



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:07 PM GMT

PDB ID : 3W67  
Title : Crystal structure of mouse alpha-tocopherol transfer protein in complex with  
alpha-tocopherol and phosphatidylinositol-(3,4)-biphosphate  
Authors : Ohto, U.; Satow, Y.  
Deposited on : 2013-02-11  
Resolution : 2.61 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) 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

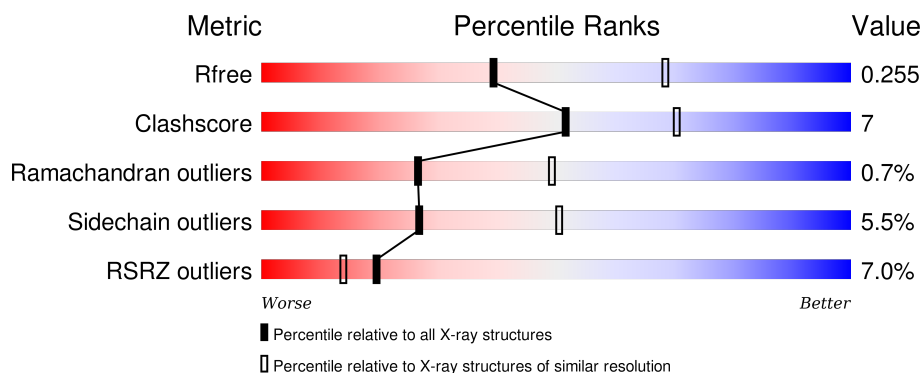
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.61 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	2700 (2.64-2.60)
Clashscore	102246	3065 (2.64-2.60)
Ramachandran outliers	100387	3015 (2.64-2.60)
Sidechain outliers	100360	3015 (2.64-2.60)
RSRZ outliers	91569	2706 (2.64-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	266	<div> <div>2%</div> <div>79%</div> <div>14%</div> <div>6%</div> </div>
1	B	266	<div> <div>73%</div> <div>20%</div> <div>5%</div> </div>
1	C	266	<div> <div>2%</div> <div>73%</div> <div>19%</div> <div>6%</div> </div>
1	D	266	<div> <div>23%</div> <div>76%</div> <div>18%</div> <div>6%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	VIV	C	301	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8568 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 Alpha-tocopherol transfer protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	0	0
			2052	1324	357	364	7			
1	B	253	Total	C	N	O	S	0	0	0
			2064	1333	358	366	7			
1	C	250	Total	C	N	O	S	0	0	0
			2039	1316	354	362	7			
1	D	251	Total	C	N	O	S	0	0	0
			2048	1321	356	364	7			

There are 32 discrepancies between the modelled and reference sequences:

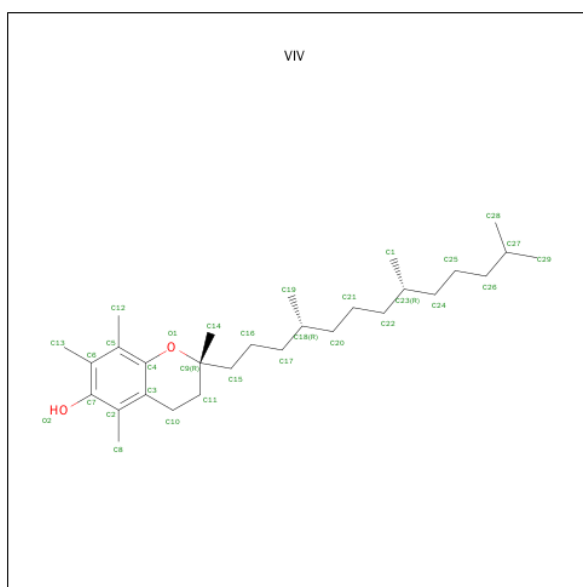
Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	-	EXPRESSION TAG	UNP Q8BWP5
A	14	PRO	-	EXPRESSION TAG	UNP Q8BWP5
A	15	LEU	-	EXPRESSION TAG	UNP Q8BWP5
A	16	GLY	-	EXPRESSION TAG	UNP Q8BWP5
A	17	SER	-	EXPRESSION TAG	UNP Q8BWP5
A	18	PRO	-	EXPRESSION TAG	UNP Q8BWP5
A	19	GLU	-	EXPRESSION TAG	UNP Q8BWP5
A	20	PHE	-	EXPRESSION TAG	UNP Q8BWP5
B	13	GLY	-	EXPRESSION TAG	UNP Q8BWP5
B	14	PRO	-	EXPRESSION TAG	UNP Q8BWP5
B	15	LEU	-	EXPRESSION TAG	UNP Q8BWP5
B	16	GLY	-	EXPRESSION TAG	UNP Q8BWP5
B	17	SER	-	EXPRESSION TAG	UNP Q8BWP5
B	18	PRO	-	EXPRESSION TAG	UNP Q8BWP5
B	19	GLU	-	EXPRESSION TAG	UNP Q8BWP5
B	20	PHE	-	EXPRESSION TAG	UNP Q8BWP5
C	13	GLY	-	EXPRESSION TAG	UNP Q8BWP5
C	14	PRO	-	EXPRESSION TAG	UNP Q8BWP5
C	15	LEU	-	EXPRESSION TAG	UNP Q8BWP5
C	16	GLY	-	EXPRESSION TAG	UNP Q8BWP5
C	17	SER	-	EXPRESSION TAG	UNP Q8BWP5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	18	PRO	-	EXPRESSION TAG	UNP Q8BWP5
C	19	GLU	-	EXPRESSION TAG	UNP Q8BWP5
C	20	PHE	-	EXPRESSION TAG	UNP Q8BWP5
D	13	GLY	-	EXPRESSION TAG	UNP Q8BWP5
D	14	PRO	-	EXPRESSION TAG	UNP Q8BWP5
D	15	LEU	-	EXPRESSION TAG	UNP Q8BWP5
D	16	GLY	-	EXPRESSION TAG	UNP Q8BWP5
D	17	SER	-	EXPRESSION TAG	UNP Q8BWP5
D	18	PRO	-	EXPRESSION TAG	UNP Q8BWP5
D	19	GLU	-	EXPRESSION TAG	UNP Q8BWP5
D	20	PHE	-	EXPRESSION TAG	UNP Q8BWP5

