



# Full wwPDB X-ray Structure Validation Report

Mar 31, 2014 – 03:37 PM BST

PDB ID : 3ED1  
Title : Crystal Structure of Rice GID1 complexed with GA3  
Authors : Shimada, A.; Nakatsu, T.; Ueguchi-Tanaka, M.; Kato, H.; Matsuoka, M.  
Deposited on : 2008-09-02  
Resolution : 1.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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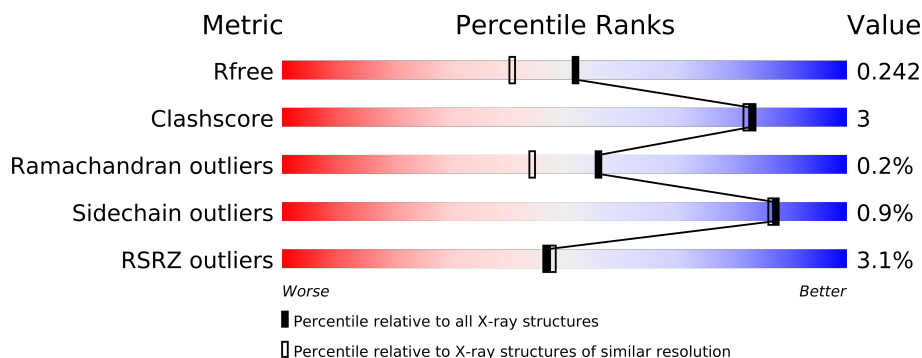
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable23004  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23004

# 1 Overall quality at a glance

The reported resolution of this entry is 1.90 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))
$R_{free}$	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	365	
1	B	365	
1	C	365	
1	D	365	
1	E	365	
1	F	365	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MPD	A	501	-	X
2	MPD	B	501	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	MPD	D	501	-	X
3	NO3	A	601	X	X
3	NO3	A	602	X	X
3	NO3	A	603	X	-
3	NO3	B	601	X	X
3	NO3	B	602	X	X
3	NO3	B	604	X	X
3	NO3	C	602	X	X
3	NO3	C	604	X	-
3	NO3	D	601	X	-
3	NO3	D	603	X	-
3	NO3	F	602	X	X
3	NO3	F	603	X	-
5	PO4	B	701	-	X
5	PO4	E	701	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15936 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Gibberellin receptor GID1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	4	0
			2510	1591	447	462	10			
1	B	316	Total	C	N	O	S	0	5	0
			2476	1572	441	453	10			
1	C	301	Total	C	N	O	S	0	3	0
			2365	1507	416	432	10			
1	D	315	Total	C	N	O	S	0	3	0
			2455	1561	429	455	10			
1	E	313	Total	C	N	O	S	0	2	0
			2390	1526	416	437	11			
1	F	305	Total	C	N	O	S	0	2	0
			2378	1518	416	434	10			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	355	GLY	-	EXPRESSION TAG	UNP Q6L545
A	356	SER	-	EXPRESSION TAG	UNP Q6L545
A	357	HIS	-	EXPRESSION TAG	UNP Q6L545
A	358	HIS	-	EXPRESSION TAG	UNP Q6L545
A	359	HIS	-	EXPRESSION TAG	UNP Q6L545
A	360	HIS	-	EXPRESSION TAG	UNP Q6L545
A	361	HIS	-	EXPRESSION TAG	UNP Q6L545
A	362	HIS	-	EXPRESSION TAG	UNP Q6L545
A	363	HIS	-	EXPRESSION TAG	UNP Q6L545
A	364	HIS	-	EXPRESSION TAG	UNP Q6L545
A	365	HIS	-	EXPRESSION TAG	UNP Q6L545
A	366	HIS	-	EXPRESSION TAG	UNP Q6L545
B	355	GLY	-	EXPRESSION TAG	UNP Q6L545
B	356	SER	-	EXPRESSION TAG	UNP Q6L545
B	357	HIS	-	EXPRESSION TAG	UNP Q6L545
B	358	HIS	-	EXPRESSION TAG	UNP Q6L545
B	359	HIS	-	EXPRESSION TAG	UNP Q6L545

