Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:41 PM GMT

PDB ID	:	1C1B
Title	:	CRYSTAL STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE IN COMPLEX WITH GCA-186
Authors	:	Hopkins, A.L.; Ren, J.; Tanaka, H.; Baba, B.; Okamato, M.; Stuart, D.I.; Stammers, D.K.
Deposited on	:	1999-07-21
Resolution	:	2.50 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:

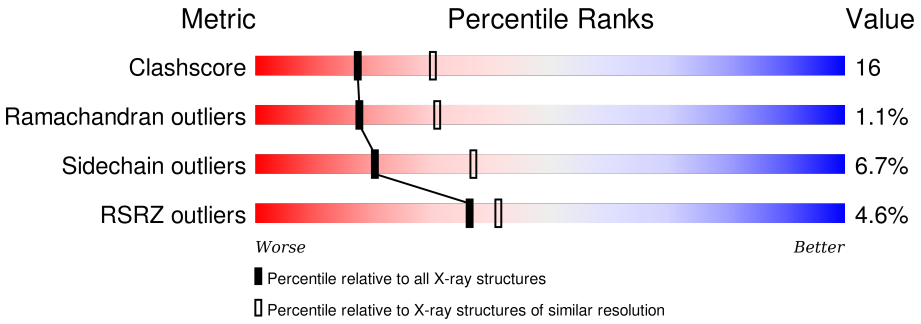
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.50 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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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% 61% 32%
2	B	440	5% 63% 28% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7888 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called HIV-1 REVERSE TRANSCRIPTASE (A-CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	537	4389	2842	732	807	8	0	0	0

There is a discrepancy between the modelled and reference sequences:

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

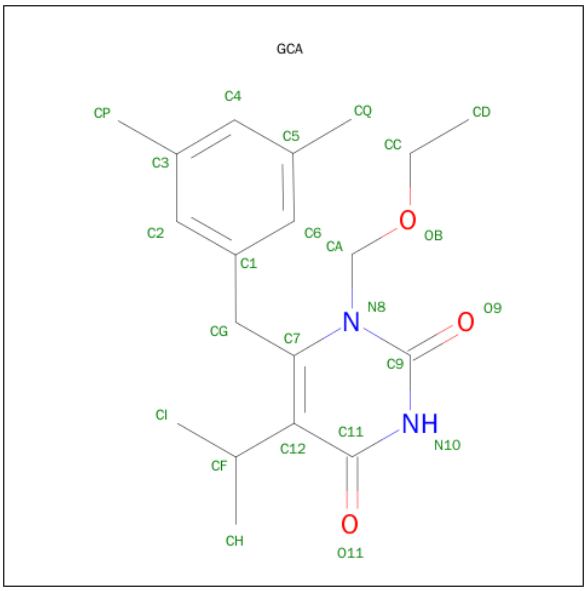
- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE (B-CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	415	3419	2225	566	621	7	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	172	LYS	ARG	CONFLICT	UNP P04585
B	428	ASN	GLN	CONFLICT	UNP P04585

- Molecule 3 is 6-(3',5'-DIMETHYLBENZYL)-1-ETHOXYMETHYL-5-ISOPROPYLURACIL (three-letter code: GCA) (formula: $C_{19}H_{26}N_2O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 24 19 2 3	0	0

- Molecule 4 is water.

