



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 12:00 pm GMT

PDB ID : 3DLE
Title : Crystal structure of hiv-1 reverse transcriptase in complex with GF128590.
Authors : Ren, J.; Chamberlain, P.P.; Stammers, D.K.
Deposited on : 2008-06-27
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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

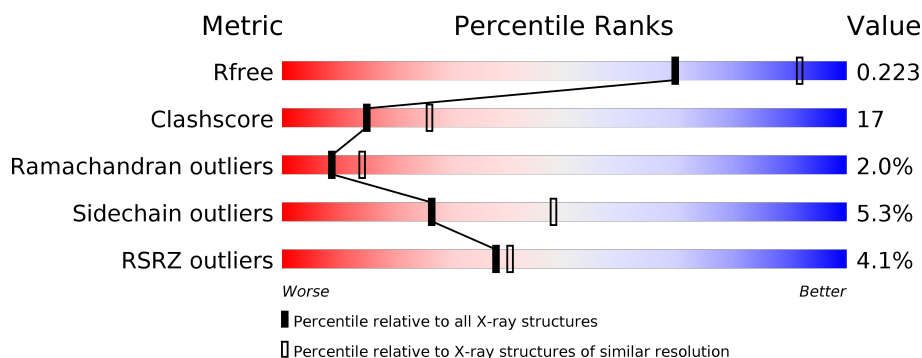
1 Overall quality at a glance

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))
R_{free}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (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 $\leq 5\%$. 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	<div> <div>4%</div> <div> <div></div> <div>57%</div> <div>35%</div> <div>• •</div> </div> </div>
2	B	440	<div> <div>3%</div> <div> <div></div> <div>59%</div> <div>31%</div> <div>• 8%</div> </div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7865 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.

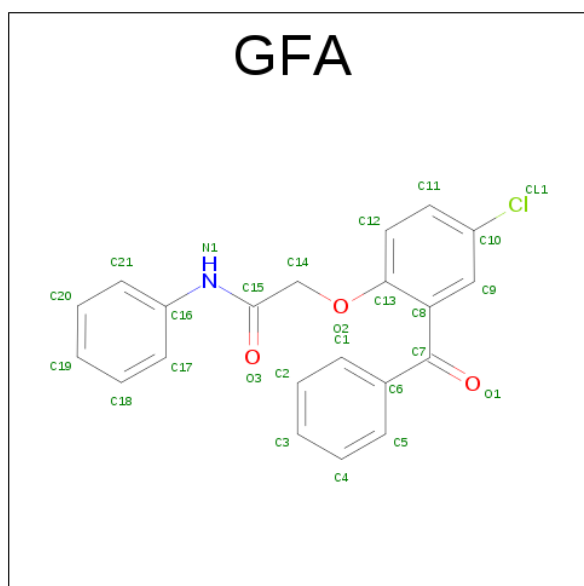
- Molecule 1 is a protein called Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	0	0	0
			4377	2834	727	808	8			

- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	403	Total	C	N	O	S	0	0	0
			3333	2165	555	606	7			

- Molecule 3 is 2-[4-CHLORO-2-(PHENYLCARBONYL)PHENOXY]-N-PHENYLACETAMIDE (three-letter code: GFA) (formula: C₂₁H₁₆ClNO₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			26	21	1	1	3		

