



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:35 AM GMT

PDB ID : 2RBE  
Title : The discovery of 2-anilinothiazolones as 11beta-HSD1 inhibitors  
Authors : Zhang, J.; Jordan, S.R.; Li, V.  
Deposited on : 2007-09-18  
Resolution : 1.90 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](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

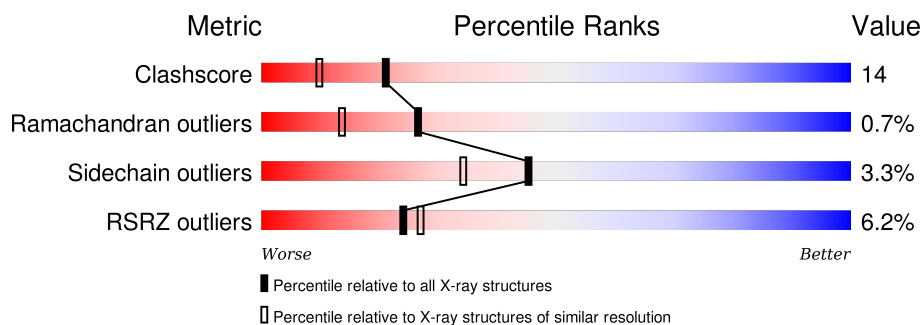
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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. 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	275	
1	B	275	
1	C	275	
1	D	275	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8618 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 Corticosteroid 11-beta-dehydrogenase isozyme 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	0	0
			1988	1270	335	368	15			
1	B	255	Total	C	N	O	S	0	0	0
			1951	1247	331	358	15			
1	C	255	Total	C	N	O	S	0	0	0
			1954	1249	331	359	15			
1	D	261	Total	C	N	O	S	0	0	0
			2002	1277	338	372	15			

There are 32 discrepancies between the modelled and reference sequences:

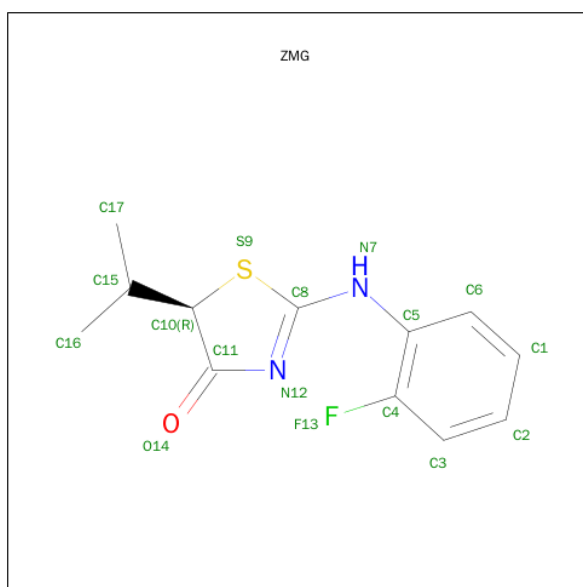
Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MET	-	EXPRESSION TAG	UNP P28845
A	19	HIS	-	EXPRESSION TAG	UNP P28845
A	20	HIS	-	EXPRESSION TAG	UNP P28845
A	21	HIS	-	EXPRESSION TAG	UNP P28845
A	22	HIS	-	EXPRESSION TAG	UNP P28845
A	23	HIS	-	EXPRESSION TAG	UNP P28845
A	24	HIS	-	EXPRESSION TAG	UNP P28845
A	272	SER	CYS	ENGINEERED	UNP P28845
B	18	MET	-	EXPRESSION TAG	UNP P28845
B	19	HIS	-	EXPRESSION TAG	UNP P28845
B	20	HIS	-	EXPRESSION TAG	UNP P28845
B	21	HIS	-	EXPRESSION TAG	UNP P28845
B	22	HIS	-	EXPRESSION TAG	UNP P28845
B	23	HIS	-	EXPRESSION TAG	UNP P28845
B	24	HIS	-	EXPRESSION TAG	UNP P28845
B	272	SER	CYS	ENGINEERED	UNP P28845
C	18	MET	-	EXPRESSION TAG	UNP P28845
C	19	HIS	-	EXPRESSION TAG	UNP P28845
C	20	HIS	-	EXPRESSION TAG	UNP P28845
C	21	HIS	-	EXPRESSION TAG	UNP P28845
C	22	HIS	-	EXPRESSION TAG	UNP P28845

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Chain	Residue	Modelled	Actual	Comment	Reference
C	23	HIS	-	EXPRESSION TAG	UNP P28845
C	24	HIS	-	EXPRESSION TAG	UNP P28845
C	272	SER	CYS	ENGINEERED	UNP P28845
D	18	MET	-	EXPRESSION TAG	UNP P28845
D	19	HIS	-	EXPRESSION TAG	UNP P28845
D	20	HIS	-	EXPRESSION TAG	UNP P28845
D	21	HIS	-	EXPRESSION TAG	UNP P28845
D	22	HIS	-	EXPRESSION TAG	UNP P28845
D	23	HIS	-	EXPRESSION TAG	UNP P28845
D	24	HIS	-	EXPRESSION TAG	UNP P28845
D	272	SER	CYS	ENGINEERED	UNP P28845

- Molecule 2 is (5R)-2-[(2-FLUOROPHENYL)AMINO]-5-(1-METHYLETHYL)-1,3-THIAZO L-4(5H)-ONE (three-letter code: ZMG) (formula: C<sub>12</sub>H<sub>13</sub>FN<sub>2</sub>OS).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 17	C 12	F 1	N 2	O 1	S 1	0	0
2	B	1	Total 17	C 12	F 1	N 2	O 1	S 1	0	0
2	C	1	Total 17	C 12	F 1	N 2	O 1	S 1	0	0
2	D	1	Total 17	C 12	F 1	N 2	O 1	S 1	0	0

