
1	A	89	GLU
1	A	217	PRO
1	A	356	ARG
2	B	160	PHE
2	B	85	GLN
1	A	13	LYS
1	A	112	GLY

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	475/498 (95%)	456 (96%)	19 (4%)	38 67
2	B	363/399 (91%)	357 (98%)	6 (2%)	68 88
All	All	838/897 (93%)	813 (97%)	25 (3%)	48 76

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	TRP
1	A	48	SER
1	A	73	LYS
1	A	83	ARG
1	A	89	GLU
1	A	94	ILE
1	A	179	VAL
1	A	205	LEU
1	A	216	THR
1	A	230	MET
1	A	241	VAL
1	A	275	LYS
1	A	340	GLN
1	A	368	LEU
1	A	386	THR

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Mol	Chain	Res	Type
1	A	402	TRP
1	A	404	GLU
1	A	465	LYS
1	A	517	LEU
2	B	24	TRP
2	B	61	PHE
2	B	193	LEU
2	B	283	LEU
2	B	300	GLU
2	B	433	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	151	GLN
1	A	207	GLN
1	A	222	GLN
1	A	242	GLN
1	A	255	ASN
1	A	278	GLN
1	A	336	GLN
1	A	475	GLN
1	A	487	GLN
1	A	500	GLN
1	A	519	ASN
1	A	520	GLN
2	B	57	ASN
2	B	137	ASN
2	B	161	GLN
2	B	174	GLN
2	B	175	ASN
2	B	182	GLN
2	B	197	GLN
2	B	269	GLN
2	B	278	GLN
2	B	332	GLN
2	B	394	GLN
2	B	428	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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	0.88	0	3,8,10	1.31	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
1	CSD	A	280	1	-	0/2/6/8	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

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
1	A	280	CSD	1	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

3 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	PO4	A	1301	-	4,4,4	1.13	0	6,6,6	0.27	0
4	GWE	A	999	-	35,38,38	2.68	10 (28%)	50,57,57	1.31	9 (18%)
3	PO4	B	1300	-	4,4,4	1.10	0	6,6,6	0.27	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	PO4	A	1301	-	-	0/0/0/0	0/0/0/0
4	GWE	A	999	-	-	0/25/29/29	0/3/3/3
3	PO4	B	1300	-	-	0/0/0/0	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	GWE	C19-C18	-3.35	1.34	1.39
4	A	999	GWE	C11-C10	2.03	1.41	1.37
4	A	999	GWE	C9-C8	2.48	1.43	1.39
4	A	999	GWE	C9-C10	2.99	1.42	1.37
4	A	999	GWE	C19-C20	4.64	1.49	1.39
4	A	999	GWE	C21-C22	5.12	1.48	1.38
4	A	999	GWE	C5-C6	5.84	1.49	1.38
4	A	999	GWE	C2-C1	5.88	1.51	1.40
4	A	999	GWE	C3-C4	5.90	1.48	1.38
4	A	999	GWE	C17-C18	6.23	1.51	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	999	GWE	C11-C10-C9	-2.51	120.21	123.52
4	A	999	GWE	O2-C15-C16	-2.38	103.89	110.83
4	A	999	GWE	O1-C7-C8	-2.36	116.35	120.12
4	A	999	GWE	C1-C2-C7	-2.32	118.90	122.78
4	A	999	GWE	C22-C17-C18	-2.32	118.02	120.67
4	A	999	GWE	F2-C14-C12	-2.16	108.33	112.95
4	A	999	GWE	C3-C2-C7	2.02	122.52	118.23
4	A	999	GWE	C15-O2-C1	2.07	122.30	117.58
4	A	999	GWE	C2-C7-C8	3.14	124.83	119.47

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	B	1300	PO4	1	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

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	531/560 (94%)	-0.31	8 (1%) 76 71	25, 56, 96, 137	0
2	B	401/440 (91%)	-0.18	15 (3%) 45 37	29, 53, 98, 123	0
All	All	932/1000 (93%)	-0.26	23 (2%) 61 54	25, 55, 98, 137	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	52	PRO	4.3
2	B	195	ILE	4.1
1	A	221	HIS	3.5
2	B	432	GLU	3.3
2	B	198	HIS	3.0
2	B	436	GLY	2.9
1	A	51	GLY	2.9
2	B	191	SER	2.7
2	B	434	ILE	2.5
2	B	240	THR	2.5
2	B	435	VAL	2.4
2	B	104	LYS	2.4
2	B	433	PRO	2.3
1	A	91	GLN	2.3
1	A	501	TYR	2.3
2	B	197	GLN	2.3
1	A	539	HIS	2.2
1	A	446	ALA	2.2
2	B	88	TRP	2.2
2	B	70	LYS	2.1
1	A	140	PRO	2.0
2	B	98	ALA	2.0
2	B	199	ARG	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, 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
1	CSD	A	280	8/9	0.93	0.14	-	45,53,58,72	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, 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	PO4	B	1300	5/5	0.84	0.23	0.51	123,126,136,137	0
4	GWE	A	999	36/36	0.97	0.14	-0.16	26,44,59,81	0
3	PO4	A	1301	5/5	0.92	0.14	-0.23	116,123,130,134	0

6.5 Other polymers (i)

There are no such residues in this entry.