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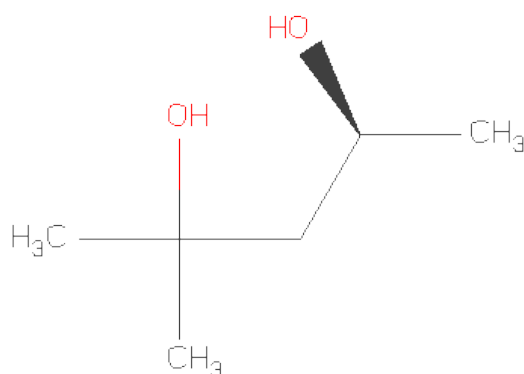
Chain	Residue	Modelled	Actual	Comment	Reference
B	360	HIS	-	EXPRESSION TAG	UNP Q6L545
B	361	HIS	-	EXPRESSION TAG	UNP Q6L545
B	362	HIS	-	EXPRESSION TAG	UNP Q6L545
B	363	HIS	-	EXPRESSION TAG	UNP Q6L545
B	364	HIS	-	EXPRESSION TAG	UNP Q6L545
B	365	HIS	-	EXPRESSION TAG	UNP Q6L545
B	366	HIS	-	EXPRESSION TAG	UNP Q6L545
C	355	GLY	-	EXPRESSION TAG	UNP Q6L545
C	356	SER	-	EXPRESSION TAG	UNP Q6L545
C	357	HIS	-	EXPRESSION TAG	UNP Q6L545
C	358	HIS	-	EXPRESSION TAG	UNP Q6L545
C	359	HIS	-	EXPRESSION TAG	UNP Q6L545
C	360	HIS	-	EXPRESSION TAG	UNP Q6L545
C	361	HIS	-	EXPRESSION TAG	UNP Q6L545
C	362	HIS	-	EXPRESSION TAG	UNP Q6L545
C	363	HIS	-	EXPRESSION TAG	UNP Q6L545
C	364	HIS	-	EXPRESSION TAG	UNP Q6L545
C	365	HIS	-	EXPRESSION TAG	UNP Q6L545
C	366	HIS	-	EXPRESSION TAG	UNP Q6L545
D	355	GLY	-	EXPRESSION TAG	UNP Q6L545
D	356	SER	-	EXPRESSION TAG	UNP Q6L545
D	357	HIS	-	EXPRESSION TAG	UNP Q6L545
D	358	HIS	-	EXPRESSION TAG	UNP Q6L545
D	359	HIS	-	EXPRESSION TAG	UNP Q6L545
D	360	HIS	-	EXPRESSION TAG	UNP Q6L545
D	361	HIS	-	EXPRESSION TAG	UNP Q6L545
D	362	HIS	-	EXPRESSION TAG	UNP Q6L545
D	363	HIS	-	EXPRESSION TAG	UNP Q6L545
D	364	HIS	-	EXPRESSION TAG	UNP Q6L545
D	365	HIS	-	EXPRESSION TAG	UNP Q6L545
D	366	HIS	-	EXPRESSION TAG	UNP Q6L545
E	355	GLY	-	EXPRESSION TAG	UNP Q6L545
E	356	SER	-	EXPRESSION TAG	UNP Q6L545
E	357	HIS	-	EXPRESSION TAG	UNP Q6L545
E	358	HIS	-	EXPRESSION TAG	UNP Q6L545
E	359	HIS	-	EXPRESSION TAG	UNP Q6L545
E	360	HIS	-	EXPRESSION TAG	UNP Q6L545
E	361	HIS	-	EXPRESSION TAG	UNP Q6L545
E	362	HIS	-	EXPRESSION TAG	UNP Q6L545
E	363	HIS	-	EXPRESSION TAG	UNP Q6L545
E	364	HIS	-	EXPRESSION TAG	UNP Q6L545
E	365	HIS	-	EXPRESSION TAG	UNP Q6L545

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Chain	Residue	Modelled	Actual	Comment	Reference
E	366	HIS	-	EXPRESSION TAG	UNP Q6L545
F	355	GLY	-	EXPRESSION TAG	UNP Q6L545
F	356	SER	-	EXPRESSION TAG	UNP Q6L545
F	357	HIS	-	EXPRESSION TAG	UNP Q6L545
F	358	HIS	-	EXPRESSION TAG	UNP Q6L545
F	359	HIS	-	EXPRESSION TAG	UNP Q6L545
F	360	HIS	-	EXPRESSION TAG	UNP Q6L545
F	361	HIS	-	EXPRESSION TAG	UNP Q6L545
F	362	HIS	-	EXPRESSION TAG	UNP Q6L545
F	363	HIS	-	EXPRESSION TAG	UNP Q6L545
F	364	HIS	-	EXPRESSION TAG	UNP Q6L545
F	365	HIS	-	EXPRESSION TAG	UNP Q6L545
F	366	HIS	-	EXPRESSION TAG	UNP Q6L545

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



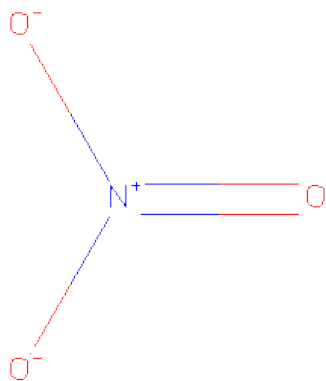
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	6	2		
2	B	1	Total	C	O	0	0
			8	6	2		
2	C	1	Total	C	O	0	0
			8	6	2		
2	D	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	C	O	0	0
			8	6	2		
2	F	1	Total	C	O	0	0
			8	6	2		

- Molecule 3 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).



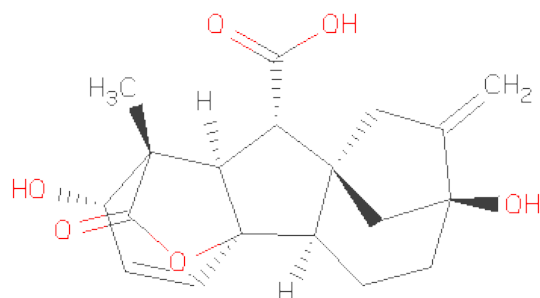
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	N	O	0	0
			4	1	3		
3	A	1	Total	N	O	0	0
			4	1	3		
3	A	1	Total	N	O	0	0
			4	1	3		
3	B	1	Total	N	O	0	0
			4	1	3		
3	B	1	Total	N	O	0	0
			4	1	3		
3	B	1	Total	N	O	0	0
			4	1	3		
3	C	1	Total	N	O	0	0
			4	1	3		
3	C	1	Total	N	O	0	0
			4	1	3		
3	D	1	Total	N	O	0	0
			4	1	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	N	O	0	0
			4	1	3		
3	F	1	Total	N	O	0	0
			4	1	3		
3	F	1	Total	N	O	0	0
			4	1	3		

