Full wwPDB X-ray Structure Validation Report (i)

PDB ID	:	1S1T
Title	:	Crystal structure of L100I mutant HIV-1 reverse transcriptase in complex with UC-781
Authors	:	Ren, J.; Nichols, C.E.; Chamberlain, P.P.; Stammers, D.K.
Deposited on	:	2004-01-07
Resolution	:	2.40 Å(reported)

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

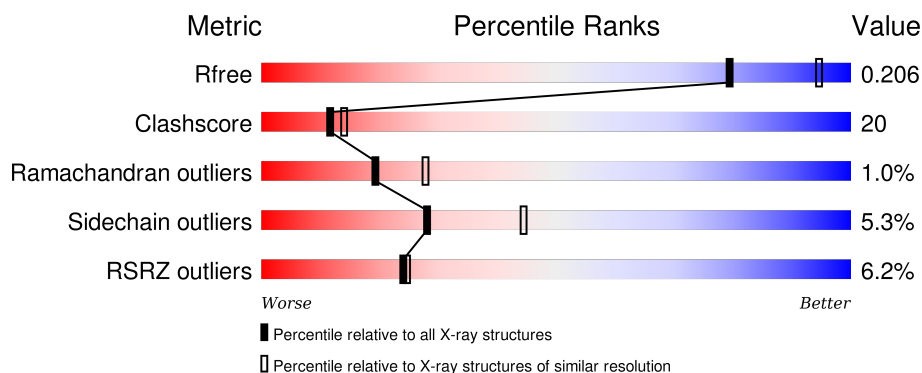|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.40 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		0.206
Clashscore		20
Ramachandran outliers		1.0%
Sidechain outliers		5.3%
RSRZ outliers		6.2%

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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	5% · 55% · 36% · 5%
2	B	440	7% · 58% · 34% · 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8012 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	534	Total	C	N	O	S	0	0	0
			4364	2825	727	804	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ILE	LEU	ENGINEERED	UNP P04585
A	280	CSD	CYS	MODIFIED RESIDUE	UNP P04585

- Molecule 2 is a protein called Reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	416	Total	C	N	O	S	0	0	0
			3432	2232	569	624	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	100	ILE	LEU	ENGINEERED	UNP P04585

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

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

- Molecule 4 is 2-METHYL-FURAN-3-CARBOTHIOIC ACID [4-CHLORO-3-(3-METHYL-BUT-2-ENYLOXY)-PHENYL]-AMIDE (three-letter code: UC1) (formula: $C_{17}H_{18}ClNO_2S$).
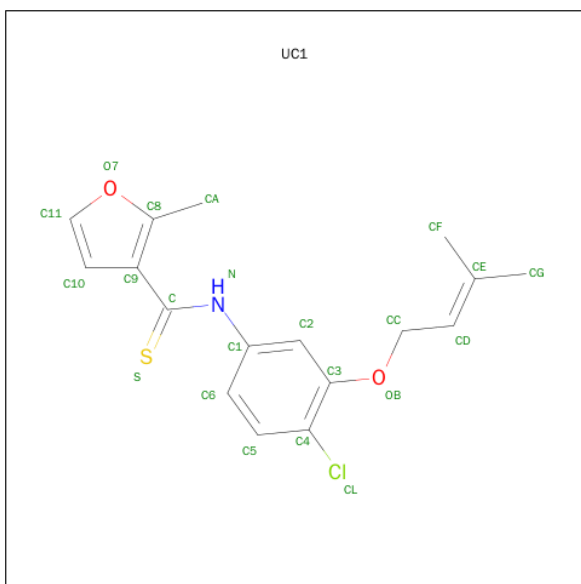
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 22	C 17	Cl 1	N 1	O 2	S 1	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	110	Total 110	O 110	0	0
5	B	74	Total 74	O 74	0	0