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			47	21	6	17	3		
3	B	1	Total	C	N	O	P	0	0
			47	21	6	17	3		
3	C	1	Total	C	N	O	P	0	0
			47	21	6	17	3		
3	D	1	Total	C	N	O	P	0	0
			47	21	6	17	3		

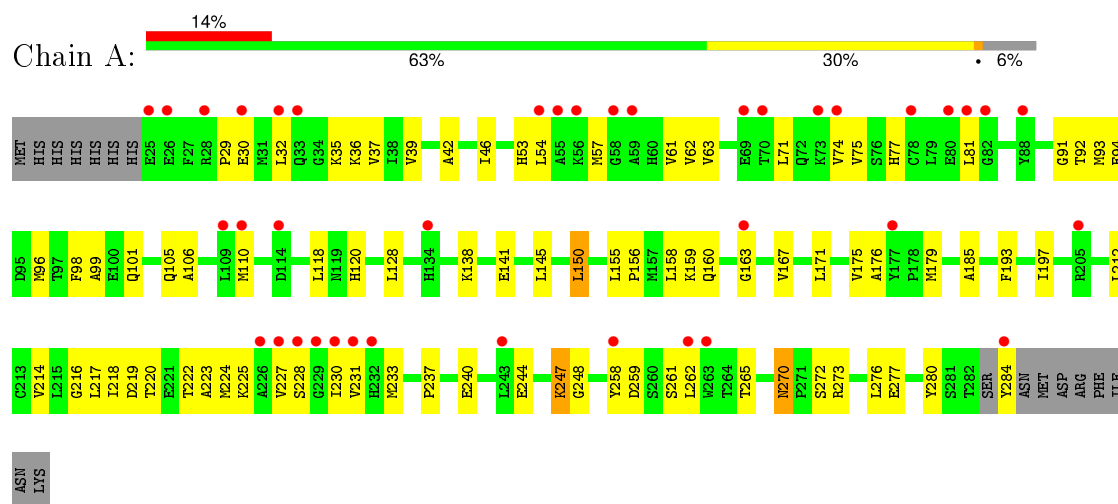
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	82	Total	O	0	0
			82	82		
4	B	114	Total	O	0	0
			114	114		
4	C	143	Total	O	0	0
			143	143		
4	D	128	Total	O	0	0
			128	128		

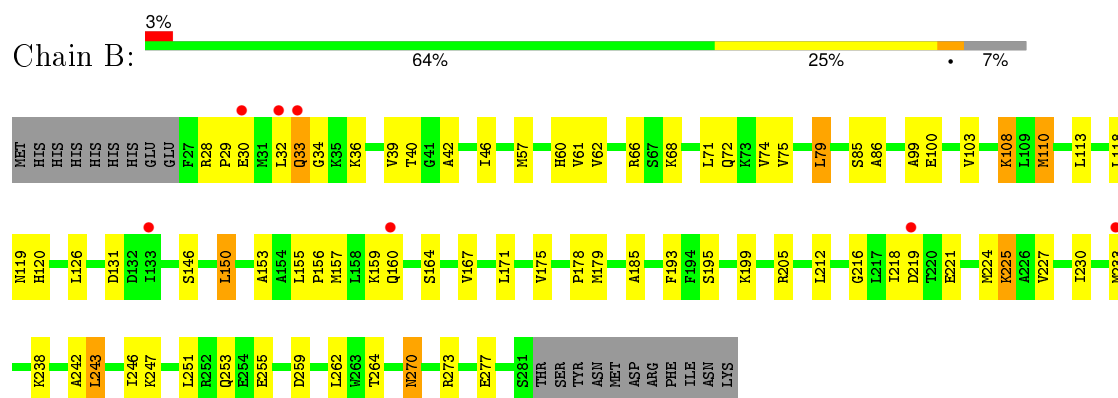
### 3 Residue-property plots

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.

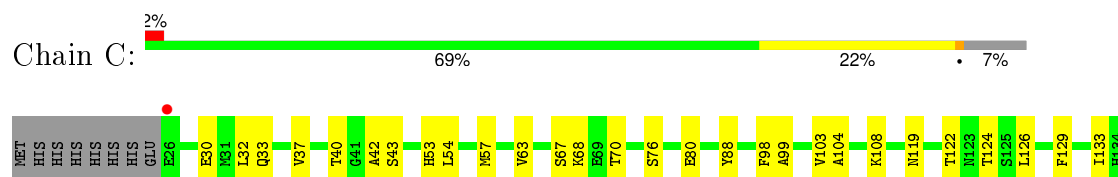
- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1

