



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 20, 2016 – 03:17 PM EDT

PDB ID : 5J1E
Title : Crystal Structure of a Hydroxypyridone Carboxylic Acid Active-Site RNase H Inhibitor in Complex with HIV Reverse Transcriptase
Authors : Kirby, K.A.; Sarafianos, S.G.
Deposited on : 2016-03-29
Resolution : 2.90 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027790
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) : rb-20027790

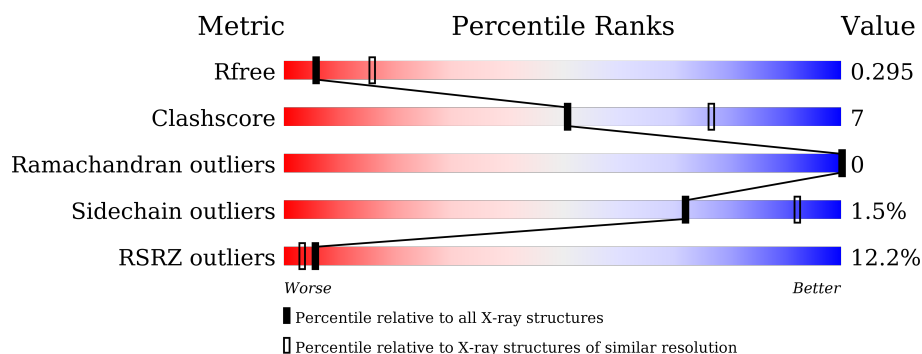
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	557	<div> <div>17%</div> <div>73%</div> <div>24%</div> <div>..</div> </div>
1	C	557	<div> <div>10%</div> <div>82%</div> <div>16%</div> <div>.</div> </div>
2	B	429	<div> <div>11%</div> <div>76%</div> <div>19%</div> <div>6%</div> </div>
2	D	429	<div> <div>7%</div> <div>74%</div> <div>17%</div> <div>8%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	6FT	C	603	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15484 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 P66 DOMAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	541	Total	C	N	O	S	0	0	0
			4407	2855	730	815	7			
1	C	548	Total	C	N	O	S	0	0	0
			4463	2889	742	825	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366
C	-1	MET	-	initiating methionine	UNP P03366
C	0	VAL	-	expression tag	UNP P03366
C	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE P51 DOMAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	405	Total	C	N	O	S	0	0	0
			3341	2175	554	606	6			
2	D	393	Total	C	N	O	S	0	0	0
			3240	2114	532	589	5			

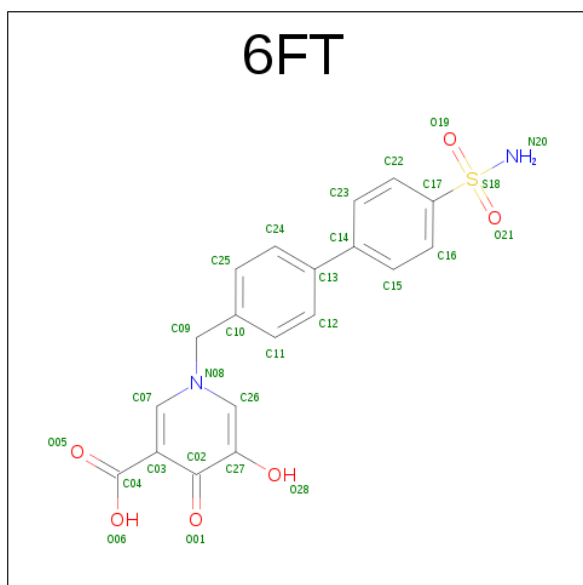
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP P03366
B	280	SER	CYS	engineered mutation	UNP P03366
D	0	GLY	-	expression tag	UNP P03366
D	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	C	2	Total Mg 2 2	0	0

- Molecule 4 is 5-hydroxy-4-oxo-1-[(4'-sulfamoyl[1,1'-biphenyl]-4-yl)methyl]-1,4-dihydropyridine-3-carboxylic acid (three-letter code: 6FT) (formula: C₁₉H₁₆N₂O₆S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	S	0	0
			28	19	2	6	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total O 1 1	0	0
5	D	1	Total O 1 1	0	0