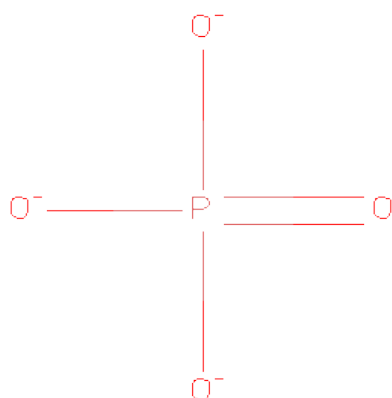
- Molecule 4 is GIBBERELLIN A3 (three-letter code: GA3) (formula: C<sub>19</sub>H<sub>22</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			25	19	6		
4	B	1	Total	C	O	0	0
			25	19	6		
4	C	1	Total	C	O	0	0
			25	19	6		
4	D	1	Total	C	O	0	0
			25	19	6		
4	E	1	Total	C	O	0	0
			25	19	6		
4	F	1	Total	C	O	0	0
			25	19	6		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).





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

- Molecule 6 is water.

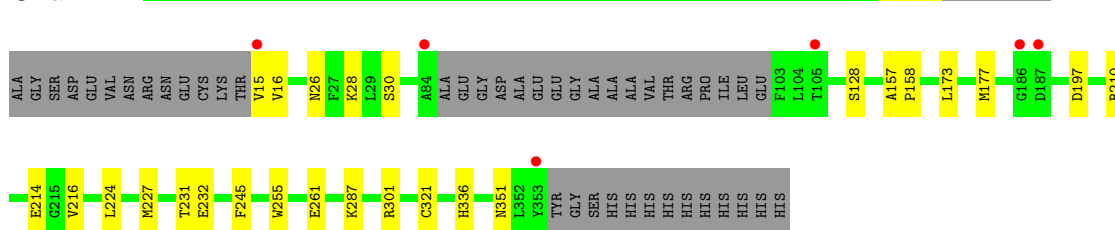
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	239	Total	O	0	0
			239	239		
6	B	193	Total	O	0	0
			193	193		
6	C	173	Total	O	0	0
			173	173		
6	D	204	Total	O	0	0
			204	204		
6	E	123	Total	O	0	0
			123	123		
6	F	174	Total	O	0	0
			174	174		

### 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.

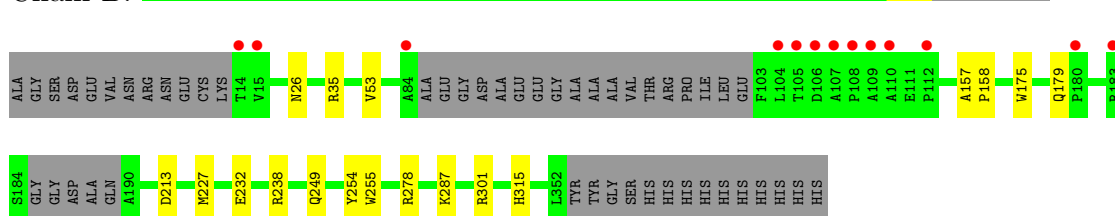
- Molecule 1: Gibberellin receptor GID1

Chain A:



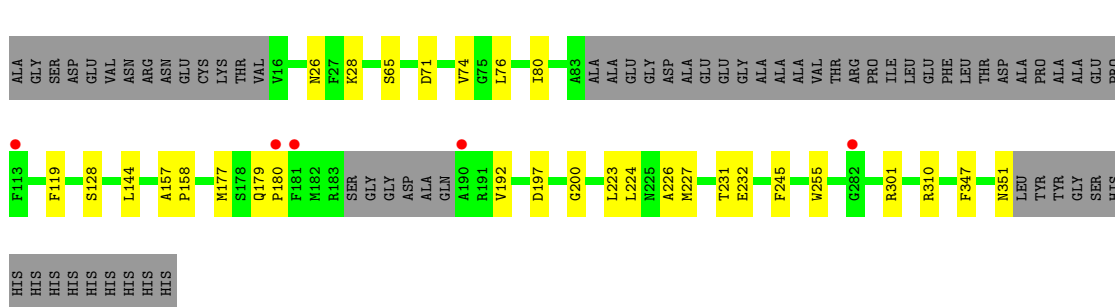
- Molecule 1: Gibberellin receptor GID1

Chain B:



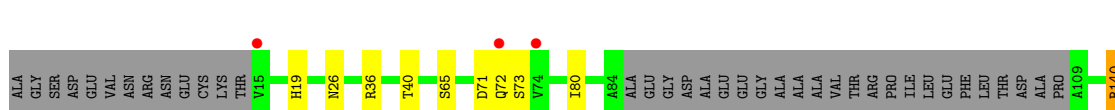
- Molecule 1: Gibberellin receptor GID1

Chain C:



- Molecule 1: Gibberellin receptor GID1

Chain D:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.72Å 134.14Å 118.87Å 90.00° 105.20° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 41.20 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-1.90) 97.4 (41.20-1.90)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.53 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.197 , 0.239 0.199 , 0.242	Depositor DCC
$R_{free}$ test set	9653 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.4	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 44.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 192187 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15936	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, GA3, MPD, NO3

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	0.75	0/2593	0.70	0/3524
1	B	0.69	0/2561	0.67	0/3480
1	C	0.65	0/2440	0.67	0/3313
1	D	0.67	0/2533	0.67	0/3446
1	E	0.58	0/2461	0.63	0/3352
1	F	0.64	0/2449	0.65	0/3328
All	All	0.66	0/15037	0.67	0/20443