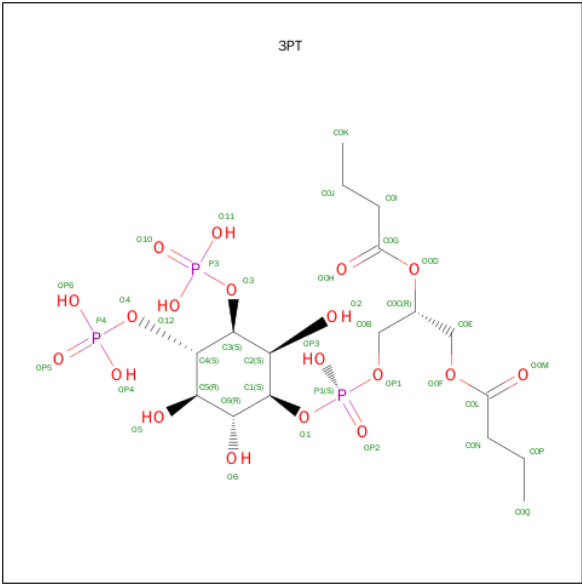
- Molecule 2 is (2R)-2,5,7,8-TETRAMETHYL-2-[(4R,8R)-4,8,12-TRIMETHYLTRIDECYL]CHROMAN-6-OL (three-letter code: VIV) (formula: C<sub>29</sub>H<sub>50</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			31	29	2		
2	B	1	Total	C	O	0	0
			31	29	2		
2	C	1	Total	C	O	0	0
			31	29	2		
2	D	1	Total	C	O	0	0
			31	29	2		

- Molecule 3 is (2R)-3-[(S)-HYDROXY{[(1S,2R,3R,4S,5S,6S)-2,3,6-TRIHYDROXY-4,5-BIS (PHOSPHONOOXY)CYCLOHEXYL]OXY}PHOSPHORYL]OXY}PROPANE-1,2-DIYL

DIBUTANOATE (three-letter code: 3PT) (formula: C<sub>17</sub>H<sub>33</sub>O<sub>19</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			39	17	19	3		
3	B	1	Total	C	O	P	0	0
			39	17	19	3		
3	C	1	Total	C	O	P	0	0
			39	17	19	3		
3	D	1	Total	C	O	P	0	0
			39	17	19	3		

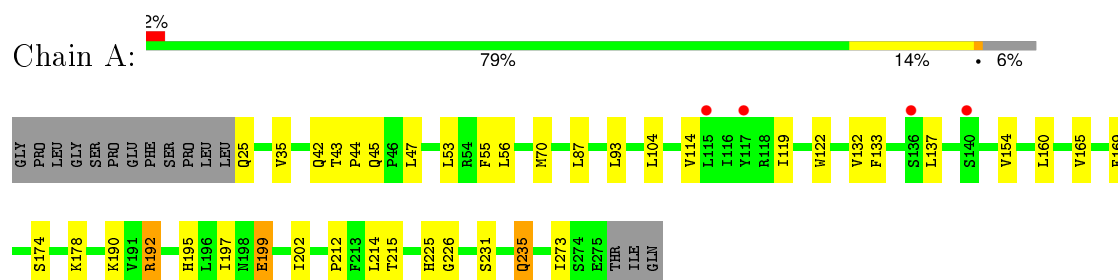
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	42	Total	O	0	0
			42	42		
4	B	42	Total	O	0	0
			42	42		
4	D	1	Total	O	0	0
			1	1		