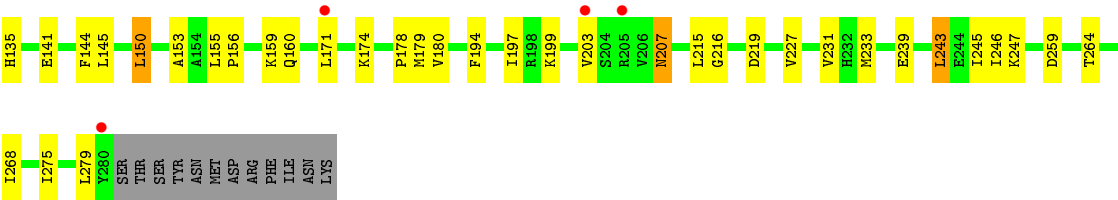


- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1

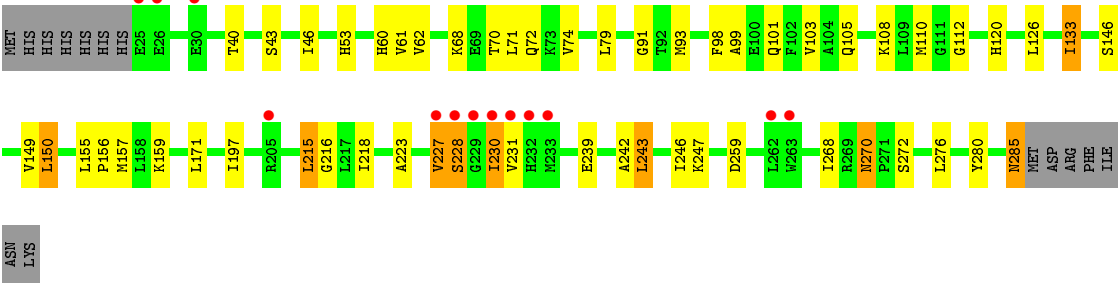


- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1





● Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1



ASN  
LYS

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.91Å 138.66Å 155.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 46.12 – 1.90	Depositor EDS
% Data completeness (in resolution range)	91.3 (50.00-1.90) 91.4 (46.12-1.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 1.90Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.219 , 0.264 0.223 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	23.1	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 46.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 77180 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8618	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% 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: NDP, ZMG

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	0.28	0/2021	0.52	0/2727
1	B	0.31	0/1984	0.56	0/2678
1	C	0.32	0/1987	0.57	0/2682
1	D	0.31	0/2036	0.58	0/2749
All	All	0.31	0/8028	0.56	0/10836

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	1988	0	2034	74	0
1	B	1951	0	2007	67	0
1	C	1954	0	2008	54	0
1	D	2002	0	2046	51	0
2	A	17	0	13	0	0
2	B	17	0	13	0	0
2	C	17	0	13	0	0
2	D	17	0	13	0	0
3	A	47	0	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	47	0	25	2	0
3	C	47	0	25	2	0
3	D	47	0	25	2	0
4	A	82	0	0	1	0
4	B	114	0	0	4	0
4	C	143	0	0	0	0
4	D	128	0	0	0	0
All	All	8618	0	8247	234	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 14.