3 Residue-property plots ⓘ

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

- Molecule 1: Reverse transcriptase
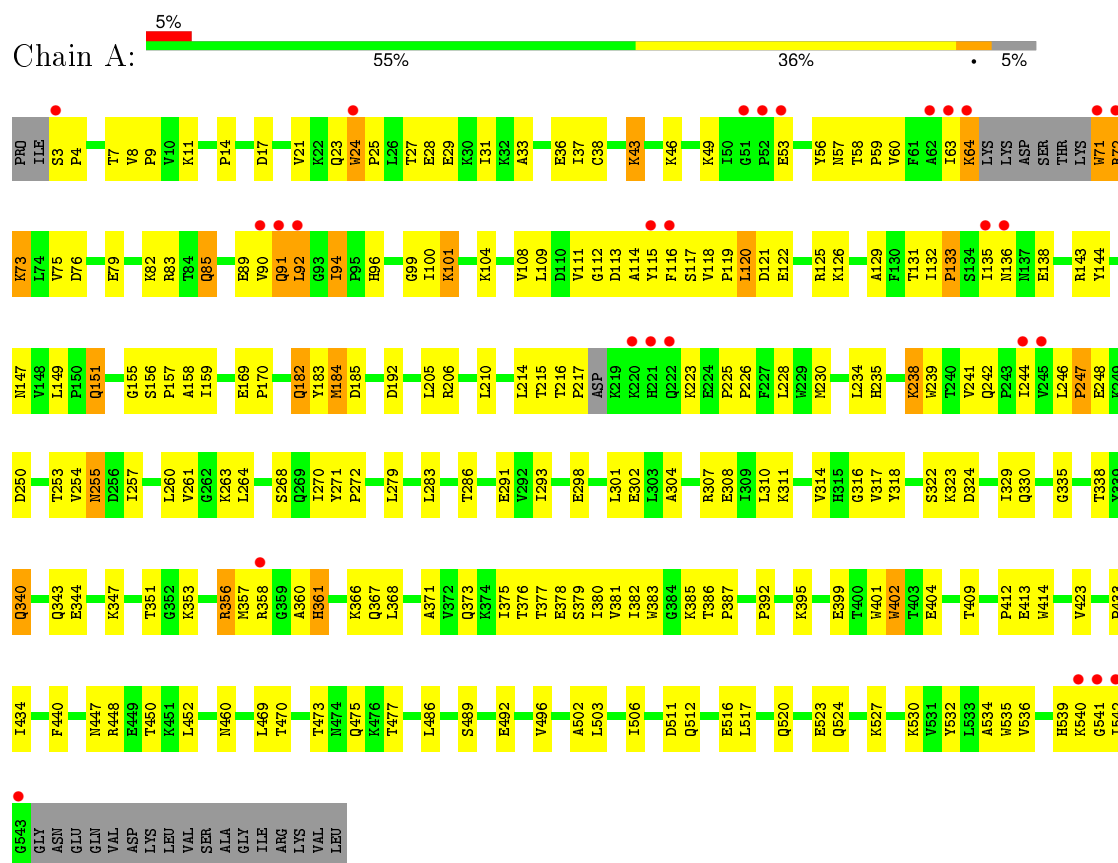
- Molecule 2: Reverse transcriptase
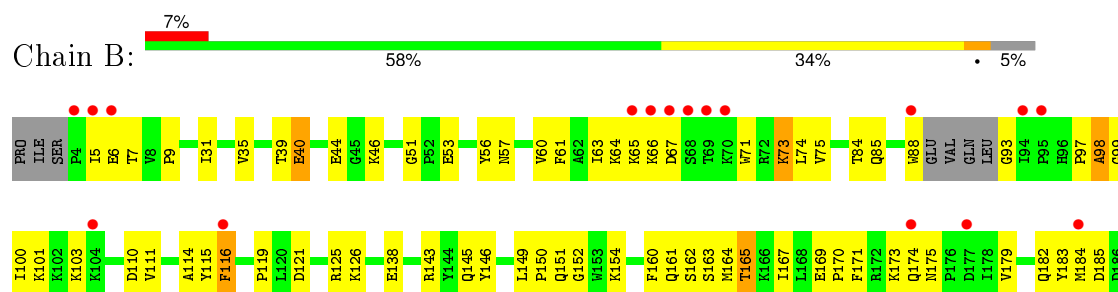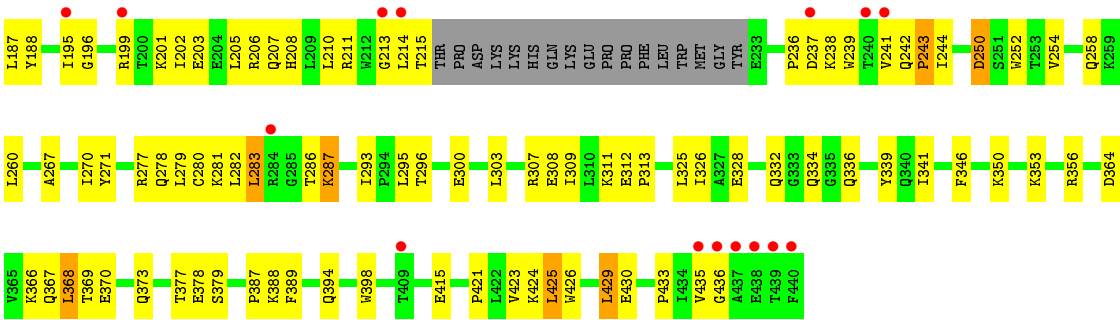
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	137.51Å 109.38Å 72.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.42 – 2.40 29.42 – 2.41	Depositor EDS
% Data completeness (in resolution range)	96.5 (29.42-2.40) 96.7 (29.42-2.41)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 2.42Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.206 , 0.274 0.200 , 0.206	Depositor DCC
R_{free} test set	2086 reflections (5.02%)	DCC
Wilson B-factor (Å^2)	44.3	Xtriage
Anisotropy	0.514	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 64.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50, < L^2 > = 0.33$	Xtriage
Outliers	0 of 41526 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8012	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CSD, PO4, UC1

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	0.38	0/4470	0.62	0/6074
2	B	0.39	0/3528	0.63	0/4790
All	All	0.38	0/7998	0.63	0/10864

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	4364	0	4402	191	0
2	B	3432	0	3465	138	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	22	0	18	1	0
5	A	110	0	0	3	0
5	B	74	0	0	11	0
All	All	8012	0	7885	319	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 20.