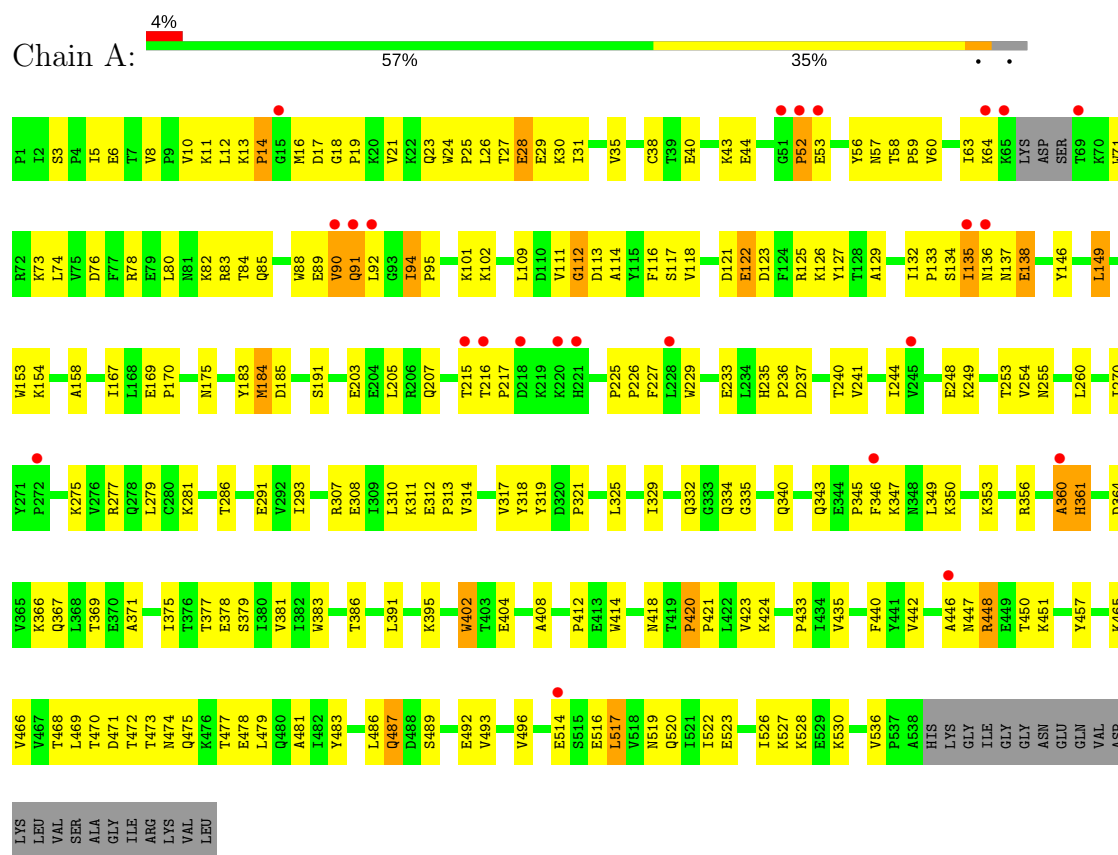
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	74	Total 74	O 74	0	0
4	B	55	Total 55	O 55	0	0

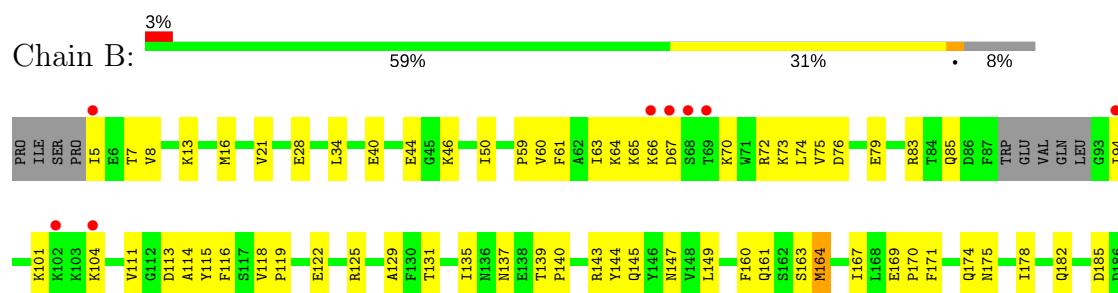
3 Residue-property plots

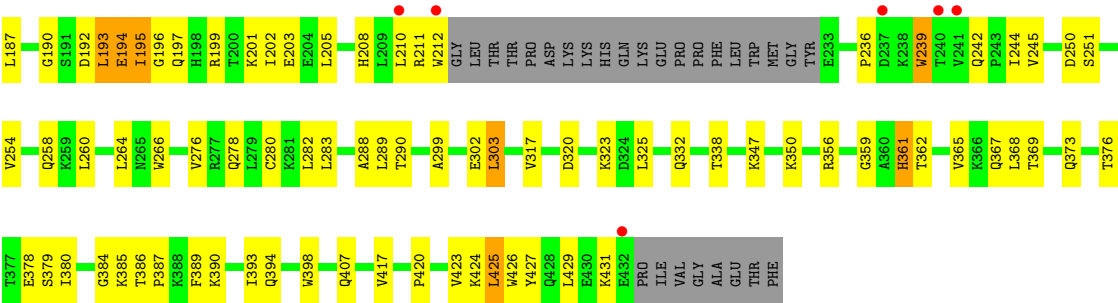
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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



• Molecule 2: p51 RT





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	137.89Å 110.25Å 72.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.79 – 2.50 25.79 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.2 (25.79-2.50) 96.3 (25.79-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.214 , 0.296 0.216 , 0.223	Depositor DCC
R_{free} test set	1863 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	50.8	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 64.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7865	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: CSD, GFA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.40	0/4484	0.64	0/6095
2	B	0.40	0/3424	0.63	0/4647
All	All	0.40	0/7908	0.63	0/10742

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

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	4377	0	4424	151	0
2	B	3333	0	3369	123	0
3	A	26	0	16	0	0
4	A	74	0	0	3	0
4	B	55	0	0	1	0
All	All	7865	0	7809	263	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 17.