All (234) 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:B:46:ILE:HD11	1:B:218:ILE:HG21	1.39	1.02
3:D:504:NDP:C6A	3:D:504:NDP:C2A	2.37	1.01
3:C:503:NDP:C6A	3:C:503:NDP:C2A	2.37	1.00
3:A:501:NDP:C6A	3:A:501:NDP:C2A	2.37	1.00
3:B:502:NDP:C6A	3:B:502:NDP:C2A	2.38	0.99
1:D:46:ILE:HD11	1:D:218:ILE:HG21	1.50	0.93
1:C:227:VAL:HG13	1:C:231:VAL:HB	1.46	0.93
1:A:46:ILE:HD11	1:A:218:ILE:HG21	1.60	0.83
1:C:67:SER:HB2	1:C:70:THR:HG22	1.61	0.82
1:D:62:VAL:HG23	1:D:110:MET:HE3	1.61	0.82
1:B:103:VAL:HG21	1:B:153:ALA:CB	2.10	0.82
1:A:227:VAL:HG13	1:A:231:VAL:HB	1.63	0.81
1:B:167:VAL:HG23	1:B:212:LEU:HA	1.65	0.77
1:A:247:LYS:HD3	1:A:248:GLY:N	1.99	0.76
1:C:227:VAL:CG1	1:C:231:VAL:HB	2.17	0.74
1:B:103:VAL:HG21	1:B:153:ALA:HB1	1.67	0.74
1:C:104:ALA:O	1:C:108:LYS:HG2	1.87	0.74
1:C:99:ALA:HB1	1:C:150:LEU:HD13	1.71	0.72
1:B:62:VAL:HG23	1:B:110:MET:HE3	1.72	0.71
1:C:67:SER:HB2	1:C:70:THR:CG2	2.21	0.69
1:B:60:HIS:HB3	1:B:110:MET:HE2	1.76	0.68
1:D:60:HIS:HB3	1:D:110:MET:HE2	1.74	0.67
1:D:61:VAL:CA	1:D:110:MET:HE1	2.25	0.67
1:D:133:ILE:HD13	1:D:133:ILE:O	1.95	0.67
1:A:96:MET:SD	1:A:145:LEU:HD22	2.36	0.66
1:B:243:LEU:HD22	1:B:247:LYS:HD2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:LEU:HD22	1:C:57:MET:SD	2.37	0.65
1:B:60:HIS:ND1	1:B:85:SER:HB3	2.12	0.65
1:C:43:SER:HB2	1:C:70:THR:CG2	2.26	0.64
1:A:225:LYS:HB3	1:A:225:LYS:NZ	2.12	0.64
1:A:167:VAL:HG23	1:A:212:LEU:HD12	1.78	0.64
1:A:37:VAL:HG11	1:A:54:LEU:HD13	1.80	0.64
1:B:103:VAL:HG21	1:B:153:ALA:HB3	1.81	0.63
1:B:156:PRO:O	1:B:160:GLN:HG3	1.99	0.62
1:D:227:VAL:HG12	1:D:228:SER:N	2.14	0.62
1:A:36:LYS:HB3	1:A:110:MET:SD	2.39	0.62
1:A:118:LEU:HD22	1:A:150:LEU:HD23	1.81	0.62
1:B:155:LEU:HG	1:B:159:LYS:HE3	1.80	0.62
1:B:171:LEU:HG	1:B:216:GLY:HA2	1.82	0.62
1:B:30:GLU:HG3	1:B:33:GLN:NE2	2.14	0.62
1:A:167:VAL:HG23	1:A:212:LEU:HA	1.82	0.62
1:C:133:ILE:HD13	1:D:149:VAL:HG22	1.81	0.62
1:A:155:LEU:HG	1:A:159:LYS:HE3	1.82	0.61
1:C:32:LEU:HD23	1:C:54:LEU:HD23	1.82	0.61
1:A:273:ARG:HG3	1:B:175:VAL:HG22	1.83	0.60
1:B:61:VAL:CA	1:B:110:MET:HE1	2.30	0.60
1:B:216:GLY:HA3	1:B:259:ASP:OD1	2.02	0.60
1:C:67:SER:CB	1:C:70:THR:HG22	2.31	0.59
1:B:103:VAL:CG2	1:B:153:ALA:HB1	2.33	0.59
1:C:37:VAL:HG11	1:C:54:LEU:HD13	1.84	0.58
1:A:32:LEU:HD23	1:A:35:LYS:HG3	1.86	0.58
1:B:167:VAL:CG2	1:B:212:LEU:HA	2.34	0.58
1:A:101:GLN:O	1:A:105:GLN:HG3	2.04	0.57
1:A:217:LEU:HD11	1:A:227:VAL:HG21	1.86	0.57
1:A:219:ASP:OD2	1:A:237:PRO:HA	2.04	0.57
1:A:175:VAL:HG22	1:B:273:ARG:HG3	1.87	0.57
1:C:43:SER:HB2	1:C:70:THR:HG21	1.85	0.57
1:D:243:LEU:HD22	1:D:247:LYS:HE3	1.86	0.57
1:A:220:THR:HG22	1:A:222:THR:H	1.68	0.57
1:B:255:GLU:HG2	4:B:706:HOH:O	2.04	0.57
1:C:126:LEU:HD13	1:C:180:VAL:HG13	1.85	0.57
1:C:122:THR:O	1:C:124:THR:HG23	2.04	0.56
1:C:216:GLY:HA3	1:C:259:ASP:OD1	2.05	0.56
1:D:126:LEU:HD23	1:D:230:ILE:HG21	1.87	0.56
1:B:62:VAL:HG23	1:B:110:MET:CE	2.36	0.56
1:B:68:LYS:HG2	1:B:72:GLN:HE21	1.70	0.56
1:C:32:LEU:HD23	1:C:54:LEU:CD2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:VAL:HG23	1:A:110:MET:HE3	1.89	0.54
1:B:46:ILE:HD13	1:B:238:LYS:HB2	1.88	0.54
1:B:167:VAL:HG23	1:B:212:LEU:HD12	1.90	0.54
1:C:194:PHE:HA	1:C:197:ILE:HG12	1.90	0.54
1:B:40:THR:OG1	1:B:120:HIS:HD2	1.90	0.54
1:C:171:LEU:HD13	1:D:280:TYR:OH	2.08	0.54
1:C:144:PHE:CD2	1:C:145:LEU:HD22	2.43	0.54
1:A:277:GLU:HG2	1:B:175:VAL:HG13	1.90	0.54
1:A:261:SER:O	1:A:265:THR:HG23	2.08	0.53
1:D:112:GLY:HA2	1:D:157:MET:CE	2.38	0.53
1:D:155:LEU:HG	1:D:159:LYS:HE3	1.88	0.53