All (319) 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:492:GLU:HG2	1:A:530:LYS:HB2	1.39	1.04
2:B:114:ALA:HB2	2:B:214:LEU:HD21	1.46	0.94
1:A:112:GLY:HA2	1:A:185:ASP:HB3	1.52	0.92
1:A:114:ALA:HB1	1:A:214:LEU:HD22	1.54	0.88
2:B:163:SER:O	2:B:167:ILE:HG23	1.75	0.86
1:A:448:ARG:NH1	1:A:473:THR:HB	1.90	0.85
1:A:101:LYS:N	1:A:101:LYS:HE3	1.92	0.85
1:A:380:ILE:HD11	1:A:386:THR:HG22	1.61	0.82
2:B:5:ILE:HG22	2:B:6:GLU:H	1.44	0.81
2:B:242:GLN:NE2	2:B:243:PRO:HD2	1.95	0.80
2:B:5:ILE:HG22	2:B:6:GLU:N	2.01	0.76
2:B:241:VAL:HG12	5:B:1124:HOH:O	1.84	0.76
1:A:241:VAL:HG21	1:A:270:ILE:HG21	1.68	0.75
1:A:108:VAL:CG1	1:A:223:LYS:HB2	2.16	0.75
1:A:94:ILE:H	1:A:94:ILE:HD13	1.50	0.74
1:A:17:ASP:O	1:A:83:ARG:HD3	1.88	0.73
2:B:161:GLN:O	2:B:165:THR:HG22	1.87	0.73
2:B:242:GLN:HE21	2:B:243:PRO:HD2	1.52	0.72
1:A:64:LYS:H	1:A:64:LYS:HD2	1.54	0.72
1:A:28:GLU:HB3	1:A:135:ILE:HD11	1.70	0.72
1:A:239:TRP:CE2	1:A:316:GLY:HA3	2.25	0.71
2:B:366:LYS:O	2:B:370:GLU:HG3	1.90	0.71
2:B:64:LYS:HE2	2:B:71:TRP:CE2	2.26	0.71
2:B:169:GLU:HB2	2:B:170:PRO:HD3	1.73	0.70
1:A:64:LYS:HE3	1:A:71:TRP:CZ3	2.25	0.70
1:A:386:THR:HG21	5:B:1047:HOH:O	1.91	0.70
1:A:108:VAL:HG11	1:A:223:LYS:HB2	1.74	0.70
1:A:238:LYS:HB2	1:A:316:GLY:O	1.92	0.69
2:B:244:ILE:HG23	2:B:429:LEU:HB3	1.74	0.69
1:A:71:TRP:HA	1:A:71:TRP:CE3	2.26	0.69
2:B:169:GLU:O	2:B:173:LYS:HD3	1.93	0.69
1:A:257:ILE:O	1:A:261:VAL:HG23	1.92	0.68
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.75	0.68
1:A:114:ALA:HA	1:A:117:SER:OG	1.94	0.68
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.75	0.67
2:B:63:ILE:HD13	2:B:74:LEU:HD22	1.77	0.67
2:B:279:LEU:HA	2:B:282:LEU:HD12	1.75	0.66
2:B:56:TYR:HE2	2:B:126:LYS:HE2	1.60	0.66
1:A:71:TRP:HA	1:A:71:TRP:HE3	1.61	0.66
1:A:73:LYS:HE3	1:A:75:VAL:HG23	1.76	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:254:VAL:O	2:B:258:GLN:HG3	1.96	0.65
2:B:175:ASN:ND2	2:B:201:LYS:HD2	2.10	0.65
2:B:161:GLN:HE22	2:B:182:GLN:NE2	1.95	0.65
1:A:46:LYS:HE2	1:A:116:PHE:HB3	1.78	0.65
1:A:357:MET:HB2	1:A:367:GLN:NE2	2.11	0.64
1:A:112:GLY:CA	1:A:185:ASP:HB3	2.26	0.64
1:A:114:ALA:CB	1:A:214:LEU:HD22	2.28	0.64
2:B:421:PRO:O	2:B:425:LEU:HD22	1.98	0.64
1:A:448:ARG:HH12	1:A:473:THR:HB	1.61	0.64
1:A:29:GLU:HG2	1:A:71:TRP:HE1	1.61	0.64
2:B:250:ASP:OD2	2:B:250:ASP:N	2.31	0.63
1:A:7:THR:HG22	1:A:119:PRO:HB2	1.80	0.62
2:B:332:GLN:NE2	2:B:424:LYS:HE2	2.13	0.62
1:A:356:ARG:CZ	1:A:358:ARG:HD3	2.29	0.62
2:B:169:GLU:HG2	2:B:173:LYS:HZ3	1.64	0.62
2:B:195:ILE:HG13	2:B:199:ARG:HE	1.64	0.62
1:A:373:GLN:HG2	5:B:1042:HOH:O	2.00	0.62
1:A:90:VAL:HG12	1:A:158:ALA:HB2	1.80	0.62
1:A:38:CYS:HB3	1:A:144:TYR:CE1	2.35	0.62
2:B:35:VAL:O	2:B:39:THR:HG23	2.00	0.62
1:A:33:ALA:O	1:A:36:GLU:HB3	2.00	0.61
2:B:169:GLU:HA	2:B:173:LYS:HZ2	1.65	0.61
2:B:161:GLN:HE22	2:B:182:GLN:HE22	1.48	0.61
2:B:84:THR:HB	2:B:154:LYS:HE2	1.82	0.61
1:A:540:LYS:HB2	1:A:542:ILE:HG13	1.81	0.61
2:B:388:LYS:HE2	2:B:415:GLU:HB3	1.82	0.61
2:B:379:SER:CB	2:B:387:PRO:HD3	2.31	0.61
1:A:409:THR:O	2:B:364:ASP:HB2	2.01	0.61
2:B:379:SER:OG	2:B:387:PRO:HD3	2.01	0.60
1:A:378:GLU:O	1:A:382:ILE:HG12	2.01	0.60
1:A:268:SER:HB3	1:A:353:LYS:HE2	1.82	0.60
1:A:293:ILE:HD12	1:A:293:ILE:N	2.16	0.60
1:A:376:THR:O	1:A:380:ILE:HG12	2.02	0.59
1:A:380:ILE:CD1	1:A:386:THR:HG22	2.31	0.59
1:A:90:VAL:O	1:A:91:GLN:C	2.41	0.59
1:A:21:VAL:HG13	1:A:59:PRO:HD3	1.84	0.59
2:B:114:ALA:CB	2:B:214:LEU:HD21	2.26	0.59
1:A:239:TRP:CZ2	1:A:316:GLY:HA3	2.37	0.59
2:B:103:LYS:HE2	2:B:179:VAL:HG23	1.85	0.59
1:A:23:GLN:HE22	1:A:60:VAL:H	1.51	0.59