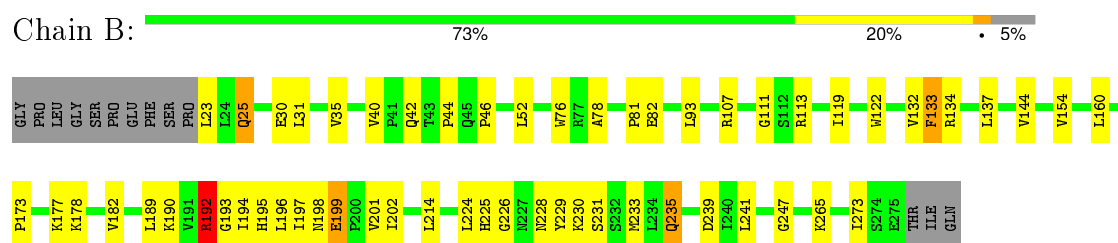
### 3 Residue-property plots [i](#)

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.

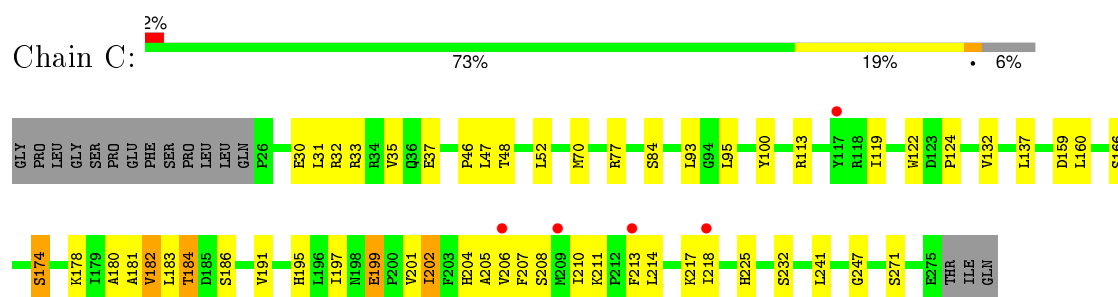
- Molecule 1: Alpha-tocopherol transfer protein



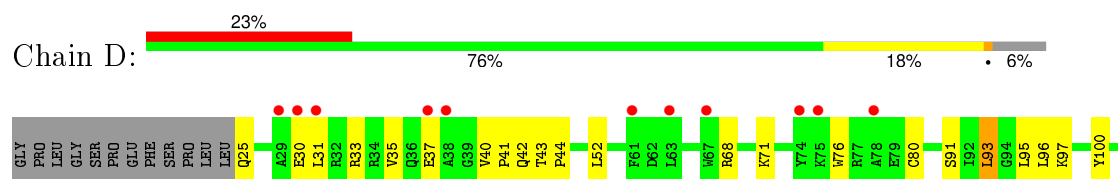
- Molecule 1: Alpha-tocopherol transfer protein

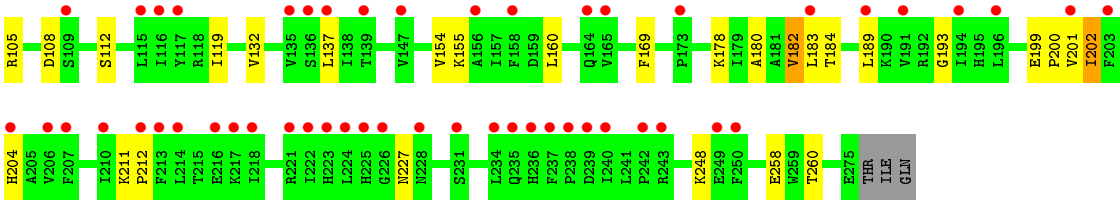


- Molecule 1: Alpha-tocopherol transfer protein



- Molecule 1: Alpha-tocopherol transfer protein







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.28Å 69.67Å 87.18Å 100.24° 109.72° 100.46°	Depositor
Resolution (Å)	28.41 – 2.61 28.41 – 2.61	Depositor EDS
% Data completeness (in resolution range)	95.5 (28.41-2.61) 87.8 (28.41-2.61)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.211 , 0.260 0.208 , 0.255	Depositor DCC
$R_{free}$ test set	1851 reflections (5.49%)	DCC
Wilson B-factor (Å <sup>2</sup> )	62.4	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 53.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 35512 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8568	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: 3PT, VIV

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	0.60	0/2104	0.71	0/2848
1	B	0.56	0/2116	0.72	3/2866 (0.1%)
1	C	0.56	0/2091	0.67	0/2831
1	D	0.43	0/2100	0.58	0/2844
All	All	0.54	0/8411	0.67	3/11389 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	23	LEU	CA-CB-CG	5.45	127.83	115.30
1	B	214	LEU	CA-CB-CG	5.26	127.40	115.30
1	B	192	ARG	NE-CZ-NH1	5.02	122.81	120.30

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	2052	0	2063	22	0
1	B	2064	0	2074	36	0
1	C	2039	0	2045	33	0
1	D	2048	0	2052	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	31	0	50	0	0
2	B	31	0	49	1	0
2	C	31	0	49	3	0
2	D	31	0	49	2	0
3	A	39	0	28	1	0
3	B	39	0	28	1	0
3	C	39	0	28	2	0
3	D	39	0	28	0	0
4	A	42	0	0	1	0
4	B	42	0	0	0	0
4	D	1	0	0	0	0
All	All	8568	0	8543	116	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 7.