All (263) 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:195:ILE:HD11	2:B:199:ARG:HE	1.14	1.07
1:A:469:LEU:HD12	1:A:477:THR:HG22	1.57	0.86
2:B:195:ILE:HD11	2:B:199:ARG:NE	1.94	0.82
1:A:448:ARG:HH11	1:A:448:ARG:HG3	1.49	0.78
2:B:195:ILE:HG23	2:B:196:GLY:H	1.45	0.78
2:B:195:ILE:CD1	2:B:199:ARG:HE	1.96	0.78
2:B:67:ASP:HB3	2:B:70:LYS:HD3	1.65	0.78
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.65	0.77
2:B:70:LYS:HD2	2:B:70:LYS:H	1.50	0.77
2:B:161:GLN:HA	2:B:161:GLN:HE21	1.48	0.76
2:B:175:ASN:HD21	2:B:201:LYS:NZ	1.82	0.76
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.68	0.75
2:B:61:PHE:CE1	2:B:74:LEU:HD23	2.21	0.75
2:B:332:GLN:NE2	2:B:424:LYS:HE2	2.02	0.74
2:B:356:ARG:HB2	2:B:367:GLN:HG2	1.70	0.74
1:A:377:THR:O	1:A:381:VAL:HG23	1.89	0.73
2:B:125:ARG:HE	2:B:147:ASN:HA	1.54	0.72
2:B:79:GLU:O	2:B:83:ARG:HG3	1.89	0.72
2:B:254:VAL:O	2:B:258:GLN:HG3	1.90	0.72
2:B:163:SER:O	2:B:167:ILE:HG23	1.89	0.71
1:A:17:ASP:O	1:A:83:ARG:HD3	1.89	0.71
2:B:175:ASN:HD21	2:B:201:LYS:HZ2	1.36	0.71
1:A:248:GLU:HG2	1:A:307:ARG:CZ	2.21	0.71
2:B:420:PRO:HB2	2:B:423:VAL:HG23	1.74	0.70
1:A:31:ILE:O	1:A:35:VAL:HG23	1.92	0.70
2:B:60:VAL:HG23	2:B:75:VAL:HG22	1.73	0.69
1:A:448:ARG:NH1	1:A:448:ARG:HG3	2.02	0.69
1:A:317:VAL:HG21	1:A:347:LYS:HB3	1.74	0.69
2:B:161:GLN:HA	2:B:161:GLN:NE2	2.07	0.68
1:A:85:GLN:O	1:A:154:LYS:HE3	1.93	0.68
1:A:335:GLY:HA2	1:A:367:GLN:OE1	1.94	0.67
1:A:277:ARG:O	1:A:281:LYS:HG3	1.94	0.67
2:B:70:LYS:N	2:B:70:LYS:HD2	2.09	0.67
1:A:516:GLU:O	1:A:520:GLN:HG3	1.95	0.67
2:B:208:HIS:O	2:B:211:ARG:HG2	1.96	0.66
2:B:365:VAL:O	2:B:369:THR:HG23	1.95	0.66
1:A:248:GLU:HG2	1:A:307:ARG:NH2	2.11	0.66
2:B:278:GLN:HB2	2:B:302:GLU:OE2	1.95	0.65
2:B:59:PRO:HG2	2:B:76:ASP:HB3	1.79	0.65
2:B:195:ILE:HG23	2:B:196:GLY:N	2.12	0.65
1:A:329:ILE:HD12	1:A:391:LEU:CD2	2.28	0.64
1:A:118:VAL:HB	1:A:149:LEU:HD22	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:ASN:ND2	2:B:201:LYS:NZ	2.45	0.64
1:A:312:GLU:HG2	1:A:313:PRO:HD2	1.80	0.63
1:A:89:GLU:C	1:A:91:GLN:H	2.01	0.63
2:B:239:TRP:CH2	2:B:378:GLU:HG2	2.34	0.63
2:B:320:ASP:OD2	2:B:323:LYS:HE3	1.99	0.63
1:A:112:GLY:C	1:A:114:ALA:H	2.02	0.63
1:A:418:ASN:O	1:A:420:PRO:HD3	1.98	0.62
2:B:260:LEU:HD21	2:B:303:LEU:HD21	1.82	0.62
1:A:73:LYS:HG2	1:A:74:LEU:N	2.13	0.62
2:B:245:VAL:CG2	2:B:431:LYS:HB2	2.29	0.62
1:A:13:LYS:HB3	1:A:14:PRO:HD2	1.81	0.62