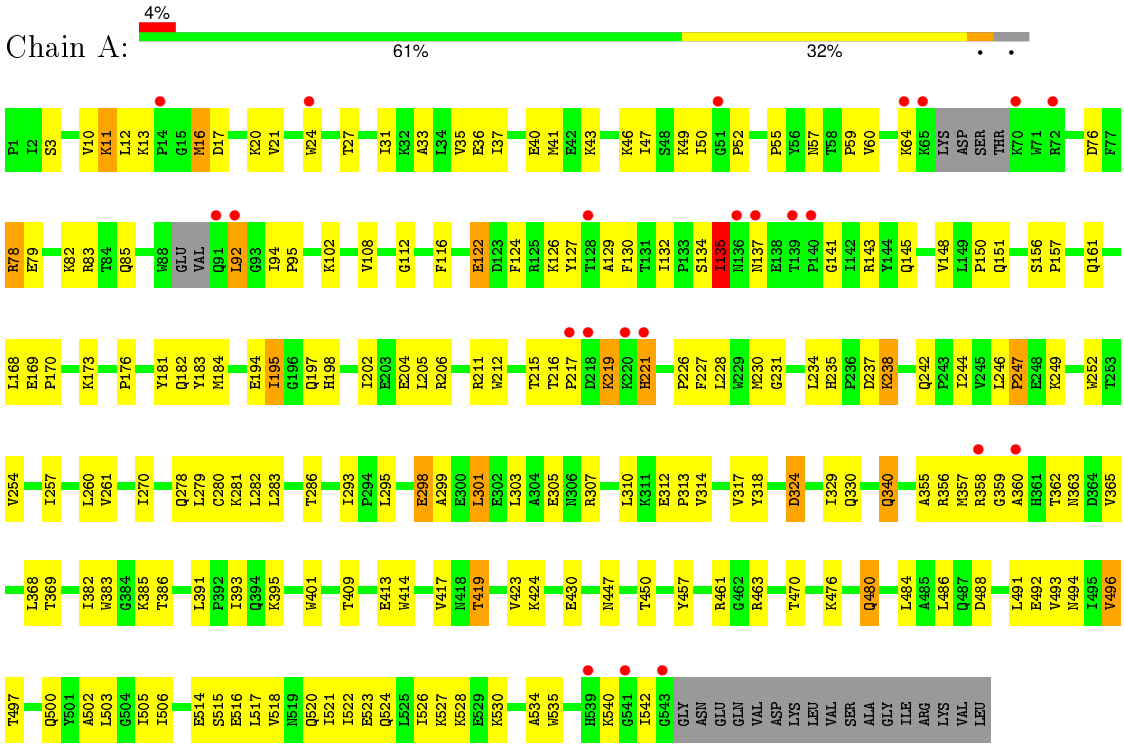
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	40	Total O 40 40	0	0
4	B	16	Total O 16 16	0	0

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.

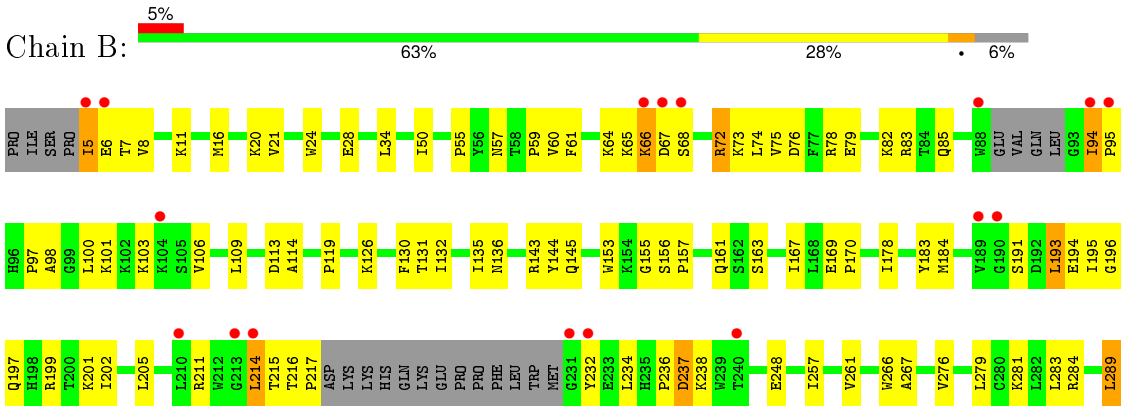
- Molecule 1: HIV-1 REVERSE TRANSCRIPTASE (A-CHAIN)

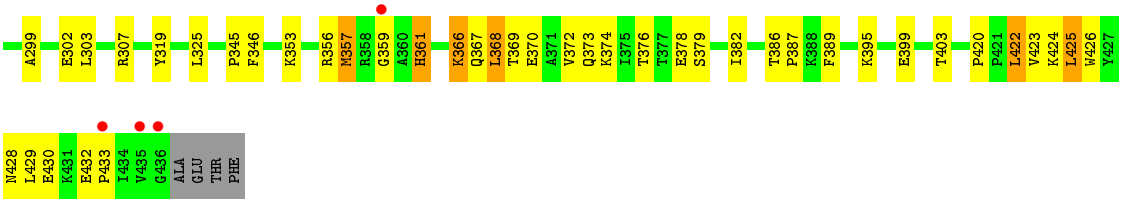
Chain A:



- Molecule 2: HIV-1 REVERSE TRANSCRIPTASE (B-CHAIN)

Chain B:




A299
E302
L303
R307
Y319
L325
P345
F346
K353
R356
M357
R358
G359
A360
H361
K366
Q367
L368
T369
E370
A371
V372
Q373
K374
I375
T376
T377
E378
S379
I382
T386
P387
K388
F389
K395
E399
T403
P420
P421
L422
V423
K424
L425
W426
Y427