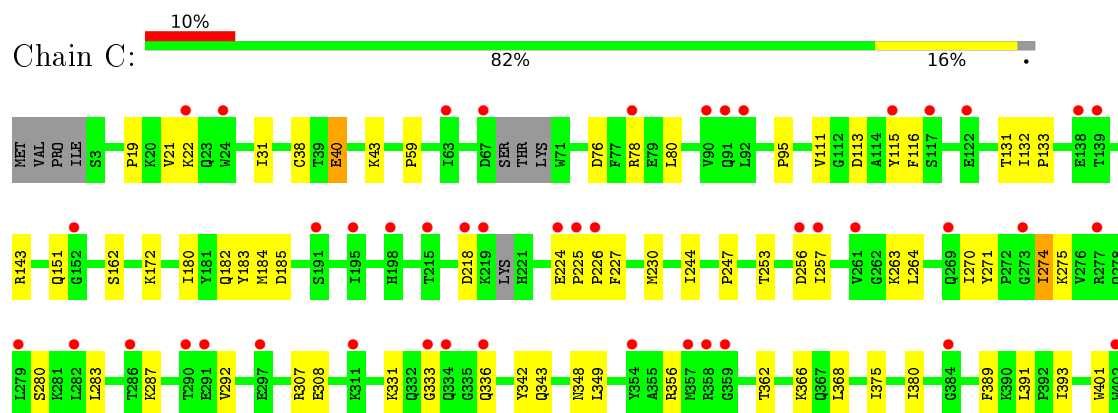
3 Residue-property plots

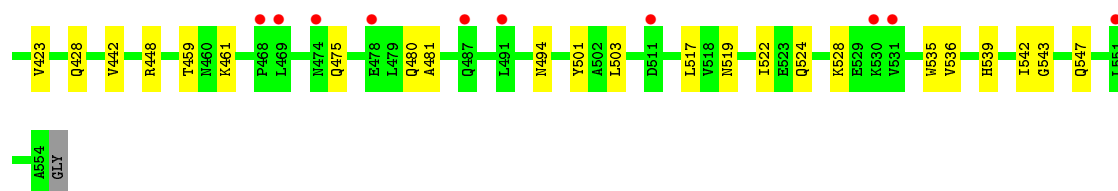
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: HIV-1 REVERSE TRANSCRIPTASE P66 DOMAIN



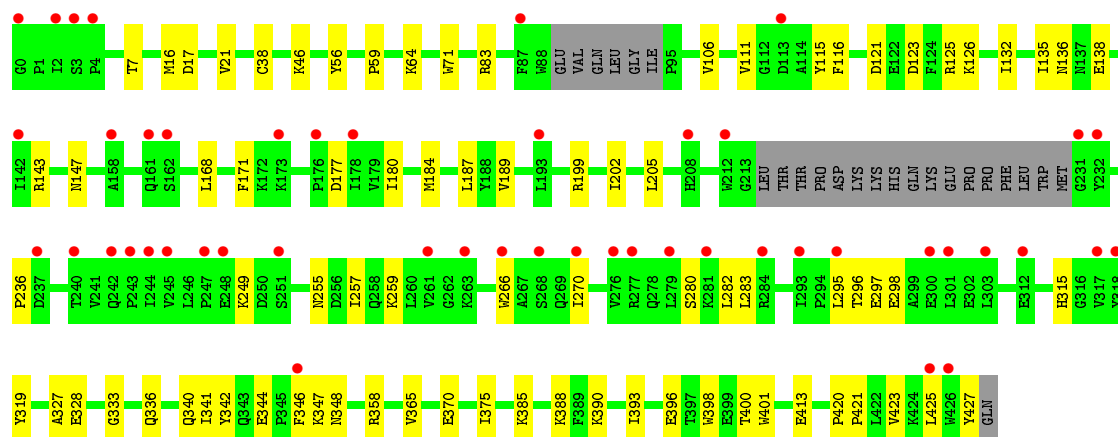
• Molecule 1: HIV-1 REVERSE TRANSCRIPTASE P66 DOMAIN





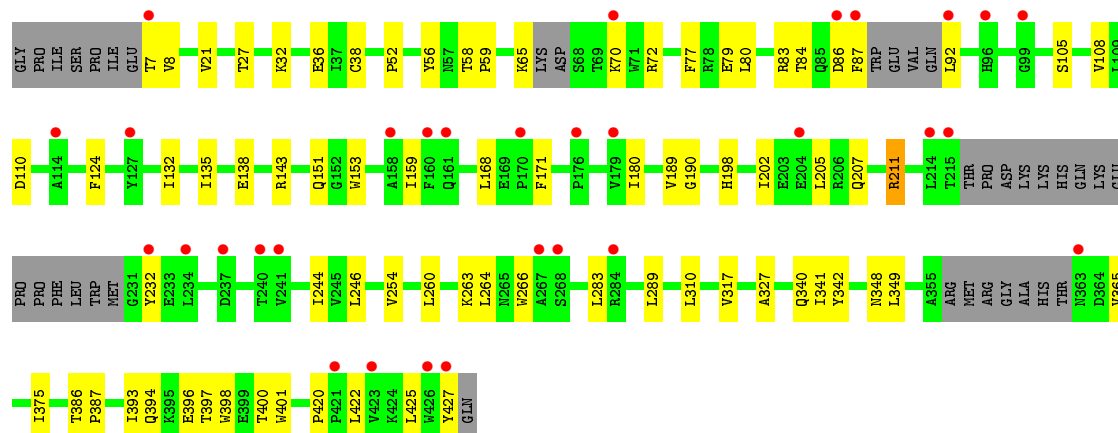
• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE P51 DOMAIN

Chain B: 11% 76% 19% 6%



• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE P51 DOMAIN

Chain D: 7% 74% 17% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	69.07Å 89.31Å 108.22Å 105.47° 92.69° 110.80°	Depositor
Resolution (Å)	63.77 – 2.90 63.77 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.8 (63.77-2.90) 87.7 (63.77-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.254 , 0.294 0.257 , 0.295	Depositor DCC
R_{free} test set	2493 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	61.9	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 28.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.014 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	15484	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 6FT