1:B:79:LEU:HD13	1:B:86:ALA:HB3	1.90	0.53
1:C:155:LEU:HG	1:C:159:LYS:HE3	1.89	0.53
1:D:112:GLY:HA2	1:D:157:MET:HE2	1.90	0.53
1:C:103:VAL:HG21	1:C:153:ALA:CB	2.38	0.53
1:C:243:LEU:HD22	1:C:247:LYS:HD2	1.89	0.53
1:D:68:LYS:O	1:D:72:GLN:HG3	2.09	0.53
1:A:277:GLU:CG	1:B:175:VAL:HG13	2.39	0.53
1:B:71:LEU:HA	1:B:74:VAL:HG22	1.90	0.53
1:A:54:LEU:HA	1:A:57:MET:HE2	1.90	0.52
1:C:76:SER:O	1:C:80:GLU:HG3	2.10	0.52
1:A:231:VAL:HG12	1:A:233:MET:HG2	1.90	0.52
1:B:243:LEU:O	1:B:247:LYS:HG3	2.10	0.52
1:C:126:LEU:HB3	1:C:179:MET:HE1	1.91	0.52
1:A:71:LEU:O	1:A:74:VAL:HG12	2.10	0.52
1:B:71:LEU:O	1:B:74:VAL:HG22	2.10	0.52
1:A:230:ILE:N	1:A:230:ILE:HD12	2.24	0.51
1:C:42:ALA:HB3	1:C:63:VAL:HB	1.91	0.51
1:A:225:LYS:HZ3	1:A:225:LYS:HB3	1.74	0.51
1:B:29:PRO:HA	1:B:57:MET:HE3	1.92	0.51
1:D:171:LEU:HD13	1:D:268:ILE:HD13	1.92	0.51
1:D:61:VAL:N	1:D:110:MET:HE1	2.25	0.51
1:A:71:LEU:O	1:A:75:VAL:HG23	2.11	0.51
1:A:193:PHE:HB2	1:B:185:ALA:HB2	1.93	0.51
1:C:231:VAL:HG12	1:C:233:MET:HG2	1.93	0.51
1:D:276:LEU:HG	1:D:280:TYR:CE2	2.45	0.51
1:D:40:THR:OG1	1:D:120:HIS:HD2	1.93	0.51
1:A:145:LEU:O	1:A:145:LEU:HD23	2.12	0.50
1:D:93:MET:HG3	1:D:120:HIS:CE1	2.46	0.50
1:C:53:HIS:HE1	1:C:239:GLU:O	1.93	0.50
1:A:92:THR:OG1	1:A:94:GLU:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:ALA:HB1	1:B:150:LEU:HD13	1.93	0.50
1:A:29:PRO:HG2	1:A:30:GLU:OE2	2.10	0.50
1:C:43:SER:HB2	1:C:70:THR:HG23	1.92	0.50
1:C:30:GLU:O	1:C:33:GLN:HG2	2.12	0.50
1:A:128:LEU:HD23	1:A:179:MET:SD	2.52	0.50
1:D:60:HIS:C	1:D:110:MET:HE1	2.31	0.50
1:D:61:VAL:HA	1:D:110:MET:HE1	1.93	0.50
1:D:71:LEU:HA	1:D:74:VAL:HG12	1.94	0.50
1:C:178:PRO:O	1:C:179:MET:HB2	2.11	0.49
1:C:103:VAL:CG2	1:C:153:ALA:HB1	2.41	0.49
1:C:199:LYS:O	1:C:203:VAL:HG23	2.11	0.49
1:B:61:VAL:HA	1:B:110:MET:HE1	1.94	0.49
1:B:66:ARG:HD2	1:D:105:GLN:HE22	1.77	0.49
1:B:100:GLU:O	1:B:103:VAL:HG22	2.12	0.49
1:C:155:LEU:HB3	1:C:156:PRO:HD3	1.95	0.49
1:D:216:GLY:HA3	1:D:259:ASP:OD1	2.11	0.49
1:B:118:LEU:HD22	1:B:150:LEU:HD23	1.95	0.49
1:D:91:GLY:HA3	1:D:98:PHE:CZ	2.48	0.49
1:B:251:LEU:HD12	1:B:253:GLN:HE21	1.78	0.48
1:A:284:TYR:HA	1:B:230:ILE:O	2.13	0.48
1:C:264:THR:HG23	1:D:280:TYR:OH	2.14	0.48
1:A:216:GLY:HA3	1:A:259:ASP:OD1	2.14	0.48
1:C:275:ILE:O	1:C:279:LEU:HD13	2.13	0.48
1:A:171:LEU:HD23	1:A:214:VAL:HG12	1.95	0.48
1:D:99:ALA:HB1	1:D:150:LEU:HD13	1.95	0.48
1:A:185:ALA:HB2	1:B:193:PHE:HB2	1.95	0.48
1:A:118:LEU:CD2	1:A:150:LEU:HD23	2.42	0.47
1:A:276:LEU:HD11	1:A:280:TYR:CZ	2.49	0.47
1:C:171:LEU:HD22	1:C:268:ILE:HD13	1.94	0.47
1:D:71:LEU:O	1:D:74:VAL:HG12	2.13	0.47
1:D:60:HIS:C	1:D:110:MET:CE	2.82	0.47
1:A:93:MET:HG3	1:A:120:HIS:CE1	2.49	0.47
1:A:62:VAL:HG23	1:A:110:MET:CE	2.43	0.47
1:B:195:SER:O	1:B:199:LYS:HG2	2.14	0.47
1:D:270:ASN:HD21	1:D:272:SER:HB2	1.80	0.47
1:C:103:VAL:HG21	1:C:153:ALA:HB1	1.96	0.47
1:A:77:HIS:O	1:A:81:LEU:HG	2.15	0.47
1:B:270:ASN:C	1:B:270:ASN:HD22	2.18	0.47
1:A:155:LEU:HB3	1:A:156:PRO:HD3	1.97	0.47
1:B:221:GLU:O	1:B:225:LYS:HE2	2.15	0.46
1:B:242:ALA:O	1:B:246:ILE:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:LYS:NZ	1:A:225:LYS:CB	2.77	0.46
1:D:53:HIS:HE1	1:D:239:GLU:O	1.98	0.46
1:D:133:ILE:HD13	1:D:133:ILE:C	2.36	0.46
1:C:32:LEU:HD21	1:C:246:ILE:CG2	2.46	0.46
1:A:53:HIS:O	1:A:57:MET:HG3	2.16	0.46
1:A:99:ALA:HB1	1:A:150:LEU:HD13	1.97	0.46
1:B:108:LYS:HE2	1:B:108:LYS:CA	2.46	0.46
1:D:108:LYS:HB3	1:D:108:LYS:NZ	2.31	0.46
1:D:242:ALA:O	1:D:246:ILE:HG12	2.16	0.46
1:C:124:THR:HG22	1:C:135:HIS:HE1	1.81	0.46
1:C:194:PHE:CD1	1:C:197:ILE:HD11	2.50	0.46