1:A:90:VAL:HG12	1:A:158:ALA:HB2	1.81	0.61
1:A:114:ALA:HA	1:A:117:SER:OG	2.00	0.61
1:A:116:PHE:HE1	1:A:146:TYR:HE1	1.48	0.61
1:A:254:VAL:HG23	1:A:293:ILE:HD11	1.81	0.61
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.83	0.61
2:B:139:THR:HG22	2:B:140:PRO:O	2.01	0.60
1:A:420:PRO:HA	1:A:421:PRO:C	2.22	0.60
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.36	0.60
2:B:359:GLY:HA2	2:B:361:HIS:CE1	2.37	0.60
2:B:137:ASN:C	2:B:139:THR:H	2.05	0.60
1:A:203:GLU:O	1:A:207:GLN:HB2	2.01	0.60
1:A:293:ILE:N	1:A:293:ILE:HD12	2.17	0.59
2:B:104:LYS:HD2	2:B:192:ASP:O	2.02	0.59
2:B:65:LYS:HG3	2:B:66:LYS:H	1.66	0.59
1:A:3:SER:HB3	1:A:5:ILE:HG13	1.83	0.59
1:A:317:VAL:HG12	1:A:318:TYR:N	2.19	0.58
1:A:408:ALA:HB3	2:B:393:ILE:HB	1.86	0.58
1:A:89:GLU:HA	4:A:1006:HOH:O	2.03	0.58
2:B:70:LYS:CD	2:B:70:LYS:H	2.17	0.58
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.04	0.58
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.39	0.57
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.39	0.57
2:B:245:VAL:HG23	2:B:431:LYS:HB2	1.87	0.57
1:A:483:TYR:O	1:A:487:GLN:HG2	2.03	0.57
1:A:492:GLU:HA	1:A:530:LYS:O	2.04	0.56
1:A:335:GLY:HA3	1:A:356:ARG:HD2	1.88	0.56
1:A:254:VAL:HG22	1:A:286:THR:HG21	1.87	0.56
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.40	0.56
1:A:76:ASP:OD2	1:A:78:ARG:HG3	2.05	0.56
2:B:239:TRP:CZ2	2:B:378:GLU:HG2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:LYS:O	2:B:236:PRO:HB2	2.07	0.55
1:A:522:ILE:O	1:A:526:ILE:HG13	2.07	0.55
2:B:356:ARG:CB	2:B:367:GLN:HG2	2.36	0.55
1:A:78:ARG:O	1:A:82:LYS:HG3	2.07	0.55
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.47	0.55
1:A:57:ASN:HA	1:A:129:ALA:O	2.07	0.55
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.88	0.54
1:A:356:ARG:HG2	1:A:356:ARG:HH11	1.72	0.54
2:B:13:LYS:HB2	2:B:16:MET:HG3	1.89	0.54
1:A:225:PRO:HA	1:A:226:PRO:C	2.28	0.54
1:A:366:LYS:NZ	2:B:394:GLN:NE2	2.56	0.54
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.89	0.54
2:B:65:LYS:HA	2:B:407:GLN:HG2	1.90	0.53
1:A:13:LYS:HB3	1:A:14:PRO:CD	2.39	0.53
2:B:426:TRP:O	2:B:429:LEU:HB2	2.09	0.53
1:A:254:VAL:CG2	1:A:293:ILE:HD11	2.38	0.53
1:A:371:ALA:O	1:A:375:ILE:HG13	2.08	0.53
1:A:317:VAL:HG12	1:A:318:TYR:H	1.73	0.53
1:A:402:TRP:CD1	1:A:402:TRP:C	2.82	0.53
2:B:129:ALA:HA	2:B:144:TYR:O	2.09	0.52
1:A:94:ILE:H	1:A:94:ILE:CD1	2.22	0.52