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	0.25	0/4521	0.46	0/6143
1	C	0.24	0/4578	0.44	0/6218
2	B	0.25	0/3437	0.42	0/4668
2	D	0.24	0/3329	0.43	0/4520
All	All	0.25	0/15865	0.44	0/21549

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	136	ASN	Peptide

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	4407	0	4450	86	1
1	C	4463	0	4509	52	1
2	B	3341	0	3373	46	0
2	D	3240	0	3276	42	0
3	A	1	0	0	0	0
3	C	2	0	0	0	0
4	C	28	0	0	1	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
All	All	15484	0	15608	215	1

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 7.

All (215) 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:D:84:THR:HG21	2:D:153:TRP:HE1	1.42	0.84
1:C:59:PRO:HG2	1:C:76:ASP:HB3	1.61	0.82
1:A:83:ARG:NH2	1:C:308:GLU:OE1	2.16	0.79
2:B:270:ILE:HG12	2:B:346:PHE:HB3	1.67	0.76
1:A:246:LEU:HD21	1:A:310:LEU:HD12	1.69	0.73
2:D:246:LEU:HD11	2:D:264:LEU:HD21	1.71	0.72
1:C:459:THR:HG22	1:C:461:LYS:H	1.54	0.70
2:B:180:ILE:HG12	2:B:189:VAL:HG12	1.72	0.69
1:A:358:ARG:HG2	1:A:360:ALA:H	1.57	0.68
1:A:135:ILE:O	1:A:139:THR:OG1	2.11	0.68
1:A:206:ARG:NH1	1:A:216:THR:O	2.27	0.65
1:A:459:THR:HG22	1:A:461:LYS:H	1.62	0.64
2:D:180:ILE:HG12	2:D:189:VAL:HG12	1.79	0.64
1:A:167:ILE:O	1:A:208:HIS:NE2	2.25	0.64
1:C:21:VAL:HB	1:C:59:PRO:HD3	1.81	0.63
1:C:224:GLU:HG2	1:C:226:PRO:HD2	1.80	0.63
2:B:135:ILE:O	2:B:138:GLU:HG2	1.99	0.63
1:A:83:ARG:HH22	1:C:308:GLU:CD	2.03	0.62
1:A:228:LEU:HA	1:A:232:TYR:O	2.00	0.62
1:A:31:ILE:HG12	1:A:133:PRO:HG2	1.81	0.61
1:C:247:PRO:O	1:C:307:ARG:NH2	2.34	0.61
2:D:422:LEU:HG	2:D:425:LEU:HD12	1.83	0.60
1:A:472:THR:HA	1:A:476:LYS:HD2	1.82	0.60
2:B:168:LEU:HD22	2:B:205:LEU:HD11	1.84	0.60
1:C:356:ARG:HD2	1:C:362:THR:HG21	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:56:TYR:O	2:D:143:ARG:NH2	2.35	0.59
1:A:341:ILE:O	1:A:349:LEU:N	2.36	0.59
2:D:72:ARG:NH2	2:D:151:GLN:OE1	2.35	0.59
1:A:284:ARG:HB3	1:A:284:ARG:HH11	1.68	0.58
2:B:266:TRP:CE2	2:B:425:LEU:HD13	2.38	0.58
2:B:115:TYR:OH	2:B:184:MET:O	2.19	0.58
1:C:503:LEU:HD22	1:C:535:TRP:HB2	1.86	0.58
1:A:503:LEU:HD13	1:A:535:TRP:HB2	1.85	0.58
1:A:64:LYS:HB2	1:A:71:TRP:HA	1.86	0.57
1:A:342:TYR:HB3	1:A:348:ASN:HA	1.87	0.57
1:A:60:VAL:HG22	1:A:75:VAL:HG13	1.86	0.57
2:D:87:PHE:HB3	2:D:92:LEU:HB3	1.87	0.56
1:C:244:ILE:HG23	1:C:263:LYS:HE2	1.87	0.56
1:C:480:GLN:HG2	1:C:517:LEU:HD11	1.87	0.56
1:A:95:PRO:HB2	1:A:230:MET:HE1	1.88	0.56
1:A:524:GLN:O	1:A:528:LYS:HG2	2.04	0.56
2:D:79:GLU:HG3	2:D:83:ARG:HE	1.71	0.56
2:D:394:GLN:HB3	2:D:397:THR:HG22	1.87	0.56