1:C:171:LEU:HG	1:C:216:GLY:HA2	1.97	0.45
1:D:216:GLY:O	3:D:504:NDP:H42N	2.16	0.45
1:D:223:ALA:O	1:D:227:VAL:HG23	2.16	0.45
1:D:103:VAL:CG2	1:D:150:LEU:HD12	2.47	0.45
1:C:129:PHE:HB3	1:D:197:ILE:CD1	2.46	0.45
1:A:193:PHE:O	1:A:197:ILE:HG12	2.16	0.45
4:B:693:HOH:O	1:D:101:GLN:HG3	2.16	0.45
1:A:276:LEU:HG	1:A:280:TYR:CE2	2.52	0.45
1:A:53:HIS:O	1:A:57:MET:HE2	2.16	0.45
1:C:174:LYS:HB2	1:C:268:ILE:HD11	1.97	0.45
1:B:36:LYS:HB2	1:B:113:LEU:HA	1.98	0.45
1:A:42:ALA:HB3	1:A:63:VAL:HB	1.99	0.45
1:D:61:VAL:N	1:D:110:MET:CE	2.80	0.45
1:B:120:HIS:HE1	1:B:146:SER:OG	1.99	0.45
1:D:227:VAL:HG12	1:D:228:SER:H	1.81	0.44
1:A:220:THR:HG22	1:A:222:THR:N	2.30	0.44
1:A:91:GLY:HA3	1:A:98:PHE:CZ	2.52	0.44
1:A:106:ALA:O	1:A:110:MET:HG2	2.17	0.44
1:D:71:LEU:O	1:D:74:VAL:CG1	2.65	0.44
1:B:29:PRO:HA	1:B:57:MET:CE	2.48	0.44
1:A:240:GLU:HB3	1:A:258:TYR:OH	2.17	0.44
1:A:94:GLU:OE1	1:A:138:LYS:NZ	2.50	0.44
1:A:223:ALA:O	1:A:227:VAL:HG23	2.17	0.44
1:B:178:PRO:O	1:B:179:MET:HB2	2.18	0.44
1:A:158:LEU:HD22	1:A:163:GLY:HA3	1.99	0.44
1:B:39:VAL:HG12	1:B:42:ALA:HB2	2.00	0.44
1:A:216:GLY:O	3:A:501:NDP:H42N	2.18	0.43
1:B:74:VAL:HG23	1:B:75:VAL:N	2.32	0.43
1:B:164:SER:HB3	4:B:683:HOH:O	2.18	0.43
1:A:54:LEU:HD23	1:A:57:MET:HE3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:VAL:HG13	1:A:61:VAL:HG12	2.00	0.43
1:D:126:LEU:HD21	1:D:231:VAL:HG23	2.00	0.43
1:D:91:GLY:HA3	1:D:98:PHE:CE2	2.54	0.43
1:C:68:LYS:HG3	1:C:88:TYR:HE2	1.83	0.43
1:A:244:GLU:HA	1:A:247:LYS:HG3	2.01	0.43
1:A:175:VAL:CG1	1:A:176:ALA:N	2.82	0.43
1:D:103:VAL:HG23	1:D:150:LEU:HD12	2.01	0.43
1:D:155:LEU:HB3	1:D:156:PRO:HD3	1.99	0.43
1:A:39:VAL:HG12	1:A:42:ALA:HB2	2.01	0.42
1:D:285:ASN:C	1:D:285:ASN:HD22	2.21	0.42
1:C:40:THR:O	1:C:119:ASN:HB3	2.19	0.42
1:D:227:VAL:HG13	1:D:231:VAL:HB	2.01	0.42
1:A:175:VAL:HG13	1:B:277:GLU:CG	2.49	0.42
1:B:119:ASN:OD1	3:B:502:NDP:H4D	2.19	0.42
1:C:227:VAL:O	1:C:227:VAL:CG1	2.67	0.42
1:C:144:PHE:HD2	1:C:145:LEU:HD22	1.82	0.42
1:B:262:LEU:HD12	1:B:262:LEU:N	2.34	0.42
1:B:36:LYS:HD2	1:B:110:MET:HB2	2.01	0.42
1:D:43:SER:HB2	1:D:70:THR:CG2	2.49	0.42
1:B:108:LYS:HE2	1:B:108:LYS:N	2.34	0.42
1:B:167:VAL:HG23	1:B:167:VAL:O	2.19	0.42
1:B:61:VAL:C	1:B:110:MET:HE1	2.41	0.42
1:A:247:LYS:HD3	1:A:247:LYS:C	2.40	0.41
1:C:207:ASN:HD22	1:C:207:ASN:HA	1.67	0.41
1:A:171:LEU:HG	1:A:216:GLY:HA2	2.02	0.41
1:A:277:GLU:HG2	1:B:175:VAL:CG1	2.50	0.41
1:A:217:LEU:CD1	1:A:227:VAL:HG21	2.48	0.41
1:B:126:LEU:HD11	1:B:227:VAL:HG12	2.02	0.41
1:B:157:MET:HG3	4:B:698:HOH:O	2.19	0.41
1:A:262:LEU:HD12	1:A:262:LEU:N	2.35	0.41
1:A:128:LEU:N	1:A:179:MET:HE3	2.36	0.41
1:A:160:GLN:OE1	1:C:98:PHE:HB2	2.20	0.41
1:A:270:ASN:HD21	1:A:272:SER:HB2	1.85	0.41
1:B:60:HIS:C	1:B:110:MET:HE2	2.41	0.41
1:A:220:THR:HG23	4:A:617:HOH:O	2.20	0.41
1:C:216:GLY:O	3:C:503:NDP:H42N	2.21	0.40
1:D:120:HIS:HE1	1:D:146:SER:OG	2.04	0.40
1:C:37:VAL:CG1	1:C:54:LEU:HD13	2.50	0.40
1:D:171:LEU:HD23	1:D:215:LEU:C	2.42	0.40
1:C:215:LEU:HD21	1:C:245:ILE:HD11	2.04	0.40
1:A:280:TYR:OH	1:B:264:THR:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:LEU:CG	1:B:159:LYS:HE3	2.50	0.40
1:C:156:PRO:O	1:C:160:GLN:HG3	2.21	0.40
1:B:32:LEU:O	1:B:34:GLY:N	2.53	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	256/275 (93%)	237 (93%)	18 (7%)	1 (0%)	39	27
1	B	253/275 (92%)	242 (96%)	9 (4%)	2 (1%)	24	11
1	C	253/275 (92%)	243 (96%)	9 (4%)	1 (0%)	39	27
1	D	259/275 (94%)	247 (95%)	9 (4%)	3 (1%)	16	5
All	All	1021/1100 (93%)	969 (95%)	45 (4%)	7 (1%)	26	14