All (116) 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:D:93:LEU:HD13	1:D:97:LYS:HE2	1.56	0.88
1:B:119:ILE:HG13	1:B:160:LEU:HD23	1.58	0.85
1:C:183:LEU:HD22	1:C:191:VAL:HG21	1.59	0.83
1:C:32:ARG:NH2	1:C:47:LEU:O	2.14	0.79
1:D:43:THR:HB	1:D:44:PRO:HA	1.66	0.76
1:A:195:HIS:ND1	1:A:225:HIS:HE1	1.85	0.75
1:B:133:PHE:CZ	1:B:182:VAL:HG21	2.26	0.71
1:A:119:ILE:HG13	1:A:160:LEU:HD23	1.72	0.69
1:D:33:ARG:O	1:D:37:GLU:HG2	1.93	0.68
1:C:210:ILE:HG22	1:C:214:LEU:HG	1.74	0.68
1:C:195:HIS:ND1	1:C:225:HIS:HE1	1.96	0.63
1:C:207:PHE:CE2	1:C:211:LYS:HG2	2.34	0.62
1:A:212:PRO:O	1:B:177:LYS:HD2	1.99	0.62
1:D:155:LYS:HD3	1:D:193:GLY:HA3	1.81	0.62
1:B:133:PHE:HZ	1:B:182:VAL:HG21	1.64	0.62
1:A:199:GLU:OE1	1:A:226:GLY:N	2.34	0.61
1:D:93:LEU:CD1	1:D:97:LYS:HE2	2.30	0.60
1:C:31:LEU:HD11	1:C:70:MET:HE3	1.83	0.59
1:A:87:LEU:HD12	1:A:273:ILE:HG13	1.83	0.59
1:B:182:VAL:HG11	2:B:301:VIV:H123	1.84	0.58
1:B:201:VAL:HG21	1:D:204:HIS:HB3	1.87	0.57
1:A:195:HIS:ND1	1:A:225:HIS:CE1	2.72	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:VAL:HG13	1:D:40:VAL:HB	1.86	0.56
1:B:35:VAL:HG13	1:B:40:VAL:HB	1.87	0.56
1:D:119:ILE:HG13	1:D:160:LEU:HD23	1.88	0.56
1:C:197:ILE:HG22	1:C:225:HIS:HB2	1.88	0.56
1:C:180:ALA:O	1:C:184:THR:OG1	2.21	0.55
1:C:241:LEU:O	1:C:247:GLY:HA3	2.06	0.55
1:C:33:ARG:O	1:C:37:GLU:HG2	2.06	0.55
1:C:181:ALA:O	1:C:186:SER:HB2	2.07	0.54
1:A:212:PRO:HG2	1:B:173:PRO:HB2	1.87	0.54
1:B:201:VAL:HG11	1:D:204:HIS:HB2	1.88	0.54
1:B:76:TRP:CZ2	1:B:182:VAL:HG22	2.43	0.54
1:B:231:SER:O	1:B:235:GLN:NE2	2.40	0.54
1:D:95:LEU:HD21	1:D:132:VAL:HG22	1.89	0.54
1:B:195:HIS:ND1	1:B:225:HIS:HE1	2.05	0.54
1:D:108:ASP:OD2	1:D:155:LYS:NZ	2.41	0.53
1:A:190:LYS:HD3	1:A:192:ARG:NH1	2.23	0.53
1:A:35:VAL:CG1	1:A:47:LEU:HD13	2.39	0.53
1:A:174:SER:O	1:A:178:LYS:HG3	2.10	0.52
1:D:68:ARG:HA	1:D:71:LYS:HE3	1.91	0.52
1:A:165:VAL:HG12	1:A:169:PHE:CE1	2.45	0.51
1:A:231:SER:O	1:A:235:GLN:NE2	2.44	0.50
1:C:46:PRO:HB2	1:C:48:THR:HG23	1.93	0.50
1:B:76:TRP:CE2	1:B:182:VAL:HG22	2.47	0.50
2:C:301:VIV:H262	2:C:301:VIV:HC11	1.93	0.50
1:D:182:VAL:HG12	1:D:183:LEU:HG	1.94	0.50
1:D:154:VAL:HG13	1:D:189:LEU:HD22	1.94	0.49
1:C:218:ILE:HD11	3:C:302:3PT:H32	1.95	0.49
1:C:33:ARG:NH1	1:C:33:ARG:HB3	2.27	0.48
1:C:182:VAL:HG11	2:C:301:VIV:H123	1.94	0.48
1:B:133:PHE:HZ	1:B:182:VAL:CG2	2.26	0.48
1:B:241:LEU:O	1:B:247:GLY:HA3	2.14	0.48
1:A:165:VAL:HG12	1:A:169:PHE:HE1	1.79	0.48
1:B:196:LEU:HG	1:B:224:LEU:HD22	1.96	0.47
1:D:43:THR:HB	1:D:44:PRO:CA	2.41	0.47
1:A:45:GLN:HG3	4:A:410:HOH:O	2.14	0.47
1:C:77:ARG:HG2	1:C:84:SER:HB2	1.96	0.47
1:C:31:LEU:HD23	1:C:52:LEU:HB3	1.96	0.47
1:C:159:ASP:HA	1:C:197:ILE:HG13	1.96	0.47
1:D:108:ASP:OD1	1:D:112:SER:N	2.46	0.47