1:A:317:VAL:HG23	1:A:349:LEU:HD23	1.87	0.56
1:C:78:ARG:NH2	1:C:287:LYS:O	2.31	0.55
2:B:125:ARG:HD3	2:B:147:ASN:HD22	1.71	0.54
2:D:168:LEU:HD22	2:D:205:LEU:HD11	1.88	0.54
2:D:254:VAL:HG13	2:D:283:LEU:HD22	1.89	0.54
1:C:368:LEU:HD11	1:C:391:LEU:HD22	1.90	0.54
1:A:303:LEU:O	1:A:307:ARG:HB3	2.08	0.54
1:A:181:TYR:CD1	2:B:138:GLU:HB3	2.43	0.54
1:A:261:VAL:O	1:A:265:ASN:ND2	2.41	0.53
2:B:64:LYS:HE3	2:B:71:TRP:CE2	2.43	0.53
2:D:365:VAL:HG11	2:D:401:TRP:HB2	1.91	0.53
1:C:31:ILE:HG12	1:C:133:PRO:HG2	1.90	0.53
1:C:475:GLN:HB3	1:C:501:TYR:CE2	2.44	0.53
1:A:268:SER:OG	1:A:269:GLN:OE1	2.24	0.52
1:A:78:ARG:NH2	1:A:287:LYS:O	2.42	0.52
1:C:270:ILE:HG23	1:C:271:TYR:HD1	1.73	0.52
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.91	0.52
2:B:106:VAL:HG12	2:B:236:PRO:HD3	1.91	0.52
1:A:330:GLN:NE2	1:A:340:GLN:OE1	2.32	0.52
1:C:442:VAL:HB	1:C:481:ALA:HB1	1.91	0.51
1:A:259:LYS:HD2	1:A:259:LYS:N	2.25	0.51
1:C:375:ILE:HD11	1:C:389:PHE:HE1	1.75	0.51
1:A:199:ARG:HA	1:A:202:ILE:HD12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:327:ALA:HA	2:B:340:GLN:O	2.11	0.51
1:C:333:GLY:H	1:C:336:GLN:HB2	1.75	0.51
1:A:244:ILE:HB	1:A:310:LEU:HD13	1.92	0.50
2:B:111:VAL:HG11	2:B:187:LEU:HD12	1.93	0.50
2:D:246:LEU:HD13	2:D:260:LEU:HD11	1.93	0.50
2:B:328:GLU:HG2	2:B:390:LYS:HB2	1.94	0.49
2:B:315:HIS:O	2:B:347:LYS:NZ	2.39	0.49
2:D:21:VAL:HB	2:D:59:PRO:HD3	1.94	0.49
1:A:431:LYS:HG3	1:A:432:GLU:HG2	1.94	0.49
2:B:121:ASP:O	2:B:125:ARG:HG3	2.12	0.49
1:A:469:LEU:HD11	1:A:480:GLN:HG2	1.94	0.49
2:B:257:ILE:HB	2:B:283:LEU:HD21	1.95	0.49
1:C:393:ILE:HB	1:C:423:VAL:HB	1.94	0.49
1:A:203:GLU:O	1:A:207:GLN:HG2	2.12	0.49
2:B:341:ILE:HD11	2:B:375:ILE:HG23	1.95	0.49
1:C:343:GLN:HG3	1:C:349:LEU:HD11	1.94	0.49
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.48	0.49
2:B:255:ASN:O	2:B:259:LYS:HG2	2.13	0.48
1:A:549:ASP:HA	1:A:552:VAL:HG22	1.95	0.48
1:A:270:ILE:HG23	1:A:271:TYR:HD1	1.77	0.48
2:B:358:ARG:HE	2:B:370:GLU:HB2	1.79	0.48
1:A:317:VAL:HG21	1:A:347:LYS:HG2	1.95	0.48
1:C:183:TYR:HD1	1:C:184:MET:HG2	1.78	0.48
2:D:84:THR:HG22	2:D:124:PHE:HZ	1.79	0.48
1:A:44:GLU:HB3	1:A:46:LYS:HE3	1.94	0.48
1:A:284:ARG:NH1	1:A:284:ARG:HB3	2.28	0.48
2:B:333:GLY:O	2:B:336:GLN:HG2	2.14	0.48
1:A:249:LYS:NZ	1:A:256:ASP:OD2	2.47	0.48
2:D:396:GLU:O	2:D:400:THR:OG1	2.20	0.48
1:A:280:SER:HA	1:A:283:LEU:HD13	1.96	0.48
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.95	0.48
2:D:135:ILE:O	2:D:138:GLU:HG3	2.14	0.48
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.96	0.47
1:C:115:TYR:HD2	1:C:151:GLN:HA	1.79	0.47