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2510	0	2387	17	0
1	B	2476	0	2367	12	0
1	C	2365	0	2245	17	0
1	D	2455	0	2315	15	0
1	E	2390	0	2242	18	0
1	F	2378	0	2246	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	8	0	14	1	0
2	B	8	0	14	2	0
2	C	8	0	14	0	0
2	D	8	0	14	0	0
2	E	8	0	14	1	0
2	F	8	0	14	1	0
3	A	12	0	0	1	0
3	B	12	0	0	1	0
3	C	8	0	0	2	0
3	D	8	0	0	0	0
3	F	8	0	0	0	0
4	A	25	0	21	0	0
4	B	25	0	21	0	0
4	C	25	0	21	0	0
4	D	25	0	21	0	0
4	E	25	0	21	0	0
4	F	25	0	21	0	0
5	B	5	0	0	0	0
5	E	5	0	0	0	0
6	A	239	0	0	1	0
6	B	193	0	0	1	0
6	C	173	0	0	1	0
6	D	204	0	0	1	0
6	E	123	0	0	0	0
6	F	174	0	0	0	0
All	All	15936	0	14012	86	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (86) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:26:ASN:HD22	1:B:26:ASN:HD22	1.29	0.81
1:A:15:VAL:HG12	1:A:16:VAL:H	1.52	0.73
2:E:501:MPD:H13	2:F:501:MPD:H13	1.77	0.67
1:E:290:ILE:HG13	1:E:290:ILE:O	1.93	0.67
1:A:28[A]:LYS:HE3	1:A:245:PHE:O	1.98	0.63
1:D:279:ARG:HD2	1:D:312:ASP:OD2	1.99	0.63
1:C:347:PHE:O	1:C:351:ASN:ND2	2.33	0.62
1:C:177:MET:HE1	1:C:192:VAL:HG11	1.82	0.62
1:F:232:GLU:O	1:F:301:ARG:NH2	2.34	0.60
1:E:109:ALA:O	1:E:110:ALA:HB3	2.02	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:26:ASN:HD22	1:D:26:ASN:HD22	1.49	0.58
1:B:175:TRP:O	1:B:179:GLN:HG2	2.03	0.57
1:A:231:THR:HG22	3:A:602:NO3:O3	2.06	0.56
1:C:231:THR:HG22	3:C:602:NO3:O2	2.05	0.56
1:D:279:ARG:HH12	1:D:311:GLU:HB2	1.70	0.55
1:F:283:LEU:O	1:F:314:HIS:HE1	1.90	0.55
1:E:144:LEU:HD11	1:E:344:ILE:HG22	1.89	0.55
1:C:232:GLU:O	1:C:301:ARG:NH2	2.41	0.54
1:A:177:MET:HE2	1:A:216:VAL:CG1	2.38	0.54
2:A:501:MPD:HM2	2:B:501:MPD:H13	1.90	0.53
1:E:26:ASN:HD22	1:F:26:ASN:HD22	1.57	0.53
1:E:232:GLU:O	1:E:301:ARG:NH2	2.42	0.53
1:D:330:LEU:O	1:D:331:LEU:HD23	2.09	0.53
1:F:227:MET:HG2	1:F:255:TRP:CZ2	2.44	0.52
1:B:301:ARG:HG2	1:B:301:ARG:HH11	1.75	0.51
1:D:232:GLU:O	1:D:301:ARG:NH2	2.43	0.51
1:A:177:MET:CE	1:A:216:VAL:CG1	2.89	0.51
1:F:191:ARG:NH1	1:F:352:LEU:O	2.44	0.51
1:A:287:LYS:HD2	1:A:351:ASN:OD1	2.11	0.50
1:D:279:ARG:HH12	1:D:311:GLU:CB	2.24	0.49
1:A:227:MET:HG2	1:A:255:TRP:CZ2	2.48	0.48
1:E:205:HIS:O	1:E:208:ALA:HB3	2.13	0.48
1:D:65:SER:HA	1:D:80:ILE:O	2.13	0.48
1:A:30[A]:SER:OG	3:B:604:NO3:O1	2.27	0.48
1:E:119:PHE:O	1:E:200:GLY:HA3	2.14	0.48
1:E:140:ARG:HD3	1:E:337:TYR:OH	2.14	0.47
1:E:159:GLU:CD	1:E:159:GLU:H	2.18	0.47
1:C:144:LEU:HD12	1:C:144:LEU:C	2.35	0.47
1:B:232:GLU:O	1:B:301:ARG:NH2	2.48	0.47