1:A:73:LYS:HE3	1:A:75:VAL:CG2	2.33	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:426:TRP:O	2:B:429:LEU:HB2	2.03	0.59
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.38	0.59
2:B:423:VAL:HG21	5:B:1140:HOH:O	2.02	0.58
1:A:413:GLU:HG3	5:A:1063:HOH:O	2.03	0.58
1:A:317:VAL:HG12	1:A:318:TYR:N	2.16	0.58
2:B:287:LYS:HE2	2:B:293:ILE:HD11	1.86	0.58
2:B:5:ILE:CG2	2:B:6:GLU:H	2.15	0.58
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.85	0.58
1:A:116:PHE:CZ	1:A:151:GLN:HB2	2.39	0.58
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.44	0.57
1:A:118:VAL:HB	1:A:149:LEU:HD22	1.85	0.57
1:A:228:LEU:HD22	1:A:242:GLN:CD	2.24	0.57
1:A:72:ARG:HG3	1:A:72:ARG:HH11	1.70	0.57
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.86	0.57
1:A:90:VAL:CG1	1:A:158:ALA:HB2	2.34	0.57
1:A:206:ARG:HG3	1:A:216:THR:CG2	2.34	0.57
1:A:516:GLU:O	1:A:520:GLN:HG3	2.05	0.56
2:B:65:LYS:HE3	2:B:110:ASP:OD1	2.05	0.56
1:A:183:TYR:CD1	1:A:184:MET:HB2	2.40	0.56
1:A:356:ARG:HG3	1:A:356:ARG:HH11	1.70	0.56
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.87	0.56
1:A:279:LEU:HD23	1:A:302:GLU:OE1	2.05	0.56
1:A:101:LYS:HE3	1:A:101:LYS:H	1.69	0.55
2:B:244:ILE:HG13	2:B:426:TRP:CZ2	2.42	0.55
1:A:536:VAL:HG12	2:B:258:GLN:HB3	1.88	0.55
1:A:270:ILE:CG2	1:A:314:VAL:HG11	2.36	0.55
2:B:170:PRO:O	2:B:174:GLN:HG3	2.06	0.55
2:B:46:LYS:HE2	2:B:116:PHE:CD1	2.41	0.55
2:B:203:GLU:HA	2:B:206:ARG:HG3	1.89	0.55
1:A:210:LEU:CD1	1:A:215:THR:HG22	2.37	0.55
1:A:253:THR:O	1:A:257:ILE:HG13	2.06	0.55
2:B:60:VAL:HG23	2:B:75:VAL:HG22	1.90	0.54
1:A:244:ILE:CG2	1:A:310:LEU:HD22	2.37	0.54
1:A:260:LEU:O	1:A:264:LEU:HD23	2.07	0.54
1:A:301:LEU:O	1:A:304:ALA:HB3	2.07	0.54
1:A:122:GLU:CD	1:A:122:GLU:H	2.10	0.54
1:A:143:ARG:HH11	1:A:143:ARG:HG2	1.73	0.54
1:A:49:LYS:HA	1:A:144:TYR:HD2	1.73	0.54
1:A:248:GLU:HA	1:A:307:ARG:NH2	2.22	0.53
1:A:330:GLN:HB2	1:A:338:THR:OG1	2.08	0.53
1:A:112:GLY:HA2	1:A:185:ASP:CB	2.33	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:206:ARG:O	2:B:210:LEU:N	2.34	0.53
2:B:88:TRP:HZ3	2:B:93:GLY:N	2.06	0.53
2:B:271:TYR:HB3	2:B:309:ILE:HG21	1.89	0.53
1:A:511:ASP:OD1	1:A:512:GLN:HG2	2.08	0.53
2:B:241:VAL:HG13	5:B:1123:HOH:O	2.08	0.53
1:A:57:ASN:ND2	1:A:131:THR:OG1	2.42	0.53
1:A:37:ILE:HD11	1:A:71:TRP:O	2.09	0.53
1:A:46:LYS:HE2	1:A:116:PHE:CB	2.38	0.52
1:A:182:GLN:HG3	5:A:1018:HOH:O	2.08	0.52
1:A:434:ILE:CD1	1:A:530:LYS:HB3	2.40	0.52
2:B:56:TYR:CE2	2:B:126:LYS:HE2	2.42	0.52
1:A:250:ASP:N	1:A:250:ASP:OD2	2.43	0.52
2:B:195:ILE:HG13	2:B:199:ARG:NE	2.25	0.52
2:B:241:VAL:HG22	5:B:1123:HOH:O	2.09	0.52
1:A:135:ILE:HG23	1:A:136:ASN:CG	2.30	0.52
2:B:98:ALA:O	2:B:101:LYS:HG2	2.09	0.52
2:B:239:TRP:CH2	2:B:378:GLU:HG2	2.45	0.52
2:B:241:VAL:HA	5:B:1123:HOH:O	2.10	0.51
1:A:9:PRO:HG2	2:B:53:GLU:HG3	1.92	0.51
2:B:169:GLU:HG2	2:B:173:LYS:NZ	2.25	0.51
1:A:539:HIS:O	1:A:540:LYS:HD2	2.10	0.51
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.45	0.51
1:A:361:HIS:CD2	1:A:361:HIS:N	2.79	0.51
2:B:169:GLU:CG	2:B:173:LYS:HZ3	2.24	0.51
2:B:31:ILE:O	2:B:35:VAL:HG23	2.11	0.51
1:A:143:ARG:NH1	1:A:143:ARG:HG2	2.25	0.51
1:A:366:LYS:HZ1	2:B:394:GLN:HE21	1.57	0.51
1:A:335:GLY:HA2	1:A:367:GLN:OE1	2.11	0.50
1:A:244:ILE:HD11	1:A:263:LYS:HB3	1.93	0.50
2:B:61:PHE:CZ	2:B:74:LEU:HD23	2.47	0.50
1:A:244:ILE:HG23	1:A:310:LEU:HD13	1.93	0.50
1:A:108:VAL:HG13	1:A:223:LYS:HB2	1.91	0.50
1:A:53:GLU:HG3	1:A:53:GLU:O	2.11	0.50
1:A:317:VAL:HG21	1:A:347:LYS:HB3	1.93	0.50
1:A:452:LEU:HD11	1:A:470:THR:HG22	1.94	0.50
1:A:452:LEU:CD1	1:A:470:THR:HG22	2.42	0.50
2:B:208:HIS:O	2:B:211:ARG:HG3	2.12	0.49