2:D:32:LYS:HE2	2:D:36:GLU:OE2	2.15	0.47
1:A:222:GLN:OE1	1:A:228:LEU:N	2.44	0.47
1:A:473:THR:H	1:A:476:LYS:HB3	1.79	0.47
2:B:342:TYR:HB3	2:B:348:ASN:HA	1.97	0.47
1:C:524:GLN:O	1:C:528:LYS:HG2	2.16	0.46
1:A:172:LYS:HD3	1:A:180:ILE:HB	1.97	0.46
1:A:39:THR:O	1:A:43:LYS:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:GLU:HB2	1:A:46:LYS:HG2	1.97	0.46
2:D:266:TRP:CG	2:D:425:LEU:HD13	2.50	0.46
1:A:60:VAL:HG21	1:A:130:PHE:CD2	2.50	0.46
1:C:536:VAL:HB	1:C:542:ILE:HD12	1.96	0.46
1:C:380:ILE:HD12	2:D:27:THR:HG22	1.98	0.46
2:D:327:ALA:HA	2:D:340:GLN:O	2.16	0.46
1:A:375:ILE:HA	1:A:378:GLU:HG2	1.98	0.46
1:A:253:THR:HG23	1:A:256:ASP:H	1.80	0.46
1:A:40:GLU:HA	1:A:43:LYS:HD2	1.98	0.46
1:C:131:THR:HG22	1:C:143:ARG:HD2	1.97	0.46
2:D:198:HIS:O	2:D:202:ILE:HG12	2.16	0.46
1:A:306:ASN:O	1:A:309:ILE:HG13	2.16	0.46
2:B:393:ILE:HD13	2:B:398:TRP:HB2	1.97	0.46
1:A:541:GLY:O	2:B:280:SER:HB2	2.17	0.45
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.98	0.45
2:D:105:SER:O	2:D:190:GLY:HA2	2.16	0.45
1:A:131:THR:HG22	1:A:143:ARG:NE	2.32	0.45
1:A:332:GLN:HB2	1:A:336:GLN:HB2	1.98	0.45
1:A:498:ASP:HB2	1:A:538:ALA:HB2	1.97	0.45
2:D:420:PRO:HG2	2:D:422:LEU:HB2	1.98	0.45
2:B:396:GLU:O	2:B:400:THR:OG1	2.18	0.45
1:C:356:ARG:CD	1:C:362:THR:HG21	2.45	0.45
1:A:177:ASP:HB2	1:A:193:LEU:HD21	1.97	0.45
1:A:371:ALA:O	1:A:375:ILE:HG22	2.17	0.45
1:C:519:ASN:HA	1:C:522:ILE:HD12	1.99	0.45
1:A:165:THR:O	1:A:169:GLU:HG2	2.17	0.45
1:A:42:GLU:OE1	1:A:49:LYS:HE3	2.17	0.44
2:D:207:GLN:O	2:D:211:ARG:HD3	2.17	0.44
2:D:342:TYR:HB3	2:D:348:ASN:HA	1.99	0.44
1:A:257:ILE:O	1:A:261:VAL:HG13	2.16	0.44
2:D:317:VAL:HG22	2:D:349:LEU:HD23	1.98	0.44
2:B:17:ASP:O	2:B:83:ARG:HD3	2.17	0.44
2:B:297:GLU:H	2:B:297:GLU:CD	2.20	0.44
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.57	0.44
1:A:376:THR:HG21	2:B:401:TRP:CH2	2.53	0.44
2:B:266:TRP:CE3	2:B:425:LEU:HD22	2.52	0.44
2:D:171:PHE:CG	2:D:205:LEU:HD13	2.53	0.44
1:A:207:GLN:O	1:A:211:ARG:HG3	2.17	0.44
2:B:199:ARG:O	2:B:202:ILE:HG13	2.18	0.44
1:C:22:LYS:HD2	1:C:22:LYS:H	1.82	0.44
1:C:543:GLY:O	1:C:547:GLN:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:PRO:O	1:A:414:TRP:HD1	2.00	0.44
2:B:56:TYR:O	2:B:143:ARG:NH2	2.50	0.43
1:C:539:HIS:HB2	4:C:603:6FT:C12	2.49	0.43
1:C:494:ASN:HB3	2:D:289:LEU:HD12	2.00	0.43
1:C:264:LEU:HD22	1:C:274:ILE:HD11	1.99	0.43
1:C:95:PRO:HB2	1:C:230:MET:HE1	2.01	0.43
1:A:305:GLU:O	1:A:309:ILE:HG23	2.19	0.43
2:B:46:LYS:HE2	2:B:116:PHE:HB3	2.00	0.43
1:C:113:ASP:HB3	1:C:116:PHE:HB2	2.00	0.43
2:D:393:ILE:HD13	2:D:398:TRP:HB2	2.00	0.43