1:E:218:VAL:HB	1:E:286:ALA:HB2	1.96	0.46
1:E:225:ASN:HA	1:E:302:GLN:OE1	2.14	0.46
1:D:140:ARG:NH1	6:D:787:HOH:O	2.47	0.46
1:C:223:LEU:HB3	1:C:226:ALA:HB2	1.97	0.46
1:A:28[A]:LYS:NZ	6:A:733:HOH:O	2.48	0.46
1:C:65:SER:HA	1:C:80:ILE:O	2.16	0.46
1:B:227:MET:HG2	1:B:255:TRP:CZ2	2.51	0.46
1:C:71:ASP:HB3	1:C:76:LEU:HB3	1.99	0.45
1:D:36:ARG:HD2	1:D:40:THR:OG1	2.17	0.45
1:B:157:ALA:HB1	1:B:158:PRO:HA	1.99	0.45
1:B:213:ASP:CG	1:B:278:ARG:HH22	2.20	0.45
1:B:26:ASN:HB3	2:B:501:MPD:HM2	1.99	0.44
1:E:109:ALA:O	1:E:110:ALA:CB	2.63	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:157:ALA:HB1	1:C:158:PRO:HA	1.98	0.44
1:A:232:GLU:O	1:A:301:ARG:NH2	2.50	0.44
1:A:157:ALA:HB1	1:A:158:PRO:HA	2.00	0.44
1:A:321:CYS:HB3	1:A:336:HIS:CG	2.53	0.44
1:D:159:GLU:H	1:D:159:GLU:HG2	1.14	0.43
1:F:175:TRP:O	1:F:179:GLN:HG2	2.18	0.43
1:A:210:ARG:O	1:A:214:GLU:HG3	2.19	0.43
1:D:281:GLY:HA2	1:D:312:ASP:O	2.18	0.43
1:E:279:ARG:HD2	1:E:312:ASP:OD2	2.19	0.43
1:C:197:ASP:HA	1:C:224:LEU:O	2.19	0.43
1:C:74:VAL:HG12	1:C:76:LEU:HB2	2.00	0.43
1:A:197:ASP:HA	1:A:224:LEU:O	2.19	0.43
1:B:213:ASP:OD1	1:B:278:ARG:NH2	2.51	0.42
1:E:144:LEU:HD12	1:E:144:LEU:C	2.40	0.42
1:B:287:LYS:HG2	1:B:315:HIS:HB3	2.01	0.42
1:B:238[A]:ARG:NH2	6:B:854:HOH:O	2.52	0.42
1:A:177:MET:CE	1:A:216:VAL:HG13	2.50	0.42
1:C:179:GLN:HA	1:C:180:PRO:HD3	1.97	0.41
1:E:197:ASP:HA	1:E:224:LEU:O	2.19	0.41
1:C:310:ARG:NH1	6:C:628:HOH:O	2.52	0.41
1:B:35:ARG:HD3	1:B:254:TYR:CZ	2.56	0.41
1:A:173:LEU:O	1:A:177:MET:HG2	2.20	0.41
1:C:119:PHE:O	1:C:200:GLY:HA3	2.20	0.41
1:D:197:ASP:HA	1:D:224:LEU:O	2.20	0.41
1:C:28[A]:LYS:HE3	1:C:245:PHE:O	2.21	0.41
1:E:231:THR:OG1	1:E:266:ASP:OD1	2.35	0.41
1:F:195:SER:HA	1:F:222:ILE:O	2.21	0.40
1:D:225:ASN:HA	1:D:302:GLN:OE1	2.21	0.40
3:C:604:NO3:O3	1:D:19:HIS:NE2	2.50	0.40
1:F:28[A]:LYS:HE3	1:F:245:PHE:O	2.21	0.40
1:C:227:MET:HG2	1:C:255:TRP:CZ2	2.56	0.40
1:D:71:ASP:C	1:D:73:SER:H	2.24	0.40
1:E:321:CYS:HB3	1:E:336:HIS:CG	2.57	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	321/365 (88%)	310 (97%)	11 (3%)	0	100	100
1	B	315/365 (86%)	303 (96%)	12 (4%)	0	100	100
1	C	298/365 (82%)	288 (97%)	10 (3%)	0	100	100
1	D	314/365 (86%)	305 (97%)	8 (2%)	1 (0%)	50	37
1	E	309/365 (85%)	297 (96%)	11 (4%)	1 (0%)	50	37
1	F	301/365 (82%)	291 (97%)	9 (3%)	1 (0%)	50	37
All	All	1858/2190 (85%)	1794 (97%)	61 (3%)	3 (0%)	56	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	72	GLN
1	E	110	ALA
1	F	73	SER