N428
L429
E430
K431
E432
P433
I434
V435
G436
ALA
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	140.00Å 111.50Å 73.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.76 – 2.51	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.50) 92.5 (19.76-2.51)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 2.50Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.198 , 0.255 0.208 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	43.3	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 69.6	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 37000 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7888	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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: GCA, CSD

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	0/4495	0.63	0/6104
2	B	0.40	0/3515	0.65	1/4775 (0.0%)
All	All	0.39	0/8010	0.64	1/10879 (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})
2	B	238	LYS	N-CA-C	-5.35	96.55	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4389	0	4436	145	0
2	B	3419	0	3454	113	0
3	A	24	0	26	1	0
4	A	40	0	0	3	0
4	B	16	0	0	0	0
All	All	7888	0	7916	254	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 16.

All (254) 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:215:THR:HG22	1:A:216:THR:H	1.29	0.97
2:B:195:ILE:HD11	2:B:199:ARG:HE	1.30	0.92
1:A:197:GLN:HE21	1:A:197:GLN:HA	1.34	0.90
1:A:260:LEU:HD23	1:A:279:LEU:HD21	1.55	0.86
1:A:542:ILE:HG23	2:B:283:LEU:HB3	1.58	0.85
2:B:57:ASN:HD22	2:B:143:ARG:NH1	1.74	0.85
2:B:236:PRO:O	2:B:237:ASP:HB3	1.76	0.84
2:B:353:LYS:HE2	2:B:430:GLU:HB3	1.57	0.84
1:A:362:THR:HG22	1:A:363:ASN:H	1.43	0.83
2:B:66:LYS:HE2	2:B:66:LYS:HA	1.63	0.80
1:A:357:MET:O	1:A:358:ARG:HG2	1.80	0.80
1:A:280:CSD:C	1:A:281:LYS:N	2.44	0.80
1:A:235:HIS:HB2	1:A:238:LYS:O	1.81	0.80
1:A:17:ASP:O	1:A:83:ARG:HD3	1.83	0.79
1:A:215:THR:HG22	1:A:216:THR:N	1.98	0.78
2:B:378:GLU:O	2:B:382:ILE:HG12	1.84	0.76
2:B:11:LYS:H	2:B:85:GLN:HE21	1.34	0.74
1:A:278:GLN:HG2	1:A:298:GLU:HB3	1.69	0.74
1:A:197:GLN:NE2	1:A:197:GLN:HA	2.02	0.74
2:B:319:TYR:HE2	2:B:325:LEU:HD11	1.51	0.74
1:A:116:PHE:CE1	1:A:151:GLN:HG2	2.24	0.73
2:B:126:LYS:HA	2:B:145:GLN:HE21	1.54	0.73
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.70	0.72
2:B:195:ILE:HD11	2:B:199:ARG:NE	2.04	0.71
2:B:319:TYR:CE2	2:B:325:LEU:HD11	2.26	0.71
1:A:360:ALA:HA	1:A:514:GLU:HG2	1.74	0.70
1:A:102:LYS:NZ	1:A:237:ASP:HA	2.07	0.69
1:A:395:LYS:HD2	1:A:414:TRP:CH2	2.27	0.69