1:C:40:GLU:HA	1:C:43:LYS:HD3	2.01	0.43
2:D:65:LYS:NZ	2:D:110:ASP:OD2	2.50	0.43
1:A:406:TRP:CZ3	1:A:407:GLN:HG3	2.54	0.43
1:C:331:LYS:HE2	1:C:333:GLY:O	2.19	0.43
1:A:57:ASN:OD1	1:A:131:THR:HG23	2.19	0.43
1:A:513:SER:O	1:A:519:ASN:ND2	2.52	0.43
2:B:297:GLU:HG2	2:B:298:GLU:H	1.84	0.43
1:C:172:LYS:HD3	1:C:180:ILE:HB	2.00	0.43
2:D:341:ILE:HD11	2:D:375:ILE:HG23	2.01	0.43
1:A:17:ASP:O	1:A:83:ARG:HD3	2.19	0.42
1:A:398:TRP:CZ2	1:A:411:ILE:HG12	2.54	0.42
1:A:450:THR:O	1:A:451:LYS:HG2	2.18	0.42
1:C:225:PRO:O	1:C:227:PHE:N	2.47	0.42
1:A:448:ARG:H	1:A:448:ARG:HG3	1.37	0.42
1:C:366:LYS:HE3	1:C:401:TRP:HH2	1.83	0.42
1:C:19:PRO:HD3	1:C:80:LEU:HD13	2.02	0.42
1:C:38:CYS:SG	1:C:132:ILE:HD11	2.59	0.42
1:C:256:ASP:OD1	1:C:257:ILE:N	2.52	0.42
1:A:503:LEU:HD12	1:A:533:LEU:HG	2.02	0.42
2:B:388:LYS:HD3	2:B:413:GLU:HB2	2.00	0.42
1:C:115:TYR:CD2	1:C:151:GLN:HA	2.54	0.42
2:D:80:LEU:O	2:D:84:THR:HG23	2.19	0.42
1:A:475:GLN:HB2	1:A:501:TYR:CD2	2.54	0.42
1:C:280:SER:HA	1:C:283:LEU:HD13	2.02	0.42
2:D:38:CYS:SG	2:D:132:ILE:HD11	2.60	0.42
1:A:278:GLN:CD	1:A:298:GLU:HB3	2.40	0.42
1:A:21:VAL:O	1:A:57:ASN:ND2	2.53	0.42
2:D:58:THR:HG21	2:D:77:PHE:CD1	2.54	0.42
1:A:412:PRO:HD3	2:B:401:TRP:CZ2	2.55	0.42
1:C:270:ILE:HG23	1:C:271:TYR:CD1	2.54	0.42
2:D:108:VAL:HB	2:D:232:TYR:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:GLN:HE22	1:A:512:LYS:HE3	1.85	0.41
2:D:263:LYS:HA	2:D:425:LEU:HD22	2.02	0.41
2:B:16:MET:HG2	1:C:292:VAL:HG11	2.01	0.41
2:D:8:VAL:HG21	2:D:159:ILE:HD13	2.02	0.41
1:C:342:TYR:HB3	1:C:348:ASN:HA	2.03	0.41
2:D:266:TRP:CD2	2:D:425:LEU:HD13	2.55	0.41
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.21	0.41
2:B:123:ASP:O	2:B:126:LYS:NZ	2.54	0.41
2:B:177:ASP:OD1	2:B:177:ASP:N	2.51	0.41
1:A:131:THR:HG22	1:A:143:ARG:HE	1.86	0.41
1:A:172:LYS:HG2	1:A:180:ILE:HD12	2.02	0.41
1:A:284:ARG:HG2	1:A:284:ARG:H	1.70	0.41
1:C:111:VAL:HG12	1:C:185:ASP:O	2.21	0.41
2:D:386:THR:HA	2:D:387:PRO:HD3	1.94	0.41
2:B:282:LEU:HD21	2:B:296:THR:HG23	2.03	0.41
1:A:361:HIS:CD2	1:A:505:ILE:HG23	2.56	0.41
2:B:420:PRO:HA	2:B:421:PRO:HD3	1.96	0.41
1:C:162:SER:HB2	2:D:52:PRO:HG3	2.03	0.41
1:C:253:THR:HG23	1:C:256:ASP:H	1.85	0.41
1:A:270:ILE:HG23	1:A:271:TYR:CD1	2.55	0.40
2:B:171:PHE:CG	2:B:205:LEU:HD13	2.57	0.40
2:B:282:LEU:HD11	2:B:295:LEU:HA	2.04	0.40
2:D:244:ILE:HB	2:D:310:LEU:HD22	2.03	0.40
1:A:252:TRP:O	1:A:293:ILE:HG22	2.21	0.40
1:A:382:ILE:O	2:B:136:ASN:HB2	2.21	0.40
2:B:319:TYR:OH	2:B:385:LYS:NZ	2.55	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:LYS:NZ	1:C:448:ARG:O[1_655]	2.18	0.02