1:A:31:ILE:HG12	1:A:133:PRO:HG2	1.93	0.49
1:A:21:VAL:CG1	1:A:59:PRO:HD3	2.42	0.49
1:A:23:GLN:HG2	1:A:131:THR:O	2.11	0.49
1:A:90:VAL:O	1:A:90:VAL:HG23	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:LYS:HE2	2:B:146:TYR:OH	2.12	0.49
2:B:287:LYS:HE2	2:B:293:ILE:CD1	2.43	0.49
2:B:207:GLN:O	2:B:210:LEU:HB3	2.13	0.49
1:A:523:GLU:O	1:A:527:LYS:HG3	2.13	0.49
1:A:539:HIS:C	1:A:540:LYS:HD2	2.33	0.49
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.47	0.49
2:B:125:ARG:HB3	2:B:145:GLN:NE2	2.28	0.48
1:A:49:LYS:HA	1:A:144:TYR:CD2	2.48	0.48
2:B:433:PRO:HB2	2:B:436:GLY:HA2	1.95	0.48
2:B:239:TRP:CZ3	2:B:378:GLU:HG2	2.49	0.48
2:B:267:ALA:HB2	2:B:426:TRP:CZ3	2.49	0.48
2:B:270:ILE:HG12	2:B:346:PHE:HB3	1.95	0.48
1:A:3:SER:HB3	1:A:4:PRO:HD2	1.96	0.48
1:A:58:THR:HG23	1:A:76:ASP:O	2.13	0.48
2:B:40:GLU:O	2:B:44:GLU:HG3	2.13	0.48
1:A:270:ILE:HG22	1:A:314:VAL:HG11	1.95	0.48
1:A:317:VAL:CG1	1:A:318:TYR:N	2.77	0.47
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.13	0.47
1:A:206:ARG:HG3	1:A:216:THR:HG23	1.95	0.47
1:A:126:LYS:HG2	5:A:1015:HOH:O	2.13	0.47
1:A:57:ASN:HA	1:A:129:ALA:O	2.14	0.47
1:A:460:ASN:HA	2:B:286:THR:O	2.14	0.47
2:B:373:GLN:O	2:B:377:THR:HG23	2.13	0.47
2:B:64:LYS:HE2	2:B:71:TRP:CZ2	2.48	0.47
2:B:350:LYS:HG3	5:B:1123:HOH:O	2.14	0.47
1:A:94:ILE:H	1:A:94:ILE:CD1	2.23	0.47
2:B:152:GLY:HA2	2:B:184:MET:HE3	1.95	0.47
2:B:161:GLN:HA	2:B:161:GLN:NE2	2.29	0.47
1:A:366:LYS:NZ	2:B:394:GLN:NE2	2.63	0.47
1:A:53:GLU:OE2	1:A:53:GLU:HA	2.15	0.47
1:A:502:ALA:O	1:A:506:ILE:HG13	2.15	0.47
2:B:57:ASN:HD22	2:B:143:ARG:NH1	2.12	0.47
1:A:434:ILE:HD13	1:A:530:LYS:HB3	1.97	0.47
1:A:23:GLN:NE2	1:A:60:VAL:H	2.12	0.47
2:B:162:SER:O	2:B:165:THR:HG23	2.14	0.46
1:A:235:HIS:HB2	1:A:238:LYS:O	2.15	0.46
2:B:332:GLN:HE22	2:B:424:LYS:HD3	1.80	0.46
2:B:67:ASP:O	2:B:67:ASP:CG	2.54	0.46
1:A:111:VAL:O	1:A:114:ALA:HB3	2.15	0.46
2:B:332:GLN:NE2	2:B:424:LYS:CE	2.79	0.46
1:A:377:THR:O	1:A:381:VAL:HG23	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ILE:O	1:A:63:ILE:HD12	2.15	0.46
1:A:226:PRO:HA	1:A:234:LEU:O	2.15	0.46
2:B:277:ARG:O	2:B:281:LYS:HG3	2.16	0.46
1:A:433:PRO:HA	1:A:532:TYR:CD2	2.50	0.46
2:B:242:GLN:HB2	5:B:1125:HOH:O	2.15	0.46
1:A:235:HIS:HB2	1:A:238:LYS:HD3	1.98	0.46
2:B:51:GLY:HA3	2:B:53:GLU:OE1	2.15	0.46
2:B:171:PHE:CG	2:B:205:LEU:HD23	2.51	0.46
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.96	0.46
1:A:120:LEU:O	1:A:121:ASP:C	2.53	0.46
1:A:101:LYS:NZ	2:B:138:GLU:OE1	2.49	0.46
1:A:329:ILE:O	1:A:392:PRO:HD3	2.16	0.46
1:A:503:LEU:HD13	1:A:535:TRP:CG	2.51	0.46
1:A:24:TRP:CD1	1:A:25:PRO:HD2	2.51	0.46
1:A:340:GLN:CB	1:A:351:THR:HG22	2.45	0.45
1:A:371:ALA:O	1:A:375:ILE:HG13	2.16	0.45
1:A:254:VAL:HG22	1:A:286:THR:HG21	1.96	0.45
2:B:308:GLU:O	2:B:311:LYS:HB2	2.16	0.45
2:B:328:GLU:O	2:B:339:TYR:HA	2.16	0.45
1:A:226:PRO:HB3	1:A:235:HIS:CE1	2.51	0.45
2:B:334:GLN:O	2:B:336:GLN:OE1	2.34	0.45
1:A:53:GLU:O	1:A:53:GLU:CG	2.65	0.45
2:B:353:LYS:NZ	2:B:430:GLU:HB2	2.31	0.45
2:B:97:PRO:O	2:B:99:GLY:N	2.50	0.45
1:A:308:GLU:HA	1:A:311:LYS:HE2	1.98	0.45
1:A:541:GLY:H	2:B:280:CYS:HB3	1.81	0.45
2:B:175:ASN:HD22	2:B:201:LYS:NZ	2.14	0.45
1:A:11:LYS:O	1:A:85:GLN:HB3	2.16	0.45
1:A:27:THR:O	1:A:31:ILE:HG13	2.17	0.45
2:B:205:LEU:HD13	2:B:205:LEU:C	2.37	0.45
2:B:195:ILE:HG23	2:B:196:GLY:N	2.32	0.45
2:B:116:PHE:C	2:B:116:PHE:CD1	2.90	0.45
1:A:206:ARG:NH2	1:A:217:PRO:C	2.70	0.45
2:B:356:ARG:HB2	2:B:367:GLN:HG2	1.97	0.45
2:B:295:LEU:HB2	2:B:300:GLU:OE1	2.17	0.45
2:B:202:ILE:O	2:B:205:LEU:HB3	2.16	0.44
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.98	0.44