1:D:200:PRO:O	1:D:202:ILE:N	2.47	0.47
1:C:174:SER:O	1:C:178:LYS:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:LYS:HE2	3:B:302:3PT:OP5	2.15	0.47
1:B:133:PHE:CE2	1:B:182:VAL:HG21	2.50	0.47
1:C:204:HIS:O	1:C:208:SER:N	2.40	0.47
1:C:122:TRP:CE2	1:C:132:VAL:HG21	2.50	0.46
1:D:76:TRP:CZ2	1:D:182:VAL:HG23	2.51	0.46
1:B:78:ALA:O	1:B:81:PRO:HD3	2.16	0.46
1:B:199:GLU:OE1	1:B:226:GLY:N	2.47	0.45
1:A:104:LEU:HD12	1:A:114:VAL:HB	1.98	0.45
1:C:122:TRP:O	1:C:124:PRO:HD3	2.17	0.45
1:C:202:ILE:HD13	1:C:202:ILE:HA	1.82	0.45
1:C:119:ILE:HG13	1:C:160:LEU:HD23	1.98	0.45
2:C:301:VIV:H211	2:C:301:VIV:H191	1.92	0.45
1:B:107:ARG:HD3	1:B:111:GLY:O	2.17	0.45
1:D:211:LYS:HB2	1:D:212:PRO:HD3	1.98	0.45
1:B:44:PRO:HB2	1:B:273:ILE:HA	1.98	0.44
1:B:76:TRP:CZ2	1:B:182:VAL:CG2	3.01	0.44
1:B:178:LYS:O	1:B:182:VAL:HG23	2.18	0.44
1:C:31:LEU:O	1:C:35:VAL:HG23	2.18	0.44
1:D:80:CYS:SG	1:D:178:LYS:HG2	2.58	0.44
1:C:199:GLU:H	1:C:199:GLU:CD	2.17	0.43
1:B:190:LYS:HD3	1:B:192:ARG:NH1	2.33	0.43
1:C:122:TRP:CD2	1:C:132:VAL:HG21	2.52	0.43
1:B:197:ILE:O	1:B:198:ASN:HB2	2.19	0.43
1:A:197:ILE:HG22	1:A:225:HIS:HB2	2.01	0.42
1:A:214:LEU:HD23	3:A:302:3PT:H12	2.01	0.42
1:D:105:ARG:NH2	1:D:258:GLU:OE1	2.45	0.42
1:C:183:LEU:O	3:C:302:3PT:H18	2.19	0.42
1:D:100:TYR:CZ	1:D:132:VAL:HG13	2.55	0.42
1:B:154:VAL:HG13	1:B:189:LEU:HD22	2.01	0.42
1:B:199:GLU:H	1:B:199:GLU:CD	2.22	0.42
1:D:96:LEU:HB3	1:D:260:THR:OG1	2.20	0.42
2:D:301:VIV:H161	2:D:301:VIV:H202	1.84	0.42
1:A:35:VAL:HG13	1:A:47:LEU:HD13	2.02	0.41
1:B:122:TRP:CE2	1:B:132:VAL:HG21	2.54	0.41
1:D:180:ALA:O	1:D:184:THR:OG1	2.28	0.41
1:B:229:TYR:O	1:B:230:LYS:C	2.58	0.41
1:B:265:LYS:HB2	1:B:265:LYS:HE2	1.87	0.41
1:D:31:LEU:HD23	1:D:52:LEU:HB3	2.02	0.41
1:B:25:GLN:HB2	1:B:25:GLN:HE21	1.62	0.41
1:A:122:TRP:CD2	1:A:132:VAL:HG21	2.55	0.41
1:C:205:ALA:C	1:C:207:PHE:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:PHE:CE1	1:A:70:MET:HA	2.56	0.41
1:B:193:GLY:O	1:B:194:ILE:HD13	2.21	0.41
2:D:301:VIV:H251	2:D:301:VIV:HC11	1.86	0.41
1:A:43:THR:HB	1:A:44:PRO:HA	2.03	0.41
1:A:53:LEU:HD23	1:A:56:LEU:HD12	2.02	0.40
1:C:100:TYR:CZ	1:C:132:VAL:HG13	2.56	0.40
1:B:31:LEU:HD23	1:B:52:LEU:HB3	2.04	0.40
1:C:35:VAL:CG1	1:C:47:LEU:HD13	2.52	0.40
1:C:95:LEU:HD21	1:C:132:VAL:HG22	2.03	0.40
1:B:44:PRO:O	1:B:46:PRO:HD3	2.21	0.40
1:B:82:GLU:O	1:B:134:ARG:NH2	2.54	0.40
1:C:35:VAL:HG11	1:C:47:LEU:HD13	2.04	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	249/266 (94%)	240 (96%)	9 (4%)	0	100	100
1	B	251/266 (94%)	244 (97%)	6 (2%)	1 (0%)	39	63
1	C	248/266 (93%)	235 (95%)	10 (4%)	3 (1%)	16	32
1	D	249/266 (94%)	229 (92%)	17 (7%)	3 (1%)	16	32
All	All	997/1064 (94%)	948 (95%)	42 (4%)	7 (1%)	26	49