### 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	260/302 (86%)	258 (99%)	2 (1%)	89	89
1	B	258/302 (85%)	256 (99%)	2 (1%)	89	89
1	C	244/302 (81%)	243 (100%)	1 (0%)	95	95
1	D	251/302 (83%)	249 (99%)	2 (1%)	89	89
1	E	239/302 (79%)	236 (99%)	3 (1%)	80	77
1	F	241/302 (80%)	238 (99%)	3 (1%)	82	80
All	All	1493/1812 (82%)	1480 (99%)	13 (1%)	87	86

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	SER

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Mol	Chain	Res	Type
1	A	261	GLU
1	B	53	VAL
1	B	249	GLN
1	C	128	SER
1	D	140	ARG
1	D	159	GLU
1	E	144	LEU
1	E	231	THR
1	E	290	ILE
1	F	128	SER
1	F	177	MET
1	F	283	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	221	ASN
1	B	26	ASN
1	B	249	GLN
1	C	26	ASN
1	C	179	GLN
1	D	68	HIS
1	E	26	ASN
1	F	19	HIS
1	F	68	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

26 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
4	GA3	A	401	-	29,29,29	1.06	1 (3%)	52,52,52	1.79	13 (25%)
2	MPD	A	501	-	7,7,7	0.37	0	10,10,10	0.47	0
3	NO3	A	601	-	3,3,3	3.34	3 (100%)	3,3,3	0.55	0
3	NO3	A	602	-	3,3,3	3.36	3 (100%)	3,3,3	0.19	0
3	NO3	A	603	-	3,3,3	3.28	3 (100%)	3,3,3	0.10	0
4	GA3	B	401	-	29,29,29	1.36	3 (10%)	52,52,52	1.64	9 (17%)
2	MPD	B	501	-	7,7,7	0.29	0	10,10,10	0.45	0
3	NO3	B	601	-	3,3,3	3.34	3 (100%)	3,3,3	0.36	0
3	NO3	B	602	-	3,3,3	3.13	3 (100%)	3,3,3	0.13	0
3	NO3	B	604	-	3,3,3	3.09	3 (100%)	3,3,3	0.17	0
5	PO4	B	701	-	4,4,4	0.23	0	6,6,6	0.31	0
4	GA3	C	401	-	29,29,29	1.08	1 (3%)	52,52,52	1.93	13 (25%)
2	MPD	C	501	-	7,7,7	0.33	0	10,10,10	0.46	0
3	NO3	C	602	-	3,3,3	3.25	3 (100%)	3,3,3	0.27	0
3	NO3	C	604	-	3,3,3	3.09	3 (100%)	3,3,3	0.24	0
4	GA3	D	401	-	29,29,29	1.23	2 (6%)	52,52,52	1.69	4 (7%)
2	MPD	D	501	-	7,7,7	0.41	0	10,10,10	0.44	0
3	NO3	D	601	-	3,3,3	3.34	3 (100%)	3,3,3	0.15	0
3	NO3	D	603	-	3,3,3	3.18	3 (100%)	3,3,3	0.18	0
4	GA3	E	401	-	29,29,29	1.26	2 (6%)	52,52,52	1.69	12 (23%)
2	MPD	E	501	-	7,7,7	0.27	0	10,10,10	0.29	0
5	PO4	E	701	-	4,4,4	0.27	0	6,6,6	0.31	0
4	GA3	F	401	-	29,29,29	1.16	1 (3%)	52,52,52	1.59	10 (19%)
2	MPD	F	501	-	7,7,7	0.23	0	10,10,10	0.47	0
3	NO3	F	602	-	3,3,3	3.17	3 (100%)	3,3,3	0.11	0
3	NO3	F	603	-	3,3,3	3.21	3 (100%)	3,3,3	0.11	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
4	GA3	A	401	-	-	0/4/84/84	0/0/5/5
2	MPD	A	501	-	-	0/5/5/5	0/0/0/0
3	NO3	A	601	-	-	0/0/0/0	0/0/0/0
3	NO3	A	602	-	-	0/0/0/0	0/0/0/0
3	NO3	A	603	-	-	0/0/0/0	0/0/0/0
4	GA3	B	401	-	-	0/4/84/84	0/0/5/5
2	MPD	B	501	-	-	0/5/5/5	0/0/0/0
3	NO3	B	601	-	-	0/0/0/0	0/0/0/0
3	NO3	B	602	-	-	0/0/0/0	0/0/0/0
3	NO3	B	604	-	-	0/0/0/0	0/0/0/0
5	PO4	B	701	-	-	0/0/0/0	0/0/0/0
4	GA3	C	401	-	-	0/4/84/84	0/0/5/5
2	MPD	C	501	-	-	0/5/5/5	0/0/0/0
3	NO3	C	602	-	-	0/0/0/0	0/0/0/0
3	NO3	C	604	-	-	0/0/0/0	0/0/0/0
4	GA3	D	401	-	-	0/4/84/84	0/0/5/5
2	MPD	D	501	-	-	0/5/5/5	0/0/0/0
3	NO3	D	601	-	-	0/0/0/0	0/0/0/0
3	NO3	D	603	-	-	0/0/0/0	0/0/0/0
4	GA3	E	401	-	-	0/4/84/84	0/0/5/5
2	MPD	E	501	-	-	0/5/5/5	0/0/0/0
5	PO4	E	701	-	-	0/0/0/0	0/0/0/0
4	GA3	F	401	-	-	0/4/84/84	0/0/5/5
2	MPD	F	501	-	-	0/5/5/5	0/0/0/0
3	NO3	F	602	-	-	0/0/0/0	0/0/0/0
3	NO3	F	603	-	-	0/0/0/0	0/0/0/0

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	401	GA3	O92-C19	4.63	1.46	1.36
4	E	401	GA3	O92-C19	4.46	1.45	1.36
3	A	602	NO3	O1-N	4.18	1.42	1.24
4	F	401	GA3	O92-C19	4.13	1.44	1.36
3	B	601	NO3	O1-N	4.12	1.41	1.24
3	D	601	NO3	O1-N	4.02	1.41	1.24
3	A	603	NO3	O1-N	3.86	1.40	1.24
3	D	603	NO3	O1-N	3.84	1.40	1.24
3	B	604	NO3	O1-N	3.83	1.40	1.24
3	C	602	NO3	O1-N	3.83	1.40	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	NO3	O1-N	3.81	1.40	1.24
3	F	603	NO3	O1-N	3.81	1.40	1.24
3	F	602	NO3	O1-N	3.80	1.40	1.24
4	D	401	GA3	O92-C19	3.78	1.44	1.36
3	A	601	NO3	O1-N	3.67	1.39	1.24
3	C	604	NO3	O1-N	3.66	1.39	1.24
3	A	601	NO3	O3-N	3.30	1.42	1.25
4	C	401	GA3	O92-C19	3.20	1.43	1.36
3	C	602	NO3	O3-N	3.15	1.42	1.25
3	A	601	NO3	O2-N	3.02	1.41	1.25
4	D	401	GA3	O92-C10	-3.00	1.41	1.49
3	A	603	NO3	O3-N	2.99	1.41	1.25
3	B	601	NO3	O2-N	2.97	1.41	1.25
3	A	602	NO3	O2-N	2.96	1.41	1.25
3	D	601	NO3	O3-N	2.95	1.41	1.25
3	D	601	NO3	O2-N	2.93	1.40	1.25
3	A	603	NO3	O2-N	2.91	1.40	1.25
4	A	401	GA3	O92-C19	2.90	1.42	1.36
3	D	603	NO3	O2-N	2.90	1.40	1.25
3	F	603	NO3	O2-N	2.88	1.40	1.25
3	F	603	NO3	O3-N	2.87	1.40	1.25
3	F	602	NO3	O2-N	2.82	1.40	1.25
4	B	401	GA3	C3-C2	2.82	1.55	1.49
3	B	602	NO3	O2-N	2.81	1.40	1.25
3	C	604	NO3	O2-N	2.81	1.40	1.25
3	F	602	NO3	O3-N	2.78	1.40	1.25
3	B	601	NO3	O3-N	2.78	1.40	1.25
3	A	602	NO3	O3-N	2.77	1.40	1.25
3	C	604	NO3	O3-N	2.72	1.39	1.25
4	B	401	GA3	O92-C10	-2.71	1.42	1.49
3	D	603	NO3	O3-N	2.68	1.39	1.25
3	C	602	NO3	O2-N	2.68	1.39	1.25
4	E	401	GA3	O92-C10	-2.67	1.42	1.49
3	B	602	NO3	O3-N	2.66	1.39	1.25
3	B	604	NO3	O3-N	2.65	1.39	1.25
3	B	604	NO3	O2-N	2.63	1.39	1.25