1:A:8:VAL:O	1:A:121:ASP:HB2	2.17	0.44
1:A:366:LYS:NZ	2:B:394:GLN:HE21	2.15	0.44
1:A:7:THR:CG2	1:A:119:PRO:HB2	2.45	0.44
2:B:326:ILE:O	2:B:341:ILE:HA	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:ALA:O	2:B:101:LYS:CG	2.66	0.44
1:A:356:ARG:NE	1:A:358:ARG:HD3	2.33	0.43
1:A:536:VAL:HB	1:A:542:ILE:HD13	1.99	0.43
1:A:379:SER:CB	1:A:387:PRO:HD3	2.48	0.43
2:B:278:GLN:HA	2:B:278:GLN:NE2	2.33	0.43
1:A:540:LYS:C	1:A:542:ILE:H	2.20	0.43
1:A:401:TRP:CZ3	1:A:409:THR:HG21	2.53	0.43
1:A:64:LYS:HE3	1:A:71:TRP:CH2	2.53	0.43
1:A:96:HIS:ND1	1:A:230:MET:HE1	2.34	0.43
2:B:421:PRO:O	2:B:425:LEU:CD2	2.63	0.43
1:A:155:GLY:O	1:A:159:ILE:HG13	2.19	0.43
2:B:236:PRO:C	2:B:238:LYS:H	2.22	0.43
1:A:360:ALA:HB3	1:A:361:HIS:HD2	1.84	0.43
1:A:383:TRP:O	1:A:385:LYS:HG3	2.18	0.43
4:A:999:UC1:H2	4:A:999:UC1:C9	2.48	0.43
2:B:160:PHE:CD1	2:B:160:PHE:O	2.72	0.43
1:A:90:VAL:HG12	1:A:158:ALA:CB	2.47	0.43
1:A:23:GLN:OE1	1:A:59:PRO:HA	2.19	0.43
2:B:260:LEU:HD21	2:B:303:LEU:HD21	2.00	0.43
1:A:28:GLU:HB3	1:A:135:ILE:CD1	2.43	0.43
1:A:56:TYR:O	1:A:143:ARG:NH2	2.51	0.43
1:A:136:ASN:OD1	1:A:138:GLU:HB2	2.18	0.43
2:B:111:VAL:HG21	2:B:164:MET:CE	2.49	0.43
1:A:255:ASN:HD22	1:A:255:ASN:HA	1.62	0.43
1:A:100:ILE:C	1:A:101:LYS:HE3	2.40	0.42
1:A:469:LEU:HD12	1:A:477:THR:HG22	2.01	0.42
2:B:350:LYS:HE2	2:B:378:GLU:OE1	2.19	0.42
1:A:540:LYS:HB3	2:B:280:CYS:SG	2.59	0.42
2:B:433:PRO:CB	2:B:436:GLY:HA2	2.49	0.42
2:B:115:TYR:HB3	2:B:149:LEU:HB2	2.00	0.42
2:B:435:VAL:HG23	2:B:436:GLY:N	2.34	0.42
1:A:246:LEU:HA	1:A:247:PRO:HD2	1.86	0.42
1:A:542:ILE:HG12	2:B:283:LEU:HD23	2.02	0.42
2:B:303:LEU:O	2:B:307:ARG:HG3	2.20	0.42
2:B:369:THR:O	2:B:373:GLN:HG3	2.20	0.42
1:A:92:LEU:O	1:A:92:LEU:HD13	2.20	0.42
2:B:149:LEU:HA	2:B:150:PRO:HD3	1.79	0.42
1:A:64:LYS:HB3	1:A:71:TRP:CE3	2.54	0.42
1:A:225:PRO:HA	1:A:226:PRO:C	2.40	0.42
2:B:282:LEU:HD21	2:B:296:THR:HG23	2.00	0.42
1:A:399:GLU:OE2	1:A:402:TRP:HZ3	2.03	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:GLY:O	1:A:101:LYS:HE2	2.20	0.42
2:B:100:ILE:HG23	2:B:101:LYS:N	2.35	0.42
2:B:183:TYR:HB3	2:B:188:TYR:HE1	1.83	0.42
1:A:184:MET:HB3	1:A:185:ASP:H	1.50	0.41
2:B:173:LYS:N	2:B:173:LYS:HD2	2.34	0.41
2:B:175:ASN:HD21	2:B:201:LYS:HD2	1.83	0.41
1:A:246:LEU:HD22	1:A:260:LEU:HD11	2.01	0.41
1:A:254:VAL:CG2	1:A:286:THR:HG21	2.50	0.41
2:B:295:LEU:HG	5:B:1136:HOH:O	2.20	0.41
1:A:271:TYR:HA	1:A:272:PRO:HD3	1.77	0.41
2:B:175:ASN:ND2	2:B:201:LYS:NZ	2.69	0.41
1:A:412:PRO:O	1:A:413:GLU:C	2.59	0.41
1:A:440:PHE:CE1	1:A:489:SER:HB3	2.56	0.41
1:A:323:LYS:NZ	1:A:344:GLU:OE2	2.53	0.41
1:A:58:THR:HG23	1:A:59:PRO:HD2	2.01	0.41
1:A:298:GLU:H	1:A:298:GLU:CD	2.15	0.41
1:A:486:LEU:HB3	1:A:524:GLN:HB3	2.00	0.41
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.55	0.41
1:A:234:LEU:HD23	1:A:239:TRP:HB3	2.02	0.41
1:A:298:GLU:OE2	1:A:298:GLU:N	2.36	0.41
2:B:9:PRO:HA	2:B:121:ASP:OD2	2.21	0.41
2:B:368:LEU:HD13	2:B:398:TRP:CZ3	2.56	0.41
2:B:312:GLU:HA	2:B:313:PRO:HD3	1.93	0.41
1:A:43:LYS:O	1:A:43:LYS:HD3	2.21	0.41
1:A:492:GLU:HA	1:A:530:LYS:O	2.22	0.40
1:A:253:THR:HA	1:A:291:GLU:O	2.21	0.40
2:B:66:LYS:O	2:B:67:ASP:HB3	2.21	0.40
2:B:97:PRO:O	2:B:98:ALA:C	2.59	0.40
2:B:73:LYS:HB3	2:B:73:LYS:NZ	2.36	0.40
1:A:79:GLU:HA	1:A:82:LYS:HG2	2.03	0.40
1:A:534:ALA:HB1	5:B:1098:HOH:O	2.21	0.40
2:B:151:GLN:HB3	2:B:185:ASP:OD1	2.22	0.40
1:A:324:ASP:O	1:A:343:GLN:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	527/560 (94%)	487 (92%)	35 (7%)	5 (1%)	21	30
2	B	410/440 (93%)	384 (94%)	22 (5%)	4 (1%)	19	28
All	All	937/1000 (94%)	871 (93%)	57 (6%)	9 (1%)	19	28