1:A:486:LEU:HB3	1:A:524:GLN:HG2	1.74	0.69
2:B:97:PRO:HG2	2:B:100:LEU:HD22	1.75	0.69
1:A:79:GLU:HG3	1:A:83:ARG:NH1	2.08	0.68
1:A:516:GLU:HA	1:A:516:GLU:OE1	1.94	0.68
1:A:116:PHE:HE1	1:A:151:GLN:HG2	1.57	0.68
1:A:13:LYS:HB2	1:A:16:MET:CE	2.24	0.68
2:B:59:PRO:HG2	2:B:76:ASP:HB3	1.76	0.68
2:B:79:GLU:O	2:B:83:ARG:HG3	1.94	0.68
1:A:217:PRO:HB2	1:A:221:HIS:CE1	2.29	0.67
1:A:13:LYS:HB2	1:A:16:MET:HE1	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:214:LEU:HD23	2:B:214:LEU:H	1.60	0.66
1:A:215:THR:CG2	1:A:216:THR:H	2.05	0.66
1:A:60:VAL:HG21	1:A:130:PHE:CD1	2.32	0.65
2:B:426:TRP:O	2:B:429:LEU:HB2	1.96	0.64
2:B:366:LYS:O	2:B:370:GLU:HG3	1.97	0.64
2:B:97:PRO:HG2	2:B:100:LEU:CD2	2.27	0.64
2:B:215:THR:O	2:B:217:PRO:HD3	1.98	0.63
2:B:359:GLY:HA2	2:B:361:HIS:CE1	2.33	0.62
1:A:11:LYS:HB3	1:A:11:LYS:NZ	2.14	0.62
1:A:279:LEU:HA	1:A:282:LEU:HD23	1.80	0.62
1:A:11:LYS:O	1:A:85:GLN:HB3	1.98	0.62
1:A:41:MET:HE2	1:A:47:ILE:HD13	1.81	0.62
2:B:57:ASN:HD22	2:B:143:ARG:HH11	1.47	0.62
1:A:486:LEU:HB3	1:A:524:GLN:CG	2.30	0.61
1:A:217:PRO:HB2	1:A:221:HIS:HE1	1.64	0.61
2:B:248:GLU:HG2	2:B:307:ARG:NH2	2.15	0.61
1:A:31:ILE:O	1:A:35:VAL:HG23	1.99	0.61
2:B:199:ARG:O	2:B:202:ILE:HB	2.01	0.61
1:A:226:PRO:HB3	1:A:235:HIS:CD2	2.35	0.61
1:A:92:LEU:N	1:A:92:LEU:HD13	2.16	0.61
2:B:50:ILE:HD13	2:B:145:GLN:HB2	1.82	0.61
2:B:420:PRO:HB2	2:B:423:VAL:HG23	1.83	0.61
2:B:64:LYS:HB2	2:B:64:LYS:NZ	2.16	0.61
1:A:516:GLU:O	1:A:520:GLN:HG2	2.01	0.60
2:B:66:LYS:O	2:B:67:ASP:HB3	2.01	0.60
2:B:163:SER:O	2:B:167:ILE:HG13	2.01	0.60
1:A:76:ASP:OD1	1:A:78:ARG:HG3	2.02	0.60
1:A:228:LEU:HD21	1:A:242:GLN:CD	2.22	0.59
2:B:114:ALA:HB2	2:B:214:LEU:HD13	1.85	0.59
1:A:20:LYS:NZ	1:A:55:PRO:HB2	2.17	0.58
2:B:195:ILE:CD1	2:B:199:ARG:HE	2.10	0.58
2:B:257:ILE:HB	2:B:283:LEU:HD11	1.84	0.58
2:B:34:LEU:CD2	2:B:73:LYS:HG3	2.33	0.58
1:A:3:SER:HB3	1:A:212:TRP:O	2.04	0.58
2:B:432:GLU:HB3	2:B:433:PRO:HD2	1.85	0.57
1:A:40:GLU:O	1:A:43:LYS:HG2	2.05	0.57
2:B:395:LYS:HG2	2:B:399:GLU:OE2	2.05	0.57
2:B:279:LEU:HD23	2:B:299:ALA:HB1	1.88	0.56
1:A:219:LYS:H	1:A:219:LYS:CD	2.19	0.56
1:A:317:VAL:HG22	1:A:318:TYR:H	1.71	0.56
2:B:100:LEU:HD23	2:B:100:LEU:H	1.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:MET:HG2	2:B:83:ARG:HB3	1.88	0.55
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.88	0.55
1:A:181:TYR:CE1	1:A:183:TYR:HB2	2.40	0.55
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.41	0.55
2:B:345:PRO:O	2:B:346:PHE:HB2	2.06	0.55
2:B:379:SER:CB	2:B:387:PRO:HD3	2.37	0.55