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	401	GA3	C15-C16-C13	7.15	113.72	107.55
4	D	401	GA3	C14-C13-C16	-6.98	98.30	102.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	401	GA3	C14-C13-C16	-6.87	98.36	102.08
4	D	401	GA3	C15-C16-C13	6.25	112.95	107.55
4	B	401	GA3	C15-C16-C13	6.16	112.87	107.55
4	A	401	GA3	C15-C16-C13	5.97	112.70	107.55
4	F	401	GA3	C15-C16-C13	5.69	112.47	107.55
4	A	401	GA3	C14-C13-C16	-5.51	99.09	102.08
4	E	401	GA3	C15-C16-C13	5.46	112.27	107.55
4	E	401	GA3	C14-C8-C15	4.50	105.22	100.81
4	A	401	GA3	O13-C13-C16	-4.13	106.40	113.26
4	B	401	GA3	C14-C13-C16	-4.06	99.88	102.08
4	F	401	GA3	C14-C13-C16	-4.04	99.89	102.08
4	E	401	GA3	C8-C6-C7	3.73	117.46	111.77
4	B	401	GA3	C8-C15-C16	-3.03	98.18	103.90
4	F	401	GA3	C8-C15-C16	-3.03	98.18	103.90
4	E	401	GA3	C18-C4-C3	2.96	114.55	109.11
4	C	401	GA3	C8-C15-C16	-2.94	98.35	103.90
4	C	401	GA3	C8-C6-C7	2.91	116.22	111.77
4	F	401	GA3	C15-C16-C17	-2.90	122.87	126.72
4	C	401	GA3	C15-C16-C17	-2.83	122.96	126.72
4	D	401	GA3	C15-C16-C17	-2.78	123.02	126.72
4	A	401	GA3	C18-C4-C3	2.69	114.05	109.11
4	B	401	GA3	C14-C8-C15	2.58	103.34	100.81
4	C	401	GA3	O92-C10-C9	2.57	113.96	110.38
4	C	401	GA3	O72-C7-C6	-2.55	116.76	123.28
4	E	401	GA3	C15-C8-C9	-2.54	105.51	110.03
4	A	401	GA3	C8-C15-C16	-2.52	99.15	103.90
4	B	401	GA3	C18-C4-C3	2.51	113.72	109.11
4	F	401	GA3	C8-C6-C7	2.44	115.50	111.77
4	A	401	GA3	O72-C7-C6	-2.41	117.11	123.28
4	C	401	GA3	C4-C5-C6	2.40	121.30	117.13
4	F	401	GA3	C18-C4-C3	2.39	113.50	109.11
4	A	401	GA3	C12-C13-C16	2.38	114.93	110.90
4	F	401	GA3	C10-O92-C19	-2.37	105.06	108.46
4	E	401	GA3	C11-C9-C8	-2.37	110.11	112.93
4	A	401	GA3	C8-C6-C7	2.34	115.34	111.77
4	E	401	GA3	C15-C16-C17	-2.33	123.62	126.72
4	F	401	GA3	C12-C13-C14	2.32	112.15	109.00
4	A	401	GA3	C4-C5-C6	2.31	121.15	117.13
4	C	401	GA3	C11-C12-C13	-2.30	109.13	112.38
4	F	401	GA3	O71-C7-C6	2.30	121.57	113.94
4	E	401	GA3	O71-C7-C6	2.29	121.56	113.94
4	B	401	GA3	O31-C3-C2	-2.29	104.54	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	401	GA3	O13-C13-C12	2.28	112.64	107.86
4	D	401	GA3	C8-C15-C16	-2.27	99.61	103.90
4	B	401	GA3	C15-C16-C17	-2.26	123.72	126.72
4	A	401	GA3	O71-C7-C6	2.25	121.40	113.94
4	A	401	GA3	C13-C16-C17	-2.23	122.81	125.17
4	E	401	GA3	O31-C3-C2	-2.23	104.67	109.75
4	C	401	GA3	C12-C13-C14	2.21	112.00	109.00
4	C	401	GA3	O31-C3-C2	-2.19	104.76	109.75
4	B	401	GA3	C15-C8-C9	-2.16	106.18	110.03
4	F	401	GA3	C11-C12-C13	-2.15	109.33	112.38
4	C	401	GA3	C14-C8-C15	2.13	102.89	100.81
4	E	401	GA3	C11-C12-C13	-2.07	109.45	112.38
4	A	401	GA3	C11-C12-C13	-2.07	109.45	112.38
4	B	401	GA3	C12-C13-C16	2.05	114.37	110.90
4	E	401	GA3	C4-C5-C6	2.04	120.68	117.13
4	E	401	GA3	C8-C15-C16	-2.01	100.12	103.90