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	239	ASP
1	C	217	LYS
1	D	201	VAL

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Mol	Chain	Res	Type
1	C	206	VAL
1	D	248	LYS
1	D	41	PRO
1	C	201	VAL

### 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	223/236 (94%)	212 (95%)	11 (5%)	31	56
1	B	224/236 (95%)	210 (94%)	14 (6%)	22	43
1	C	221/236 (94%)	208 (94%)	13 (6%)	24	46
1	D	222/236 (94%)	211 (95%)	11 (5%)	30	55
All	All	890/944 (94%)	841 (94%)	49 (6%)	27	50

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	42	GLN
1	A	93	LEU
1	A	133	PHE
1	A	137	LEU
1	A	154	VAL
1	A	192	ARG
1	A	199	GLU
1	A	202	ILE
1	A	215	THR
1	A	235	GLN
1	B	25	GLN
1	B	30	GLU
1	B	42	GLN
1	B	93	LEU
1	B	113	ARG
1	B	133	PHE

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Mol	Chain	Res	Type
1	B	137	LEU
1	B	144	VAL
1	B	192	ARG
1	B	199	GLU
1	B	202	ILE
1	B	228	ASN
1	B	233	MET
1	B	235	GLN
1	C	30	GLU
1	C	93	LEU
1	C	113	ARG
1	C	137	LEU
1	C	166	SER
1	C	174	SER
1	C	182	VAL
1	C	184	THR
1	C	199	GLU
1	C	202	ILE
1	C	213	PHE
1	C	232	SER
1	C	271	SER
1	D	25	GLN
1	D	30	GLU
1	D	42	GLN
1	D	91	SER
1	D	93	LEU
1	D	137	LEU
1	D	169	PHE
1	D	182	VAL
1	D	199	GLU
1	D	202	ILE
1	D	227	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	225	HIS
1	A	235	GLN
1	B	25	GLN
1	B	225	HIS
1	B	235	GLN

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Mol	Chain	Res	Type
1	B	257	GLN
1	C	225	HIS
1	C	235	GLN
1	C	257	GLN
1	D	198	ASN
1	D	225	HIS
1	D	236	HIS
1	D	257	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](#)

8 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	$\# Z  > 2$
2	VIV	A	301	-	32,32,32	0.89	2 (6%)	41,45,45	1.22	3 (7%)
3	3PT	A	302	-	39,39,39	1.88	7 (17%)	49,57,57	1.80	10 (20%)
2	VIV	B	301	-	32,32,32	0.94	2 (6%)	41,45,45	1.23	6 (14%)
3	3PT	B	302	-	39,39,39	2.07	7 (17%)	49,57,57	1.48	8 (16%)
2	VIV	C	301	-	32,32,32	0.99	2 (6%)	41,45,45	1.56	6 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	3PT	C	302	-	39,39,39	1.81	5 (12%)	49,57,57	1.55	7 (14%)
2	VIV	D	301	-	32,32,32	0.88	2 (6%)	41,45,45	1.23	5 (12%)
3	3PT	D	302	-	39,39,39	1.80	4 (10%)	49,57,57	1.59	8 (16%)