1:A:442:VAL:HG12	1:A:457:TYR:HB3	1.90	0.52
2:B:211:ARG:HG3	2:B:212:TRP:CD1	2.45	0.52
1:A:248:GLU:O	1:A:249:LYS:HG3	2.09	0.52
1:A:63:ILE:O	1:A:63:ILE:HD12	2.10	0.52
2:B:194:GLU:HG3	2:B:197:GLN:H	1.74	0.52
2:B:28:GLU:HG3	2:B:135:ILE:HD11	1.92	0.52
2:B:65:LYS:HE2	2:B:72:ARG:HD2	1.91	0.52
1:A:345:PRO:O	1:A:346:PHE:HB2	2.09	0.52
1:A:122:GLU:CD	1:A:122:GLU:H	2.13	0.52
1:A:244:ILE:HG23	1:A:310:LEU:HD13	1.92	0.51
1:A:95:PRO:HB2	1:A:229:TRP:HH2	1.75	0.51
1:A:244:ILE:O	1:A:244:ILE:HG23	2.11	0.51
1:A:314:VAL:HG23	1:A:314:VAL:O	2.10	0.51
2:B:317:VAL:HG22	2:B:347:LYS:HB3	1.92	0.51
1:A:479:LEU:HB2	1:A:517:LEU:HD13	1.93	0.51
1:A:88:TRP:CE3	1:A:88:TRP:HA	2.45	0.51
2:B:390:LYS:HD2	2:B:417:VAL:HG11	1.93	0.51
1:A:241:VAL:HG21	1:A:270:ILE:HG21	1.93	0.50
1:A:307:ARG:O	1:A:311:LYS:HG3	2.10	0.50
1:A:94:ILE:HD13	1:A:94:ILE:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:ASN:HA	1:A:448:ARG:NH2	2.27	0.50
2:B:245:VAL:HG21	2:B:431:LYS:HB2	1.94	0.50
1:A:402:TRP:CZ2	2:B:362:THR:HA	2.46	0.50
2:B:376:THR:O	2:B:380:ILE:HG13	2.11	0.50
1:A:225:PRO:HG3	1:A:227:PHE:CZ	2.46	0.49
2:B:266:TRP:HZ3	2:B:426:TRP:CD1	2.30	0.49
1:A:312:GLU:CG	1:A:313:PRO:HD2	2.42	0.49
1:A:440:PHE:CE1	1:A:489:SER:HB3	2.47	0.49
1:A:84:THR:HG21	1:A:153:TRP:CZ2	2.48	0.49
1:A:448:ARG:HH11	1:A:448:ARG:CG	2.19	0.49
1:A:475:GLN:HA	1:A:478:GLU:OE1	2.12	0.49
2:B:13:LYS:HB2	2:B:16:MET:CG	2.43	0.49
1:A:95:PRO:HG3	2:B:137:ASN:HB2	1.94	0.49
1:A:134:SER:O	1:A:135:ILE:C	2.50	0.49
1:A:486:LEU:O	1:A:528:LYS:NZ	2.42	0.48
1:A:30:LYS:HE2	1:A:71:TRP:CH2	2.48	0.48
2:B:63:ILE:C	2:B:64:LYS:HG3	2.33	0.48
2:B:356:ARG:HB2	2:B:367:GLN:CG	2.42	0.48
2:B:94:ILE:HG21	2:B:182:GLN:O	2.14	0.48
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.95	0.48
2:B:369:THR:O	2:B:373:GLN:HG3	2.13	0.48
1:A:112:GLY:O	1:A:114:ALA:N	2.46	0.48
2:B:125:ARG:NE	2:B:147:ASN:HA	2.24	0.48
2:B:276:VAL:HA	2:B:302:GLU:OE1	2.14	0.48
1:A:102:LYS:HE3	1:A:236:PRO:O	2.13	0.48
2:B:276:VAL:CA	2:B:302:GLU:OE1	2.62	0.48
1:A:112:GLY:C	1:A:114:ALA:N	2.66	0.48
2:B:175:ASN:ND2	2:B:201:LYS:HZ1	2.11	0.48
2:B:242:GLN:OE1	2:B:242:GLN:HA	2.13	0.48
1:A:5:ILE:HD11	1:A:167:ILE:HD11	1.96	0.47
2:B:376:THR:CG2	2:B:386:THR:HG22	2.45	0.47
1:A:126:LYS:HE2	1:A:127:TYR:CZ	2.50	0.47
1:A:23:GLN:OE1	1:A:60:VAL:HG12	2.15	0.47
1:A:260:LEU:HD23	1:A:279:LEU:HD22	1.97	0.47
1:A:334:GLN:O	1:A:356:ARG:HD3	2.14	0.47