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	228	SER
1	B	33	GLN
1	B	219	ASP
1	D	227	VAL
1	D	228	SER
1	C	219	ASP
1	D	230	ILE

### 5.3.2 Protein sidechains [i](#)

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	216/232 (93%)	211 (98%)	5 (2%)	58	51
1	B	212/232 (91%)	200 (94%)	12 (6%)	25	13
1	C	212/232 (91%)	208 (98%)	4 (2%)	65	59
1	D	218/232 (94%)	211 (97%)	7 (3%)	46	35
All	All	858/928 (92%)	830 (97%)	28 (3%)	45	34

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	GLU
1	A	150	LEU
1	A	224	MET
1	A	247	LYS
1	A	270	ASN
1	B	28	ARG
1	B	79	LEU
1	B	108	LYS
1	B	110	MET
1	B	131	ASP
1	B	150	LEU
1	B	205	ARG
1	B	224	MET
1	B	225	LYS
1	B	233	MET
1	B	243	LEU
1	B	270	ASN
1	C	141	GLU
1	C	150	LEU
1	C	207	ASN
1	C	243	LEU
1	D	79	LEU
1	D	133	ILE
1	D	150	LEU
1	D	215	LEU
1	D	243	LEU
1	D	270	ASN
1	D	285	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	A	120	HIS
1	A	123	ASN
1	A	162	ASN
1	A	270	ASN
1	B	33	GLN
1	B	53	HIS
1	B	72	GLN
1	B	101	GLN
1	B	105	GLN
1	B	120	HIS
1	B	134	HIS
1	B	207	ASN
1	B	253	GLN
1	B	270	ASN
1	C	33	GLN
1	C	53	HIS
1	C	77	HIS
1	C	123	ASN
1	C	127	ASN
1	C	135	HIS
1	C	162	ASN
1	C	207	ASN
1	C	234	GLN
1	C	253	GLN
1	D	53	HIS
1	D	72	GLN
1	D	105	GLN
1	D	120	HIS
1	D	123	ASN
1	D	127	ASN
1	D	270	ASN
1	D	285	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