4	C	401	GA3	O71-C7-C6	2.00	120.59	113.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	321/365 (87%)	-0.20	6 (1%) 64 65	15, 24, 42, 54	0
1	B	316/365 (86%)	0.01	13 (4%) 35 36	16, 28, 49, 66	0
1	C	301/365 (82%)	-0.04	5 (1%) 67 69	18, 31, 48, 57	0
1	D	315/365 (86%)	-0.02	7 (2%) 59 60	16, 28, 48, 56	0
1	E	313/365 (85%)	0.41	21 (6%) 17 17	22, 39, 56, 68	0
1	F	305/365 (83%)	-0.17	6 (1%) 62 63	19, 31, 50, 58	0
All	All	1871/2190 (85%)	-0.00	58 (3%) 47 48	15, 30, 51, 68	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	107	ALA	5.8
1	E	110	ALA	5.1
1	B	14	THR	5.0
1	E	109	ALA	4.2
1	E	181	PHE	3.9
1	F	73	SER	3.8
1	B	107	ALA	3.7
1	B	180	PRO	3.7
1	B	105	THR	3.7
1	D	15	VAL	3.5
1	C	113	PHE	3.5
1	E	313	GLY	3.5
1	D	74	VAL	3.4
1	E	74	VAL	3.4
1	A	186	GLY	3.4
1	D	275	PRO	3.4
1	A	105	THR	3.3
1	F	74	VAL	3.3
1	B	84	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	282	GLY	3.2
1	D	274	GLY	3.2
1	B	110	ALA	3.0
1	B	104	LEU	3.0
1	A	15	VAL	3.0
1	E	285	PHE	2.9
1	E	352	LEU	2.8
1	D	280	LEU	2.8
1	E	113	PHE	2.8
1	C	190	ALA	2.7
1	C	181	PHE	2.7
1	F	15	VAL	2.7
1	B	112	PRO	2.7
1	F	66	PHE	2.7
1	B	183	ARG	2.6
1	B	108	PRO	2.6
1	D	282	GLY	2.6
1	E	108	PRO	2.5
1	B	106	ASP	2.5
1	E	240	LEU	2.5
1	E	283	LEU	2.5
1	E	280	LEU	2.5
1	F	352	LEU	2.5
1	E	75	GLY	2.4
1	A	187	ASP	2.4
1	A	84	ALA	2.4
1	E	111	GLU	2.3
1	E	72	GLN	2.3
1	E	189	GLN	2.3
1	B	15	VAL	2.3
1	A	353	TYR	2.2
1	D	72	GLN	2.2
1	E	15	VAL	2.2
1	C	282	GLY	2.2
1	E	112	PRO	2.2
1	B	109	ALA	2.2
1	C	180	PRO	2.2
1	F	180	PRO	2.1
1	E	277	GLY	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NO3	C	602	4/4	0.25	12.92	42,43,43,43	0
3	NO3	B	604	4/4	0.20	9.96	50,51,51,51	0
3	NO3	F	602	4/4	0.29	9.06	51,51,51,53	0
5	PO4	B	701	5/5	0.18	6.15	89,89,89,90	0
3	NO3	A	602	4/4	0.18	5.42	42,43,44,45	0
5	PO4	E	701	5/5	0.20	4.44	97,98,98,98	0
3	NO3	A	601	4/4	0.18	3.72	45,45,46,46	0
3	NO3	B	601	4/4	0.18	3.57	49,50,50,51	0
3	NO3	B	602	4/4	0.20	3.05	45,46,46,46	0
2	MPD	A	501	8/8	0.11	3.01	28,31,37,37	0
2	MPD	B	501	8/8	0.12	2.65	33,36,36,37	0
2	MPD	D	501	8/8	0.16	2.09	34,38,38,40	0
2	MPD	E	501	8/8	0.10	1.91	38,41,42,43	0
3	NO3	D	601	4/4	0.13	1.35	61,61,61,61	0
3	NO3	A	603	4/4	0.12	0.67	61,61,62,62	0
2	MPD	F	501	8/8	0.10	0.43	32,34,35,35	0
3	NO3	D	603	4/4	0.12	0.30	51,51,51,52	0
2	MPD	C	501	8/8	0.11	0.01	31,33,35,35	0
3	NO3	F	603	4/4	0.10	-0.07	62,62,62,62	0
4	GA3	B	401	25/25	0.09	-0.21	15,17,21,21	0
4	GA3	D	401	25/25	0.09	-0.39	19,21,23,26	0
4	GA3	A	401	25/25	0.07	-0.45	15,17,20,20	0
4	GA3	C	401	25/25	0.07	-0.94	16,19,22,23	0
4	GA3	E	401	25/25	0.09	-0.96	24,28,30,32	0
3	NO3	C	604	4/4	0.09	-1.18	44,45,45,46	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GA3	F	401	25/25	0.07	-1.28	20,23,26,27	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.