1:A:500:GLN:HA	1:A:500:GLN:OE1	2.05	0.55
1:A:494:ASN:HB3	2:B:289:LEU:HD22	1.89	0.55
2:B:5:ILE:HG13	2:B:6:GLU:N	2.22	0.55
1:A:417:VAL:HG13	1:A:419:THR:HG22	1.89	0.55
1:A:227:PHE:HB2	1:A:234:LEU:HB2	1.89	0.54
1:A:102:LYS:HZ2	1:A:237:ASP:HA	1.72	0.54
1:A:278:GLN:CG	1:A:298:GLU:HB3	2.37	0.54
2:B:74:LEU:HD12	2:B:75:VAL:N	2.22	0.54
1:A:503:LEU:HA	1:A:506:ILE:HD12	1.89	0.54
2:B:368:LEU:O	2:B:372:VAL:HG23	2.08	0.54
3:A:999:GCA:HG2	3:A:999:GCA:HH3	1.90	0.54
1:A:260:LEU:CD2	1:A:279:LEU:HD21	2.33	0.53
2:B:425:LEU:O	2:B:429:LEU:HD13	2.08	0.53
2:B:281:LYS:HD3	2:B:284:ARG:NH2	2.23	0.53
2:B:85:GLN:O	2:B:85:GLN:HG3	2.08	0.53
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.91	0.53
1:A:226:PRO:HB3	1:A:235:HIS:HD2	1.72	0.53
2:B:369:THR:HG22	2:B:373:GLN:HE21	1.73	0.53
2:B:236:PRO:O	2:B:237:ASP:CB	2.49	0.53
1:A:102:LYS:HZ1	1:A:237:ASP:HA	1.73	0.53
1:A:514:GLU:HG3	1:A:515:SER:N	2.24	0.52
2:B:359:GLY:HA2	2:B:361:HIS:NE2	2.24	0.52
2:B:191:SER:HB2	2:B:193:LEU:HD13	1.91	0.52
2:B:395:LYS:O	2:B:399:GLU:HG3	2.09	0.52
1:A:329:ILE:HD12	1:A:391:LEU:CD2	2.40	0.52
1:A:480:GLN:C	1:A:480:GLN:HE21	2.14	0.52
1:A:206:ARG:HG3	1:A:216:THR:HG21	1.93	0.51
2:B:357:MET:CE	2:B:357:MET:HA	2.41	0.51
2:B:66:LYS:C	2:B:68:SER:H	2.14	0.51
1:A:195:ILE:HD13	1:A:195:ILE:N	2.25	0.51
1:A:270:ILE:HG21	1:A:314:VAL:HG21	1.93	0.51
2:B:424:LYS:O	2:B:428:ASN:HB2	2.10	0.51
2:B:214:LEU:N	2:B:214:LEU:HD23	2.25	0.51
1:A:228:LEU:HD11	1:A:242:GLN:HE22	1.76	0.51
1:A:486:LEU:HD13	1:A:524:GLN:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:ARG:NH1	1:A:488:ASP:O	2.44	0.51
1:A:355:ALA:O	1:A:356:ARG:HD3	2.11	0.51
1:A:317:VAL:HG22	1:A:318:TYR:N	2.26	0.50
1:A:126:LYS:HE3	1:A:127:TYR:CZ	2.45	0.50
1:A:480:GLN:O	1:A:480:GLN:NE2	2.45	0.50
1:A:244:ILE:HB	1:A:310:LEU:HD13	1.93	0.50
2:B:126:LYS:HA	2:B:145:GLN:NE2	2.25	0.50
1:A:329:ILE:HD12	1:A:391:LEU:HD22	1.94	0.50
2:B:195:ILE:O	2:B:199:ARG:HG3	2.11	0.50
1:A:78:ARG:O	1:A:82:LYS:HG3	2.11	0.50
1:A:204:GLU:HG2	4:A:1049:HOH:O	2.11	0.50
1:A:231:GLY:HA2	1:A:242:GLN:NE2	2.27	0.50
1:A:393:ILE:HB	1:A:423:VAL:HG22	1.93	0.50
1:A:324:ASP:OD2	1:A:324:ASP:N	2.45	0.50
2:B:276:VAL:HA	2:B:302:GLU:OE2	2.12	0.50
2:B:267:ALA:HB2	2:B:426:TRP:CZ3	2.47	0.49
1:A:503:LEU:HD21	2:B:422:LEU:HD22	1.94	0.49
2:B:109:LEU:HD23	2:B:216:THR:HG21	1.94	0.49
1:A:522:ILE:O	1:A:526:ILE:HG13	2.12	0.49
1:A:228:LEU:HD21	1:A:242:GLN:NE2	2.27	0.49
2:B:57:ASN:HD22	2:B:143:ARG:HH12	1.56	0.49
2:B:28:GLU:HG3	2:B:135:ILE:HD11	1.95	0.49
2:B:103:LYS:HD2	2:B:191:SER:HA	1.95	0.49