2:B:50:ILE:CG2	2:B:145:GLN:HG2	2.44	0.47
2:B:350:LYS:HE3	2:B:378:GLU:OE1	2.15	0.47
4:A:1117:HOH:O	2:B:288:ALA:HB1	2.14	0.47
2:B:34:LEU:CD2	2:B:73:LYS:HG3	2.45	0.47
2:B:423:VAL:O	2:B:427:TYR:HD2	1.98	0.47
1:A:89:GLU:C	1:A:91:GLN:N	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:GLU:CG	2:B:135:ILE:HD11	2.45	0.46
1:A:28:GLU:HG3	1:A:29:GLU:N	2.30	0.46
1:A:319:TYR:CE2	1:A:343:GLN:NE2	2.83	0.46
1:A:446:ALA:HB2	1:A:477:THR:HG21	1.98	0.46
1:A:90:VAL:O	1:A:90:VAL:HG23	2.14	0.46
2:B:122:GLU:HA	2:B:125:ARG:NH1	2.31	0.46
2:B:380:ILE:O	2:B:384:GLY:N	2.45	0.46
2:B:61:PHE:CZ	2:B:74:LEU:HD23	2.51	0.46
1:A:472:THR:OG1	1:A:473:THR:N	2.48	0.46
1:A:38:CYS:SG	1:A:73:LYS:NZ	2.74	0.46
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.96	0.46
1:A:94:ILE:O	1:A:94:ILE:HG12	2.15	0.46
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.51	0.46
1:A:27:THR:O	1:A:31:ILE:HG13	2.16	0.46
2:B:67:ASP:CB	2:B:70:LYS:HD3	2.42	0.46
1:A:350:LYS:HE2	1:A:378:GLU:OE2	2.16	0.46
1:A:440:PHE:CZ	1:A:489:SER:HB3	2.50	0.46
2:B:111:VAL:HG22	2:B:185:ASP:O	2.15	0.46
2:B:379:SER:CB	2:B:387:PRO:HD3	2.46	0.46
1:A:329:ILE:HD12	1:A:391:LEU:HD22	1.98	0.45
1:A:360:ALA:O	1:A:361:HIS:HB3	2.15	0.45
1:A:18:GLY:HA3	1:A:56:TYR:CD1	2.51	0.45
1:A:3:SER:CB	1:A:5:ILE:HG13	2.46	0.45
2:B:61:PHE:HE1	2:B:74:LEU:HD23	1.77	0.45
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.98	0.45
2:B:423:VAL:HG21	4:B:1088:HOH:O	2.15	0.45
1:A:215:THR:HG22	1:A:216:THR:N	2.31	0.45
1:A:40:GLU:O	1:A:44:GLU:HG3	2.16	0.45
1:A:88:TRP:O	1:A:89:GLU:C	2.54	0.45
2:B:282:LEU:HD11	2:B:299:ALA:CB	2.46	0.45
1:A:183:TYR:CD1	1:A:184:MET:HB2	2.52	0.45
1:A:253:THR:HA	1:A:291:GLU:O	2.16	0.45
1:A:101:LYS:HD3	1:A:321:PRO:CG	2.46	0.45
1:A:519:ASN:O	1:A:523:GLU:HG2	2.17	0.45
2:B:376:THR:HG23	2:B:386:THR:HG22	1.98	0.45
1:A:135:ILE:HG22	1:A:136:ASN:N	2.32	0.45
2:B:325:LEU:HD12	2:B:385:LYS:HG3	1.99	0.45
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.98	0.45
1:A:122:GLU:HA	1:A:125:ARG:CD	2.47	0.44
1:A:94:ILE:CD1	1:A:94:ILE:N	2.80	0.44
1:A:517:LEU:HA	1:A:520:GLN:OE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:202:ILE:O	2:B:205:LEU:N	2.50	0.44
1:A:137:ASN:O	1:A:138:GLU:O	2.35	0.44
1:A:8:VAL:O	1:A:121:ASP:HB2	2.17	0.44
2:B:195:ILE:CG2	2:B:196:GLY:H	2.24	0.44
2:B:425:LEU:O	2:B:429:LEU:HD13	2.18	0.44
2:B:170:PRO:O	2:B:174:GLN:HG3	2.17	0.44