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
2	B	85	GLN
1	A	91	GLN
2	B	98	ALA
1	A	247	PRO
1	A	133	PRO
2	B	237	ASP
1	A	14	PRO
2	B	213	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	476/499 (95%)	444 (93%)	32 (7%)	20	31
2	B	377/400 (94%)	364 (97%)	13 (3%)	44	65
All	All	853/899 (95%)	808 (95%)	45 (5%)	28	44

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	TRP
1	A	43	LYS
1	A	64	LYS
1	A	71	TRP
1	A	72	ARG
1	A	73	LYS
1	A	89	GLU
1	A	92	LEU
1	A	94	ILE
1	A	101	LYS
1	A	109	LEU
1	A	113	ASP
1	A	115	TYR
1	A	120	LEU
1	A	151	GLN
1	A	182	GLN
1	A	184	MET
1	A	205	LEU
1	A	238	LYS
1	A	255	ASN
1	A	283	LEU
1	A	322	SER
1	A	340	GLN
1	A	356	ARG
1	A	361	HIS
1	A	368	LEU
1	A	402	TRP
1	A	404	GLU
1	A	423	VAL
1	A	475	GLN
1	A	496	VAL
1	A	517	LEU
2	B	40	GLU
2	B	73	LYS
2	B	116	PHE
2	B	165	THR
2	B	215	THR
2	B	243	PRO
2	B	250	ASP
2	B	283	LEU
2	B	287	LYS
2	B	325	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	368	LEU
2	B	425	LEU
2	B	429	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	147	ASN
1	A	174	GLN
1	A	242	GLN
1	A	255	ASN
1	A	278	GLN
1	A	332	GLN
1	A	361	HIS
1	A	475	GLN
1	A	500	GLN
2	B	57	ASN
2	B	175	ASN
2	B	182	GLN
2	B	197	GLN
2	B	208	HIS
2	B	235	HIS
2	B	242	GLN
2	B	269	GLN
2	B	278	GLN
2	B	332	GLN
2	B	394	GLN
2	B	407	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	0.78	0	3,8,10	2.04	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	2.98	110.36	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)