1:A:497:THR:O	1:A:535:TRP:HA	2.12	0.49
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.95	0.49
1:A:11:LYS:HB3	1:A:11:LYS:HZ3	1.77	0.48
1:A:515:SER:HB3	1:A:518:VAL:CG2	2.43	0.48
1:A:383:TRP:O	1:A:385:LYS:HG3	2.13	0.48
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.49	0.48
2:B:100:LEU:HD23	2:B:100:LEU:N	2.27	0.48
2:B:61:PHE:CE2	2:B:74:LEU:HG	2.48	0.48
1:A:515:SER:HB3	1:A:518:VAL:HG23	1.94	0.48
1:A:270:ILE:CG2	1:A:314:VAL:HG21	2.43	0.48
1:A:365:VAL:O	1:A:369:THR:HG23	2.13	0.48
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.96	0.48
2:B:94:ILE:HD12	2:B:95:PRO:HD2	1.95	0.47
1:A:50:ILE:CG2	1:A:145:GLN:HG2	2.45	0.47
2:B:106:VAL:HB	2:B:234:LEU:HB2	1.96	0.47
1:A:523:GLU:O	1:A:527:LYS:HD3	2.14	0.47
2:B:5:ILE:CG1	2:B:6:GLU:N	2.78	0.47
1:A:132:ILE:O	1:A:141:GLY:HA3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:THR:HG22	1:A:363:ASN:N	2.20	0.47
2:B:211:ARG:O	2:B:211:ARG:HD3	2.15	0.46
1:A:13:LYS:HB2	1:A:16:MET:HE3	1.95	0.46
2:B:156:SER:HB2	2:B:157:PRO:CD	2.45	0.46
1:A:382:ILE:O	2:B:136:ASN:HB2	2.16	0.46
2:B:237:ASP:CG	2:B:237:ASP:O	2.54	0.46
1:A:476:LYS:O	1:A:480:GLN:HB2	2.16	0.46
1:A:161:GLN:NE2	1:A:182:GLN:NE2	2.63	0.46
1:A:228:LEU:HD22	1:A:228:LEU:HA	1.82	0.46
1:A:148:VAL:O	1:A:150:PRO:HD3	2.16	0.45
1:A:37:ILE:O	1:A:40:GLU:HB3	2.16	0.45
1:A:17:ASP:O	1:A:83:ARG:CD	2.60	0.45
2:B:72:ARG:HH11	2:B:72:ARG:HG3	1.81	0.45
2:B:281:LYS:HD3	2:B:284:ARG:CZ	2.46	0.45
1:A:122:GLU:CD	1:A:122:GLU:H	2.19	0.45
2:B:100:LEU:H	2:B:100:LEU:CD2	2.29	0.45
2:B:94:ILE:HA	2:B:95:PRO:HD3	1.86	0.45
2:B:425:LEU:HD12	2:B:425:LEU:HA	1.83	0.45
2:B:65:LYS:O	2:B:68:SER:HB3	2.17	0.45
1:A:254:VAL:HG22	1:A:286:THR:HG21	1.99	0.45
1:A:542:ILE:O	1:A:542:ILE:HG22	2.16	0.45
1:A:502:ALA:O	1:A:506:ILE:HG13	2.16	0.45
1:A:83:ARG:HG3	1:A:83:ARG:HH11	1.81	0.44
1:A:413:GLU:HG3	4:A:1014:HOH:O	2.15	0.44
1:A:246:LEU:HB2	1:A:307:ARG:NH1	2.32	0.44
2:B:131:THR:OG1	2:B:143:ARG:HD2	2.17	0.44
1:A:20:LYS:HZ1	1:A:55:PRO:HB2	1.82	0.44
2:B:132:ILE:HD12	2:B:132:ILE:N	2.32	0.44
1:A:401:TRP:CZ3	1:A:409:THR:HG21	2.53	0.44
2:B:266:TRP:CZ3	2:B:426:TRP:CG	3.06	0.44
2:B:183:TYR:O	2:B:184:MET:HB2	2.17	0.44
2:B:11:LYS:HE3	2:B:11:LYS:HB2	1.76	0.44
2:B:261:VAL:HG13	2:B:276:VAL:HG21	1.99	0.44
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.17	0.44
2:B:195:ILE:HG23	2:B:196:GLY:N	2.33	0.44
2:B:178:ILE:CD1	2:B:201:LYS:HG2	2.47	0.44
1:A:492:GLU:HA	1:A:530:LYS:O	2.17	0.44
2:B:57:ASN:ND2	2:B:143:ARG:NH1	2.53	0.44
1:A:283:LEU:O	1:A:286:THR:HG23	2.18	0.43