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
2	VIV	A	301	-	-	0/19/30/30	0/2/2/2
3	3PT	A	302	-	-	0/36/60/60	0/1/1/1
2	VIV	B	301	-	-	0/19/30/30	0/2/2/2
3	3PT	B	302	-	-	1/36/60/60	0/1/1/1
2	VIV	C	301	-	-	0/19/30/30	0/2/2/2
3	3PT	C	302	-	-	1/36/60/60	0/1/1/1
2	VIV	D	301	-	-	0/19/30/30	0/2/2/2
3	3PT	D	302	-	-	0/36/60/60	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	VIV	C21-C22	-2.75	1.39	1.52
2	C	301	VIV	C21-C20	-2.68	1.39	1.52
2	B	301	VIV	C21-C22	-2.57	1.40	1.52
2	A	301	VIV	C21-C22	-2.53	1.40	1.52
2	B	301	VIV	C21-C20	-2.51	1.40	1.52
2	D	301	VIV	C21-C22	-2.50	1.40	1.52
2	D	301	VIV	C21-C20	-2.42	1.41	1.52
2	A	301	VIV	C21-C20	-2.29	1.41	1.52
3	A	302	3PT	P3-O11	-2.18	1.46	1.54
3	B	302	3PT	P1-OP1	2.10	1.68	1.59
3	B	302	3PT	P3-O12	2.21	1.62	1.54
3	D	302	3PT	P3-O12	2.25	1.62	1.54
3	A	302	3PT	P3-O12	2.28	1.62	1.54
3	C	302	3PT	P1-OP3	2.40	1.65	1.54
3	C	302	3PT	P4-OP4	2.46	1.63	1.54
3	A	302	3PT	C0I-C0G	2.87	1.59	1.50
3	B	302	3PT	C0I-C0G	2.91	1.59	1.50
3	A	302	3PT	P1-OP3	2.96	1.67	1.54
3	B	302	3PT	P3-O10	3.13	1.61	1.51
3	C	302	3PT	P3-O10	3.22	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	3PT	O0D-C0G	3.25	1.44	1.34
3	B	302	3PT	P1-OP3	3.33	1.69	1.54
3	D	302	3PT	P3-O10	3.63	1.63	1.51
3	A	302	3PT	P3-O10	3.89	1.64	1.51
3	D	302	3PT	O0D-C0G	4.01	1.46	1.34
3	C	302	3PT	O0D-C0G	4.13	1.46	1.34
3	B	302	3PT	O0D-C0G	5.20	1.49	1.34
3	D	302	3PT	O0H-C0G	7.01	1.43	1.22
3	C	302	3PT	O0H-C0G	7.39	1.44	1.22
3	A	302	3PT	O0H-C0G	7.78	1.45	1.22
3	B	302	3PT	O0H-C0G	8.66	1.48	1.22

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	3PT	O0D-C0G-O0H	-7.46	103.66	123.67
3	C	302	3PT	O0D-C0G-O0H	-5.97	107.66	123.67
3	D	302	3PT	O0D-C0G-O0H	-5.40	109.17	123.67
2	C	301	VIV	O1-C4-C3	-5.10	118.44	122.55
3	B	302	3PT	O0D-C0G-O0H	-4.50	111.60	123.67
3	A	302	3PT	C0B-C0C-C0E	-4.35	101.91	112.07
3	B	302	3PT	C0B-C0C-C0E	-3.79	103.20	112.07
2	C	301	VIV	C15-C16-C17	-3.75	104.58	112.69
3	D	302	3PT	O0H-C0G-C0I	-3.53	109.61	123.72
3	C	302	3PT	O0H-C0G-C0I	-3.50	109.73	123.72
3	B	302	3PT	O0H-C0G-C0I	-3.41	110.06	123.72
3	A	302	3PT	C0E-O0F-C0L	-3.38	107.39	116.85
3	B	302	3PT	O12-P3-O10	-2.51	102.49	110.58
3	D	302	3PT	C0B-C0C-C0E	-2.49	106.23	112.07
2	B	301	VIV	C15-C16-C17	-2.27	107.77	112.69
3	A	302	3PT	O12-P3-O10	-2.23	103.40	110.58
3	A	302	3PT	C0C-O0D-C0G	-2.13	112.77	117.89
3	C	302	3PT	C0B-C0C-C0E	-2.09	107.19	112.07
3	A	302	3PT	O0F-C0L-O0M	-2.09	118.11	123.49
3	A	302	3PT	O11-P3-O12	2.00	115.00	107.38
2	D	301	VIV	C4-C5-C6	2.02	120.57	118.67
3	C	302	3PT	O0F-C0L-C0N	2.06	118.18	111.90
3	D	302	3PT	C5-C6-C1	2.07	114.14	109.60
3	B	302	3PT	O0F-C0L-C0N	2.07	118.22	111.90
3	B	302	3PT	C2-C1-C6	2.10	113.65	110.89
2	B	301	VIV	O1-C4-C5	2.12	117.77	115.31
2	A	301	VIV	C7-C2-C3	2.14	121.14	118.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	VIV	O1-C4-C5	2.28	117.94	115.31
2	B	301	VIV	C22-C21-C20	2.34	124.60	112.99
3	B	302	3PT	O11-P3-O12	2.35	116.34	107.38
3	B	302	3PT	O0D-C0G-C0I	2.47	116.90	111.53
2	B	301	VIV	O1-C9-C14	2.48	111.79	105.28
3	D	302	3PT	O0F-C0L-C0N	2.50	119.51	111.90
2	B	301	VIV	C7-C2-C3	2.53	121.57	118.79
3	C	302	3PT	C3-C2-C1	2.55	114.20	109.06
2	C	301	VIV	C22-C21-C20	2.55	125.63	112.99
3	C	302	3PT	O4-P4-OP5	2.61	113.63	107.11
2	C	301	VIV	C21-C22-C23	2.65	124.29	115.49
2	D	301	VIV	C7-C2-C3	2.70	121.76	118.79
2	D	301	VIV	C22-C21-C20	2.71	126.43	112.99
2	A	301	VIV	C22-C21-C20	2.79	126.80	112.99
3	A	302	3PT	O0F-C0L-C0N	2.86	120.61	111.90
2	D	301	VIV	C21-C22-C23	2.91	125.15	115.49
2	A	301	VIV	C21-C22-C23	3.03	125.55	115.49
3	D	302	3PT	O4-P4-OP5	3.06	114.74	107.11
2	C	301	VIV	O1-C4-C5	3.13	118.94	115.31
3	A	302	3PT	C2-C1-C6	3.14	115.02	110.89
3	A	302	3PT	O0F-C0E-C0C	3.28	117.51	108.69
2	B	301	VIV	C21-C22-C23	3.53	127.19	115.49
3	D	302	3PT	C2-C1-C6	3.76	115.83	110.89
2	C	301	VIV	O1-C9-C14	3.92	115.56	105.28
3	D	302	3PT	C3-C2-C1	3.95	117.03	109.06
3	C	302	3PT	C2-C1-C6	4.32	116.57	110.89