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	535/557 (96%)	516 (96%)	19 (4%)	0	100	100
1	C	542/557 (97%)	526 (97%)	16 (3%)	0	100	100
2	B	399/429 (93%)	389 (98%)	10 (2%)	0	100	100
2	D	383/429 (89%)	374 (98%)	9 (2%)	0	100	100
All	All	1859/1972 (94%)	1805 (97%)	54 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	483/497 (97%)	474 (98%)	9 (2%)	65	89
1	C	489/497 (98%)	483 (99%)	6 (1%)	78	94
2	B	367/390 (94%)	362 (99%)	5 (1%)	74	93
2	D	357/390 (92%)	352 (99%)	5 (1%)	74	93
All	All	1696/1774 (96%)	1671 (98%)	25 (2%)	72	92

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

Mol	Chain	Res	Type
1	A	142	ILE
1	A	218	ASP
1	A	259	LYS
1	A	264	LEU
1	A	276	VAL
1	A	284	ARG
1	A	307	ARG
1	A	448	ARG
1	A	449	GLU
2	B	7	THR

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Mol	Chain	Res	Type
2	B	249	LYS
2	B	344	GLU
2	B	423	VAL
2	B	427	TYR
1	C	40	GLU
1	C	182	GLN
1	C	218	ASP
1	C	274	ILE
1	C	275	LYS
1	C	428	GLN
2	D	7	THR
2	D	70	LYS
2	D	86	ASP
2	D	211	ARG
2	D	427	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	161	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
4	6FT	C	603	3	24,30,30	4.41	8 (33%)	34,44,44	2.68	6 (17%)

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
4	6FT	C	603	3	-	0/14/18/18	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	603	6FT	O21-S18	2.45	1.46	1.43
4	C	603	6FT	O19-S18	2.52	1.46	1.43
4	C	603	6FT	C17-S18	3.31	1.81	1.77
4	C	603	6FT	S18-N20	6.09	1.71	1.60
4	C	603	6FT	C07-C03	7.07	1.53	1.38
4	C	603	6FT	C07-N08	10.07	1.49	1.35
4	C	603	6FT	C26-N08	10.13	1.49	1.35
4	C	603	6FT	C26-C27	11.95	1.53	1.39

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	603	6FT	O21-S18-O19	-12.98	101.43	118.87
4	C	603	6FT	C07-N08-C26	-3.12	119.37	121.47
4	C	603	6FT	O19-S18-N20	3.05	111.04	107.25
4	C	603	6FT	O19-S18-C17	3.08	110.88	107.41
4	C	603	6FT	O21-S18-N20	3.46	111.54	107.25
4	C	603	6FT	O21-S18-C17	3.64	111.51	107.41

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
4	C	603	6FT	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, 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	541/557 (97%)	0.98	97 (17%) 2 1	36, 77, 138, 213	0
1	C	548/557 (98%)	0.75	55 (10%) 9 5	43, 70, 124, 166	0
2	B	405/429 (94%)	0.76	48 (11%) 6 3	36, 66, 124, 159	0
2	D	393/429 (91%)	0.67	31 (7%) 15 10	40, 60, 108, 126	0
All	All	1887/1972 (95%)	0.80	231 (12%) 5 3	36, 68, 126, 213	0