1:A:280:CSD:O	1:A:281:LYS:N	2.51	0.43
2:B:34:LEU:HD21	2:B:73:LYS:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:ASN:ND2	2:B:143:ARG:HH11	2.14	0.43
1:A:198:HIS:O	1:A:202:ILE:HG12	2.19	0.43
2:B:109:LEU:HG	2:B:216:THR:HG22	2.00	0.43
2:B:72:ARG:NH1	2:B:72:ARG:HG3	2.33	0.43
1:A:496:VAL:HA	1:A:534:ALA:O	2.18	0.43
1:A:417:VAL:O	1:A:417:VAL:HG13	2.19	0.43
2:B:178:ILE:HD11	2:B:201:LYS:HG2	2.00	0.43
1:A:64:LYS:HE2	1:A:64:LYS:HB3	1.82	0.43
1:A:330:GLN:OE1	1:A:340:GLN:OE1	2.37	0.43
1:A:503:LEU:HD21	2:B:422:LEU:CD2	2.48	0.43
1:A:254:VAL:HG22	1:A:293:ILE:HD11	2.00	0.43
1:A:46:LYS:HE3	1:A:116:PHE:O	2.19	0.42
1:A:33:ALA:O	1:A:36:GLU:HB3	2.19	0.42
1:A:169:GLU:N	1:A:170:PRO:HD2	2.34	0.42
2:B:78:ARG:O	2:B:82:LYS:HG3	2.19	0.42
2:B:11:LYS:N	2:B:85:GLN:HE21	2.09	0.42
1:A:27:THR:O	1:A:31:ILE:HG13	2.19	0.42
1:A:94:ILE:HA	1:A:95:PRO:HD3	1.86	0.42
2:B:98:ALA:O	2:B:101:LYS:HG2	2.19	0.42
1:A:10:VAL:HG12	1:A:124:PHE:CD1	2.54	0.42
1:A:430:GLU:HG2	4:A:1018:HOH:O	2.19	0.42
1:A:362:THR:CG2	1:A:363:ASN:H	2.24	0.42
1:A:13:LYS:HD2	1:A:16:MET:HE1	2.01	0.42
2:B:11:LYS:O	2:B:85:GLN:HG2	2.19	0.42
1:A:252:TRP:CD1	1:A:295:LEU:HD11	2.54	0.42
1:A:194:GLU:O	1:A:197:GLN:N	2.53	0.41
1:A:486:LEU:O	1:A:528:LYS:NZ	2.52	0.41
1:A:116:PHE:HE1	1:A:151:GLN:CG	2.29	0.41
2:B:376:THR:CG2	2:B:386:THR:HG22	2.50	0.41
1:A:312:GLU:OE1	1:A:313:PRO:HD2	2.20	0.41
1:A:134:SER:O	1:A:135:ILE:C	2.58	0.41
1:A:282:LEU:HD21	1:A:299:ALA:HB2	2.02	0.41
1:A:173:LYS:O	1:A:176:PRO:HD3	2.20	0.41
1:A:301:LEU:O	1:A:305:GLU:HG3	2.21	0.41
2:B:21:VAL:HB	2:B:59:PRO:HD3	2.03	0.41
1:A:480:GLN:HE22	1:A:484:LEU:HG	1.86	0.41
2:B:194:GLU:HG3	2:B:196:GLY:H	1.85	0.41
1:A:486:LEU:CD1	1:A:521:ILE:HG23	2.51	0.41
1:A:257:ILE:O	1:A:261:VAL:HG23	2.21	0.41
2:B:215:THR:C	2:B:217:PRO:HD3	2.41	0.40
2:B:64:LYS:HB2	2:B:64:LYS:HZ2	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:LEU:HA	1:A:247:PRO:HD2	1.87	0.40
1:A:57:ASN:HA	1:A:129:ALA:O	2.21	0.40
2:B:61:PHE:CD1	2:B:403:THR:HB	2.56	0.40
1:A:252:TRP:NE1	1:A:295:LEU:HD11	2.37	0.40
1:A:457:TYR:C	1:A:457:TYR:CD1	2.94	0.40
2:B:57:ASN:ND2	2:B:131:THR:OG1	2.55	0.40
1:A:298:GLU:OE1	1:A:298:GLU:N	2.54	0.40
1:A:12:LEU:HD22	1:A:83:ARG:HB3	2.03	0.40
1:A:49:LYS:HA	1:A:143:ARG:O	2.21	0.40
2:B:153:TRP:CH2	2:B:155:GLY:HA3	2.57	0.40
2:B:356:ARG:HB2	2:B:367:GLN:HG2	2.03	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	529/560 (94%)	485 (92%)	38 (7%)	6 (1%)	17	31
2	B	409/440 (93%)	377 (92%)	28 (7%)	4 (1%)	19	34
All	All	938/1000 (94%)	862 (92%)	66 (7%)	10 (1%)	17	31