2:B:28:GLU:CB	2:B:135:ILE:HD11	2.47	0.44
2:B:193:LEU:HD13	2:B:197:GLN:NE2	2.33	0.44
2:B:171:PHE:CD2	2:B:205:LEU:HD12	2.52	0.44
1:A:447:ASN:O	1:A:451:LYS:N	2.47	0.43
2:B:131:THR:HG1	2:B:143:ARG:HH11	1.66	0.43
1:A:58:THR:CG2	1:A:59:PRO:HD2	2.48	0.43
1:A:402:TRP:CH2	2:B:362:THR:HA	2.52	0.43
1:A:319:TYR:HE2	1:A:343:GLN:NE2	2.17	0.43
1:A:63:ILE:C	1:A:63:ILE:HD12	2.38	0.43
2:B:244:ILE:HG13	2:B:426:TRP:CZ2	2.54	0.43
2:B:46:LYS:HE3	2:B:116:PHE:CD1	2.54	0.43
1:A:457:TYR:C	1:A:457:TYR:CD1	2.92	0.42
1:A:470:THR:O	1:A:471:ASP:HB3	2.19	0.42
1:A:325:LEU:HA	1:A:325:LEU:HD12	1.82	0.42
1:A:379:SER:HA	1:A:383:TRP:CE3	2.54	0.42
1:A:364:ASP:HB3	1:A:423:VAL:HG13	2.00	0.42
2:B:137:ASN:C	2:B:139:THR:N	2.72	0.42
2:B:266:TRP:CZ3	2:B:426:TRP:CG	3.08	0.42
1:A:448:ARG:H	1:A:448:ARG:CZ	2.32	0.42
1:A:225:PRO:HG3	1:A:227:PHE:CE2	2.54	0.42
1:A:536:VAL:HG12	2:B:258:GLN:HB3	2.01	0.42
1:A:233:GLU:HB2	1:A:240:THR:OG1	2.20	0.42
2:B:160:PHE:CE1	2:B:164:MET:HG2	2.55	0.42
2:B:7:THR:HG22	2:B:119:PRO:HG2	2.01	0.42
1:A:235:HIS:N	1:A:235:HIS:CD2	2.87	0.41
2:B:332:GLN:HG3	2:B:338:THR:HG23	2.02	0.41
1:A:64:LYS:HE3	1:A:64:LYS:HB2	1.90	0.41
2:B:369:THR:HG22	2:B:398:TRP:CZ3	2.55	0.41
2:B:178:ILE:HG23	2:B:190:GLY:O	2.18	0.41
1:A:332:GLN:HE22	1:A:353:LYS:NZ	2.18	0.41
1:A:31:ILE:HG12	1:A:133:PRO:HG2	2.02	0.41
2:B:5:ILE:HG23	2:B:119:PRO:CD	2.51	0.41
1:A:111:VAL:HG22	1:A:185:ASP:O	2.20	0.41
1:A:169:GLU:N	1:A:170:PRO:CD	2.84	0.41
2:B:118:VAL:HB	2:B:149:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:VAL:CG2	2:B:289:LEU:HD11	2.51	0.41
2:B:40:GLU:O	2:B:44:GLU:HG3	2.21	0.41
1:A:26:LEU:HD12	1:A:133:PRO:HG3	2.03	0.41
1:A:366:LYS:HZ1	2:B:394:GLN:NE2	2.19	0.41
2:B:264:LEU:HD23	2:B:264:LEU:HA	1.91	0.41
1:A:433:PRO:HB3	2:B:289:LEU:HD23	2.02	0.41
2:B:356:ARG:HG3	2:B:356:ARG:O	2.21	0.40
1:A:10:VAL:HG12	1:A:11:LYS:N	2.36	0.40
1:A:5:ILE:CD1	1:A:167:ILE:HD11	2.50	0.40
1:A:465:LYS:CG	1:A:466:VAL:N	2.83	0.40
1:A:92:LEU:HA	1:A:92:LEU:HD12	1.91	0.40
2:B:303:LEU:HD23	2:B:303:LEU:HA	1.89	0.40
1:A:217:PRO:HD2	4:A:1010:HOH:O	2.22	0.40
2:B:161:GLN:CA	2:B:161:GLN:NE2	2.75	0.40
1:A:24:TRP:CD1	1:A:25:PRO:HD2	2.57	0.40
1:A:366:LYS:HZ2	2:B:394:GLN:NE2	2.19	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	530/560 (95%)	481 (91%)	35 (7%)	14 (3%)	6	9
2	B	397/440 (90%)	372 (94%)	20 (5%)	5 (1%)	14	25
All	All	927/1000 (93%)	853 (92%)	55 (6%)	19 (2%)	9	14