All (231) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	295	LEU	7.8
1	A	216	THR	6.7
2	B	426	TRP	6.7
2	D	240	THR	6.5
2	B	247	PRO	6.3
1	A	31	ILE	6.2
2	B	240	THR	6.1
1	A	283	LEU	6.0
2	D	232	TYR	5.8
1	A	217	PRO	5.8
1	A	249	LYS	5.5
1	C	551	LEU	5.5
2	D	7	THR	5.4
1	A	71	TRP	5.2
1	A	115	TYR	5.0
1	C	297	GLU	5.0
1	A	255	ASN	4.8
1	A	117	SER	4.8
1	A	333	GLY	4.7
1	A	38	CYS	4.7
1	A	293	ILE	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	538	ALA	4.6
1	A	93	GLY	4.6
2	D	204	GLU	4.6
2	B	301	LEU	4.5
1	A	252	TRP	4.5
2	D	114	ALA	4.5
1	A	273	GLY	4.5
2	D	423	VAL	4.5
2	B	270	ILE	4.4
1	A	132	ILE	4.4
2	B	3	SER	4.4
1	A	259	LYS	4.4
1	A	306	ASN	4.3
1	A	72	ARG	4.3
1	A	297	GLU	4.3
2	D	241	VAL	4.3
1	C	474	ASN	4.2
2	B	2	ILE	4.2
1	C	273	GLY	4.1
1	A	144	TYR	4.1
1	A	73	LYS	4.1
2	D	268	SER	4.1
1	A	60	VAL	4.0
2	B	277	ARG	4.0
1	A	280	SER	4.0
1	C	63	ILE	4.0
1	A	361	HIS	4.0
1	C	531	VAL	3.9
2	D	267	ALA	3.9
1	A	197	GLN	3.9
1	A	180	ILE	3.8
1	C	269	GLN	3.8
2	D	70	LYS	3.8
1	A	63	ILE	3.8
1	A	35	VAL	3.8
1	C	219	LYS	3.8
2	B	208	HIS	3.7
1	C	402	TRP	3.7
1	A	223	LYS	3.7
1	A	274	ILE	3.7
1	A	307	ARG	3.7
1	C	334	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	126	LYS	3.7
1	A	248	GLU	3.6
1	A	250	ASP	3.6
1	C	91	GLN	3.6
2	D	160	PHE	3.6
1	C	290	THR	3.6
1	A	183	TYR	3.5
1	C	22	LYS	3.5
2	D	215	THR	3.5
2	D	421	PRO	3.4
1	A	34	LEU	3.3
2	B	251	SER	3.3
2	D	176	PRO	3.3
1	A	24	TRP	3.3
1	A	129	ALA	3.2
1	A	33	ALA	3.2
1	A	222	GLN	3.2
1	C	333	GLY	3.2
1	A	81	ASN	3.2
1	C	277	ARG	3.2
1	C	359	GLY	3.2
1	C	261	VAL	3.2
1	A	266	TRP	3.1
1	A	137	ASN	3.1
2	B	281	LYS	3.1
2	B	300	GLU	3.1
2	D	237	ASP	3.1
2	B	279	LEU	3.1
1	A	247	PRO	3.1
1	C	139	THR	3.1
1	C	226	PRO	3.1
1	A	130	PHE	3.0
1	C	357	MET	3.0
2	B	268	SER	3.0
1	A	124	PHE	3.0
2	B	346	PHE	3.0
1	C	256	ASP	3.0
2	B	237	ASP	3.0
1	A	128	THR	3.0
1	C	286	THR	3.0
2	B	142	ILE	3.0
2	B	261	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	184	MET	3.0
1	A	446	ALA	2.9
2	B	193	LEU	2.9
1	A	36	GLU	2.9
2	B	158	ALA	2.9
2	D	158	ALA	2.8
1	A	236	PRO	2.8
1	A	194	GLU	2.8
2	D	87	PHE	2.8
1	A	260	LEU	2.8
2	B	0	GLY	2.8
1	A	131	THR	2.8
1	A	334	GLN	2.8
1	A	145	GLN	2.8
1	C	138	GLU	2.8
2	D	86	ASP	2.8
2	B	243	PRO	2.7
1	A	200	THR	2.7
1	C	279	LEU	2.7
1	A	304	ALA	2.7
2	B	318	TYR	2.7
2	D	92	LEU	2.7
2	D	161	GLN	2.7
1	C	225	PRO	2.7
2	B	317	VAL	2.6
1	A	28	GLU	2.6
1	C	257	ILE	2.6
2	B	276	VAL	2.6
2	B	245	VAL	2.6
1	A	265	ASN	2.6
2	B	87	PHE	2.6
2	D	127	TYR	2.6
1	A	312	GLU	2.6
2	B	176	PRO	2.6
1	A	29	GLU	2.6
1	C	195	ILE	2.6
1	A	190	GLY	2.6
2	D	96	HIS	2.6
1	A	292	VAL	2.6
1	C	67	ASP	2.5
2	B	284	ARG	2.5
1	A	25	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	468	PRO	2.5
2	B	293	ILE	2.5
1	A	261	VAL	2.5
1	A	477	THR	2.5
2	B	231	GLY	2.5
1	A	289	LEU	2.5
1	C	24	TRP	2.5
2	D	426	TRP	2.5
1	A	150	PRO	2.5
1	C	491	LEU	2.5
2	B	425	LEU	2.5
1	C	358	ARG	2.5
1	C	191	SER	2.5
1	C	282	LEU	2.5
2	D	284	ARG	2.5
2	B	266	TRP	2.5
2	B	178	ILE	2.5
2	B	173	LYS	2.4
2	B	113	ASP	2.4
1	A	10	VAL	2.4
2	B	244	ILE	2.4
1	A	186	ASP	2.4
1	A	545	ASN	2.4
1	A	83	ARG	2.4
1	C	152	GLY	2.4
1	A	438	GLU	2.4
1	A	138	GLU	2.4
2	D	170	PRO	2.4
2	B	212	TRP	2.4
1	A	198	HIS	2.3
1	A	15	GLY	2.3
1	C	311	LYS	2.3
1	C	354	TYR	2.3
1	C	224	GLU	2.3
1	C	90	VAL	2.3
1	A	64	LYS	2.3
2	B	303	LEU	2.3
2	D	99	GLY	2.3
1	A	133	PRO	2.3
1	C	115	TYR	2.3
2	B	242	GLN	2.3
1	A	225	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	311	LYS	2.2
1	C	487	GLN	2.2
2	D	234	LEU	2.2
1	C	78	ARG	2.2
1	C	92	LEU	2.2
1	C	117	SER	2.2
2	B	161	GLN	2.2
2	B	248	GLU	2.2
2	D	363	ASN	2.2
1	A	227	PHE	2.2
2	B	263	LYS	2.2
1	C	469	LEU	2.2
1	C	511	ASP	2.2
1	A	551	LEU	2.2
1	C	218	ASP	2.2
2	D	214	LEU	2.2
1	A	149	LEU	2.1
1	C	215	THR	2.1
2	D	427	TYR	2.1
1	C	336	GLN	2.1
1	A	218	ASP	2.1
1	C	198	HIS	2.1
1	C	384	GLY	2.1
1	C	478	GLU	2.1
1	C	291	GLU	2.1
1	A	122	GLU	2.1
1	A	140	PRO	2.1
2	B	312	GLU	2.1
1	A	257	ILE	2.1
2	B	162	SER	2.0
2	B	232	TYR	2.0
1	A	55	PRO	2.0
2	B	4	PRO	2.0
2	D	179	VAL	2.0
1	A	426	TRP	2.0
1	A	549	ASP	2.0
1	A	546	GLU	2.0
1	A	102	LYS	2.0
1	A	44	GLU	2.0
1	C	122	GLU	2.0
1	A	90	VAL	2.0
1	C	530	LYS	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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
4	6FT	C	603	28/28	0.73	0.49	2.21	60,82,99,101	28
3	MG	C	601	1/1	0.61	0.24	-0.10	66,66,66,66	0
3	MG	A	601	1/1	0.46	0.22	-0.39	113,113,113,113	0
3	MG	C	602	1/1	0.43	0.14	-2.29	67,67,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.