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	2001	-	4,4,4	0.98	0	6,6,6	0.27	0
4	UC1	A	999	-	19,23,23	1.38	1 (5%)	21,31,31	1.47	3 (14%)
3	PO4	B	1000	-	4,4,4	1.17	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	2001	-	-	0/0/0/0	0/0/0/0
4	UC1	A	999	-	-	1/10/14/14	0/1/2/2
3	PO4	B	1000	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	UC1	CA-C8	3.48	1.53	1.48

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	999	UC1	C3-C4-CL	2.53	122.53	119.42
4	A	999	UC1	OB-C3-C4	3.24	120.61	116.36
4	A	999	UC1	C9-C-N	3.71	118.77	114.12

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	999	UC1	S-C-N-C1

There are no ring outliers.

Full wwPDB X-ray Structure Validation Report

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	999	UC1	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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	533/560 (95%)	-0.09	27 (5%)	32	32	22, 46, 98, 138	0
2	B	416/440 (94%)	0.09	32 (7%)	16	16	22, 47, 101, 146	0
All	All	949/1000 (94%)	-0.01	59 (6%)	24	25	22, 47, 101, 146	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	88	TRP	6.9
2	B	67	ASP	6.7
2	B	69	THR	5.9
2	B	65	LYS	5.8
1	A	541	GLY	5.5
1	A	543	GLY	5.3
1	A	221	HIS	5.1
1	A	542	ILE	4.9
2	B	440	PHE	4.8
2	B	435	VAL	4.6
1	A	52	PRO	4.6
2	B	5	ILE	4.6
2	B	4	PRO	4.4
2	B	213	GLY	4.3
2	B	240	THR	4.1
2	B	214	LEU	4.0
2	B	195	ILE	3.8
2	B	68	SER	3.6
1	A	90	VAL	3.5
1	A	53	GLU	3.4
1	A	136	ASN	3.4
1	A	64	LYS	3.3
2	B	116	PHE	3.2
1	A	135	ILE	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	91	GLN	3.1
2	B	184	MET	3.1
2	B	94	ILE	3.0
1	A	115	TYR	3.0
2	B	439	THR	2.9
1	A	116	PHE	2.9
2	B	284	ARG	2.9
2	B	436	GLY	2.9
1	A	71	TRP	2.9
2	B	6	GLU	2.8
2	B	66	LYS	2.7
1	A	24	TRP	2.6
2	B	241	VAL	2.6
2	B	95	PRO	2.5
1	A	540	LYS	2.4
2	B	199	ARG	2.4
1	A	63	ILE	2.4
1	A	62	ALA	2.4
1	A	244	ILE	2.3
2	B	174	GLN	2.3
1	A	92	LEU	2.3
2	B	177	ASP	2.2
1	A	3	SER	2.2
1	A	72	ARG	2.2
2	B	104	LYS	2.2
2	B	438	GLU	2.2
2	B	437	ALA	2.2
1	A	220	LYS	2.1
1	A	358	ARG	2.1
2	B	70	LYS	2.1
1	A	222	GLN	2.1
2	B	409	THR	2.1
1	A	51	GLY	2.0
2	B	237	ASP	2.0
1	A	245	VAL	2.0

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

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	0.95	0.11	-	42,50,73,77	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	PO4	A	2001	5/5	0.82	0.15	0.89	106,109,116,126	0
4	UC1	A	999	22/22	0.96	0.13	0.35	26,35,43,47	0
3	PO4	B	1000	5/5	0.89	0.13	-0.98	102,105,111,114	0

6.5 Other polymers (i)

There are no such residues in this entry.