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	193	LEU
2	B	237	ASP
1	A	112	GLY
1	A	135	ILE
2	B	232	TYR
1	A	359	GLY
2	B	361	HIS

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Mol	Chain	Res	Type
1	A	247	PRO
1	A	16	MET
1	A	52	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	479/499 (96%)	443 (92%)	36 (8%)	17	31
2	B	376/400 (94%)	355 (94%)	21 (6%)	26	47
All	All	855/899 (95%)	798 (93%)	57 (7%)	20	37

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	24	TRP
1	A	78	ARG
1	A	92	LEU
1	A	108	VAL
1	A	122	GLU
1	A	135	ILE
1	A	137	ASN
1	A	168	LEU
1	A	184	MET
1	A	195	ILE
1	A	205	LEU
1	A	211	ARG
1	A	219	LYS
1	A	221	HIS
1	A	230	MET
1	A	238	LYS
1	A	249	LYS
1	A	298	GLU
1	A	301	LEU

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Mol	Chain	Res	Type
1	A	303	LEU
1	A	324	ASP
1	A	340	GLN
1	A	368	LEU
1	A	386	THR
1	A	419	THR
1	A	424	LYS
1	A	461	ARG
1	A	470	THR
1	A	480	GLN
1	A	491	LEU
1	A	493	VAL
1	A	496	VAL
1	A	505	ILE
1	A	517	LEU
1	A	540	LYS
2	B	5	ILE
2	B	8	VAL
2	B	20	LYS
2	B	24	TRP
2	B	55	PRO
2	B	66	LYS
2	B	72	ARG
2	B	94	ILE
2	B	113	ASP
2	B	161	GLN
2	B	197	GLN
2	B	205	LEU
2	B	214	LEU
2	B	289	LEU
2	B	303	LEU
2	B	357	MET
2	B	366	LYS
2	B	368	LEU
2	B	374	LYS
2	B	422	LEU
2	B	425	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN

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Mol	Chain	Res	Type
1	A	161	GLN
1	A	182	GLN
1	A	197	GLN
1	A	235	HIS
1	A	242	GLN
1	A	330	GLN
1	A	361	HIS
1	A	480	GLN
2	B	57	ASN
2	B	85	GLN
2	B	145	GLN
2	B	147	ASN
2	B	151	GLN
2	B	161	GLN
2	B	269	GLN
2	B	278	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	0.69	0	3,8,10	4.11	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	6.91	116.91	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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	280	CSD	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GCA	A	999	-	17,25,25	1.23	2 (11%)	23,35,35	3.33	5 (21%)

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	GCA	A	999	-	-	0/10/12/12	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	GCA	C7-C12	2.24	1.42	1.39
3	A	999	GCA	C11-N10	3.77	1.40	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	999	GCA	C12-C11-N10	-5.69	116.08	125.18
3	A	999	GCA	C11-C12-CF	-2.73	114.21	122.83
3	A	999	GCA	CA-N8-C7	2.82	123.49	120.26
3	A	999	GCA	C7-C12-CF	4.49	126.51	122.10
3	A	999	GCA	C11-N10-C9	13.17	126.64	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	GCA	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	536/560 (95%)	-0.17	23 (4%)	39	44	20, 52, 109, 150	0
2	B	415/440 (94%)	-0.16	21 (5%)	32	36	18, 51, 111, 145	0
All	All	951/1000 (95%)	-0.17	44 (4%)	36	41	18, 51, 111, 150	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	88	TRP	8.8
1	A	91	GLN	6.0
1	A	137	ASN	6.0
1	A	92	LEU	5.9
2	B	231	GLY	5.5
1	A	539	HIS	4.6
2	B	67	ASP	4.5
1	A	139	THR	4.4
2	B	232	TYR	4.4
2	B	5	ILE	4.3
1	A	221	HIS	4.2
2	B	214	LEU	4.0
2	B	6	GLU	3.7
1	A	358	ARG	3.7
2	B	435	VAL	3.7
1	A	218	ASP	3.6
2	B	66	LYS	3.3
1	A	64	LYS	3.3
1	A	65	LYS	3.2
2	B	189	VAL	3.2
2	B	94	ILE	3.2
1	A	360	ALA	3.0
1	A	136	ASN	3.0
2	B	190	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	213	GLY	3.0
2	B	240	THR	2.9
1	A	24	TRP	2.8
2	B	68	SER	2.8
1	A	70	LYS	2.7
1	A	217	PRO	2.7
1	A	220	LYS	2.5
1	A	541	GLY	2.4
1	A	140	PRO	2.3
1	A	543	GLY	2.3
2	B	95	PRO	2.3
2	B	104	LYS	2.3
1	A	51	GLY	2.3
2	B	210	LEU	2.2
2	B	433	PRO	2.1
2	B	436	GLY	2.1
1	A	14	PRO	2.1
1	A	72	ARG	2.1
2	B	359	GLY	2.1
1	A	128	THR	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	0.92	0.12	-	43,52,66,67	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	GCA	A	999	24/24	0.97	0.16	1.00	13,29,39,40	0

6.5 Other polymers (i)

There are no such residues in this entry.