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$
3	NDP	A	501	-	39,50,52	2.00	5 (12%)	53,76,80	1.20	5 (9%)
2	ZMG	A	601	-	17,18,18	1.32	1 (5%)	15,25,25	0.93	1 (6%)
3	NDP	B	502	-	39,50,52	2.10	5 (12%)	53,76,80	1.17	5 (9%)
2	ZMG	B	602	-	17,18,18	1.32	2 (11%)	15,25,25	0.97	1 (6%)
3	NDP	C	503	-	39,50,52	2.03	5 (12%)	53,76,80	1.18	6 (11%)
2	ZMG	C	603	-	17,18,18	1.44	2 (11%)	15,25,25	1.19	1 (6%)
3	NDP	D	504	-	39,50,52	2.00	5 (12%)	53,76,80	1.03	4 (7%)
2	ZMG	D	604	-	17,18,18	1.42	3 (17%)	15,25,25	1.10	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDP	A	501	-	-	0/30/77/77	0/4/4/5
2	ZMG	A	601	-	-	0/8/20/20	0/2/2/2
3	NDP	B	502	-	-	0/30/77/77	0/4/4/5
2	ZMG	B	602	-	-	0/8/20/20	0/2/2/2
3	NDP	C	503	-	-	0/30/77/77	0/4/4/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ZMG	C	603	-	-	0/8/20/20	0/2/2/2
3	NDP	D	504	-	-	0/30/77/77	0/4/4/5
2	ZMG	D	604	-	-	0/8/20/20	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	NDP	C6A-C5A	-9.56	1.39	1.51
3	D	504	NDP	C6A-C5A	-9.04	1.39	1.51
3	C	503	NDP	C6A-C5A	-8.88	1.40	1.51
3	A	501	NDP	C6A-C5A	-8.79	1.40	1.51
3	A	501	NDP	C2A-N3A	-4.69	1.36	1.45
3	B	502	NDP	C4N-C5N	-4.49	1.39	1.49
3	B	502	NDP	C2A-N3A	-4.47	1.37	1.45
3	A	501	NDP	C4N-C5N	-4.22	1.40	1.49
3	C	503	NDP	C2A-N3A	-4.02	1.37	1.45
3	D	504	NDP	C4N-C5N	-3.91	1.40	1.49
3	D	504	NDP	C2A-N3A	-3.88	1.38	1.45
3	C	503	NDP	C4N-C5N	-3.72	1.41	1.49
2	C	603	ZMG	C5-N7	-3.54	1.35	1.41
2	A	601	ZMG	C5-N7	-2.84	1.36	1.41
2	B	602	ZMG	C5-N7	-2.72	1.36	1.41
2	D	604	ZMG	C5-N7	-2.25	1.37	1.41
2	C	603	ZMG	C8-N7	-2.16	1.33	1.36
2	B	602	ZMG	C8-N12	2.30	1.34	1.31
2	D	604	ZMG	C8-N12	2.37	1.34	1.31
3	B	502	NDP	C2N-C3N	2.67	1.41	1.34
3	A	501	NDP	C2N-C3N	2.75	1.41	1.34
3	D	504	NDP	C2N-C3N	2.77	1.41	1.34
2	D	604	ZMG	C5-C4	2.83	1.42	1.38
3	A	501	NDP	C6N-C5N	3.18	1.39	1.33
3	D	504	NDP	C6N-C5N	3.52	1.40	1.33
3	B	502	NDP	C6N-C5N	3.58	1.40	1.33
3	C	503	NDP	C2N-C3N	3.76	1.43	1.34
3	C	503	NDP	C6N-C5N	4.19	1.41	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	NDP	C4N-C5N-C6N	-3.23	117.25	122.58
3	B	502	NDP	C4N-C5N-C6N	-3.23	117.26	122.58
3	C	503	NDP	C4N-C5N-C6N	-3.02	117.60	122.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	503	NDP	C6A-C5A-C4A	-2.71	115.22	125.40
3	B	502	NDP	C6A-C5A-C4A	-2.71	115.24	125.40
3	B	502	NDP	O3B-C3B-C4B	-2.69	102.97	111.05
3	A	501	NDP	C6A-C5A-C4A	-2.69	115.33	125.40
3	D	504	NDP	C4N-C5N-C6N	-2.66	118.19	122.58
3	D	504	NDP	C6A-C5A-C4A	-2.55	115.82	125.40
3	C	503	NDP	O3D-C3D-C2D	-2.28	104.42	111.83
3	C	503	NDP	O3B-C3B-C4B	-2.19	104.48	111.05
2	A	601	ZMG	C6-C5-C4	2.09	119.17	117.11
3	D	504	NDP	O4D-C4D-C3D	2.16	109.49	105.15
2	B	602	ZMG	C6-C5-C4	2.18	119.25	117.11
3	A	501	NDP	O4D-C1D-N1N	2.20	112.71	108.07
2	D	604	ZMG	F13-C4-C5	2.46	119.97	117.50
3	B	502	NDP	O2D-C2D-C1D	2.53	118.78	109.94
3	C	503	NDP	O2D-C2D-C3D	2.62	120.35	111.83
3	C	503	NDP	C5N-C4N-C3N	2.74	120.06	112.52
3	D	504	NDP	C5N-C4N-C3N	2.83	120.33	112.52
3	B	502	NDP	C5N-C4N-C3N	3.01	120.80	112.52
3	A	501	NDP	C5N-C4N-C3N	3.08	121.00	112.52
3	A	501	NDP	O2D-C2D-C1D	3.45	122.00	109.94
2	C	603	ZMG	C6-C5-C4	3.58	120.63	117.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	NDP	2	0
3	B	502	NDP	2	0
3	C	503	NDP	2	0
3	D	504	NDP	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	259/275 (94%)	0.96	39 (15%) 3 3	14, 38, 61, 77	0
1	B	255/275 (92%)	0.22	7 (2%) 58 61	15, 27, 44, 53	0
1	C	255/275 (92%)	0.03	5 (1%) 68 71	11, 23, 36, 52	0
1	D	261/275 (94%)	0.28	13 (4%) 32 35	11, 24, 43, 61	0
All	All	1030/1100 (93%)	0.37	64 (6%) 24 27	11, 27, 52, 77	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	232	HIS	13.9
1	A	230	ILE	10.6
1	D	232	HIS	7.7
1	D	231	VAL	6.6
1	A	229	GLY	6.3
1	A	262	LEU	6.1
1	D	228	SER	5.0
1	D	229	GLY	4.7
1	A	227	VAL	4.6
1	D	230	ILE	4.6
1	D	262	LEU	4.5
1	A	25	GLU	3.8
1	A	58	GLY	3.6
1	A	243	LEU	3.6
1	A	33	GLN	3.5
1	A	82	GLY	3.3
1	D	227	VAL	3.2
1	A	32	LEU	3.2
1	A	26	GLU	3.2
1	A	228	SER	3.2
1	A	56	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	28	ARG	3.1
1	A	81	LEU	3.1
1	A	231	VAL	3.1
1	A	70	THR	3.0
1	D	233	MET	3.0
1	A	205	ARG	3.0
1	B	32	LEU	3.0
1	C	26	GLU	3.0
1	A	30	GLU	2.9
1	C	171	LEU	2.9
1	A	163	GLY	2.9
1	D	205	ARG	2.8
1	A	263	TRP	2.8
1	C	280	TYR	2.8
1	A	226	ALA	2.7
1	B	33	GLN	2.6
1	A	74	VAL	2.6
1	A	114	ASP	2.6
1	A	109	LEU	2.6
1	A	54	LEU	2.5
1	D	26	GLU	2.5
1	B	233	MET	2.4
1	A	55	ALA	2.4
1	A	177	TYR	2.4
1	A	258	TYR	2.4
1	A	80	GLU	2.4
1	C	205	ARG	2.4
1	A	284	TYR	2.3
1	A	73	LYS	2.3
1	B	30	GLU	2.3
1	C	203	VAL	2.2
1	B	133	ILE	2.2
1	D	25	GLU	2.2
1	D	263	TRP	2.2
1	A	134	HIS	2.2
1	B	219	ASP	2.1
1	A	110	MET	2.1
1	A	69	GLU	2.1
1	B	160	GLN	2.1
1	D	30	GLU	2.0
1	A	59	ALA	2.0
1	A	88	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	78	CYS	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	ZMG	B	602	17/17	0.96	0.11	-0.03	21,24,30,31	0
3	NDP	D	504	47/48	0.96	0.10	-0.06	14,16,20,23	0
2	ZMG	C	603	17/17	0.97	0.10	-0.31	18,21,24,25	0
3	NDP	B	502	47/48	0.96	0.09	-0.48	17,21,23,28	0
3	NDP	C	503	47/48	0.97	0.08	-0.50	14,19,23,26	0
3	NDP	A	501	47/48	0.93	0.11	-0.54	21,26,32,34	0
2	ZMG	D	604	17/17	0.96	0.10	-0.66	20,25,27,27	0
2	ZMG	A	601	17/17	0.94	0.11	-0.72	27,31,34,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.