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	302	3PT	C0C-O0D-C0G-O0H
3	C	302	3PT	C0C-O0D-C0G-O0H

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	3PT	1	0
2	B	301	VIV	1	0
3	B	302	3PT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	VIV	3	0
3	C	302	3PT	2	0
2	D	301	VIV	2	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	251/266 (94%)	-0.35	4 (1%) 74 69	28, 51, 82, 113	0
1	B	253/266 (95%)	-0.42	0 100 100	26, 55, 83, 114	0
1	C	250/266 (93%)	-0.27	5 (2%) 68 63	33, 62, 108, 124	0
1	D	251/266 (94%)	1.11	61 (24%) 1 0	65, 124, 244, 281	0
All	All	1005/1064 (94%)	0.02	70 (6%) 19 14	26, 62, 175, 281	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	213	PHE	11.8
1	D	234	LEU	6.4
1	D	210	ILE	5.9
1	D	201	VAL	5.8
1	D	237	PHE	5.8
1	D	203	PHE	5.5
1	D	165	VAL	5.3
1	D	249	GLU	5.2
1	D	109	SER	5.1
1	D	235	GLN	4.9
1	D	115	LEU	4.5
1	D	207	PHE	4.2
1	D	194	ILE	4.1
1	D	136	SER	4.1
1	D	228	ASN	4.1
1	D	204	HIS	4.1
1	D	221	ARG	4.0
1	D	31	LEU	3.8
1	D	231	SER	3.7
1	D	218	ILE	3.7
1	D	240	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	196	LEU	3.6
1	D	243	ARG	3.5
1	C	209	MET	3.5
1	D	214	LEU	3.5
1	D	30	GLU	3.5
1	D	37	GLU	3.4
1	C	218	ILE	3.3
1	D	156	ALA	3.2
1	D	63	LEU	3.1
1	D	224	LEU	3.0
1	D	78	ALA	3.0
1	D	191	VAL	2.9
1	D	216	GLU	2.9
1	D	236	HIS	2.8
1	D	164	GLN	2.8
1	D	147	VAL	2.8
1	D	38	ALA	2.8
1	D	189	LEU	2.7
1	D	225	HIS	2.7
1	C	206	VAL	2.7
1	D	206	VAL	2.7
1	D	223	HIS	2.6
1	A	136	SER	2.6
1	D	135	VAL	2.6
1	D	212	PRO	2.5
1	D	173	PRO	2.5
1	C	213	PHE	2.5
1	D	74	TYR	2.4
1	D	217	LYS	2.4
1	D	238	PRO	2.4
1	D	137	LEU	2.4
1	D	29	ALA	2.4
1	D	250	PHE	2.4
1	D	61	PHE	2.3
1	C	117	TYR	2.3
1	A	117	TYR	2.3
1	D	222	ILE	2.2
1	D	117	TYR	2.2
1	D	239	ASP	2.2
1	D	139	THR	2.2
1	D	242	PRO	2.2
1	D	226	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	115	LEU	2.1
1	D	67	TRP	2.1
1	D	75	LYS	2.1
1	D	183	LEU	2.1
1	A	140	SER	2.1
1	D	158	PHE	2.0
1	D	116	ILE	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	VIV	C	301	31/31	0.95	0.33	2.81	45,50,60,61	0
2	VIV	B	301	31/31	0.95	0.25	1.39	41,51,54,55	0
2	VIV	A	301	31/31	0.95	0.30	1.37	38,47,53,55	0
2	VIV	D	301	31/31	0.93	0.34	0.31	75,78,84,85	0
3	3PT	C	302	39/39	0.80	0.27	0.21	120,132,142,142	0
3	3PT	D	302	39/39	0.75	0.35	0.06	163,167,172,173	0
3	3PT	A	302	39/39	0.94	0.12	-0.39	37,61,78,78	0
3	3PT	B	302	39/39	0.96	0.12	-0.54	37,56,73,74	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.