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	GLU
1	A	135	ILE

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Mol	Chain	Res	Type
1	A	138	GLU
1	A	360	ALA
2	B	193	LEU
1	A	90	VAL
1	A	113	ASP
2	B	85	GLN
2	B	239	TRP
1	A	16	MET
1	A	52	PRO
1	A	91	GLN
1	A	361	HIS
1	A	14	PRO
2	B	195	ILE
2	B	210	LEU
1	A	412	PRO
1	A	420	PRO
1	A	112	GLY

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%)	447 (93%)	32 (7%)	19	35
2	B	367/400 (92%)	354 (96%)	13 (4%)	41	68
All	All	846/899 (94%)	801 (95%)	45 (5%)	26	48

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

Mol	Chain	Res	Type
1	A	6	GLU
1	A	21	VAL
1	A	28	GLU
1	A	43	LYS
1	A	52	PRO
1	A	94	ILE

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Mol	Chain	Res	Type
1	A	109	LEU
1	A	122	GLU
1	A	123	ASP
1	A	149	LEU
1	A	175	ASN
1	A	184	MET
1	A	191	SER
1	A	205	LEU
1	A	237	ASP
1	A	255	ASN
1	A	275	LYS
1	A	308	GLU
1	A	340	GLN
1	A	369	THR
1	A	386	THR
1	A	402	TRP
1	A	404	GLU
1	A	424	LYS
1	A	448	ARG
1	A	468	THR
1	A	474	ASN
1	A	487	GLN
1	A	493	VAL
1	A	514	GLU
1	A	517	LEU
1	A	527	LYS
2	B	8	VAL
2	B	113	ASP
2	B	164	MET
2	B	194	GLU
2	B	203	GLU
2	B	250	ASP
2	B	251	SER
2	B	280	CYS
2	B	283	LEU
2	B	303	LEU
2	B	361	HIS
2	B	368	LEU
2	B	425	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	174	GLN
1	A	197	GLN
1	A	242	GLN
1	A	255	ASN
1	A	278	GLN
1	A	332	GLN
1	A	334	GLN
1	A	336	GLN
1	A	474	ASN
1	A	500	GLN
2	B	147	ASN
2	B	151	GLN
2	B	161	GLN
2	B	174	GLN
2	B	175	ASN
2	B	197	GLN
2	B	235	HIS
2	B	278	GLN
2	B	332	GLN
2	B	334	GLN
2	B	361	HIS
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	4,7,8	2.00	1 (25%)	2,8,10	1.80	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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	CSD	CA-C	3.65	1.55	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GFA	A	999	-	28,28,28	1.26	5 (17%)	37,37,37	0.85	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	GFA	A	999	-	-	0/17/17/17	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	GFA	C10-CL1	-2.44	1.69	1.74
3	A	999	GFA	C15-N1	2.03	1.40	1.35
3	A	999	GFA	C1-C6	2.18	1.42	1.39
3	A	999	GFA	C9-C8	2.18	1.43	1.39
3	A	999	GFA	O2-C13	2.60	1.42	1.37

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	534/560 (95%)	-0.04	24 (4%)	34 36	25, 53, 95, 134	0
2	B	403/440 (91%)	-0.08	14 (3%)	44 47	25, 50, 90, 131	0
All	All	937/1000 (93%)	-0.05	38 (4%)	38 40	25, 52, 93, 134	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	94	ILE	4.8
1	A	92	LEU	4.5
2	B	241	VAL	4.3
2	B	210	LEU	4.3
2	B	5	ILE	4.2
1	A	221	HIS	3.8
2	B	67	ASP	3.8
2	B	104	LYS	3.4
1	A	65	LYS	3.3
1	A	52	PRO	3.3
2	B	240	THR	3.3
1	A	446	ALA	3.2
1	A	346	PHE	3.2
2	B	69	THR	3.1
1	A	91	GLN	3.1
1	A	53	GLU	3.1
1	A	64	LYS	3.0
2	B	237	ASP	2.9
1	A	90	VAL	2.8
1	A	136	ASN	2.8
1	A	69	THR	2.7
1	A	272	PRO	2.7
1	A	245	VAL	2.7
2	B	432	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	135	ILE	2.5
2	B	212	TRP	2.5
1	A	51	GLY	2.3
1	A	215	THR	2.3
1	A	216	THR	2.3
2	B	66	LYS	2.3
2	B	102	LYS	2.3
1	A	218	ASP	2.3
1	A	514	GLU	2.2
2	B	68	SER	2.2
1	A	15	GLY	2.1
1	A	228	LEU	2.0
1	A	360	ALA	2.0
1	A	220	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	CSD	A	280	8/9	0.95	0.12	-	50,54,67,72	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, 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(\AA^2)	Q<0.9
3	GFA	A	999	26/26	0.96	0.19	1.07	27,35,44,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.