



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:38 am GMT

PDB ID : 4DTC  
Title : Crystal Structure of DPP-IV with Compound C5  
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Deposited on : 2012-02-21  
Resolution : 3.00 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

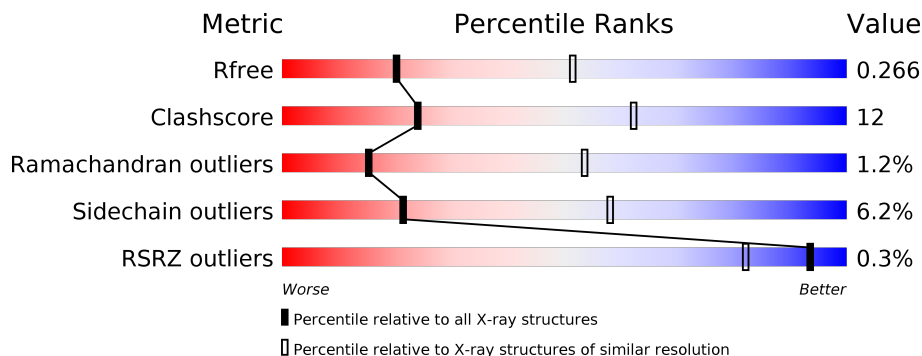
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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	728	
1	B	728	

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	D5C	A	801	-	-	-	X

## 2 Entry composition [i](#)

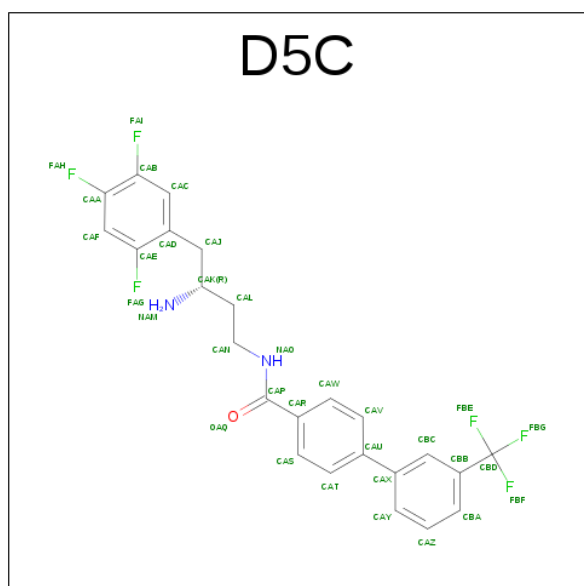
There are 2 unique types of molecules in this entry. The entry contains 11992 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			
1	B	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			

- Molecule 2 is N-[(3R)-3-AMINO-4-(2,4,5-TRIFLUOROPHENYL)BUTYL]-3'-(TRIFLUOROMETHYL)BIPHENYL-4-CARBOXAMIDE (three-letter code: D5C) (formula:  $C_{24}H_{20}F_6N_2O$ ).

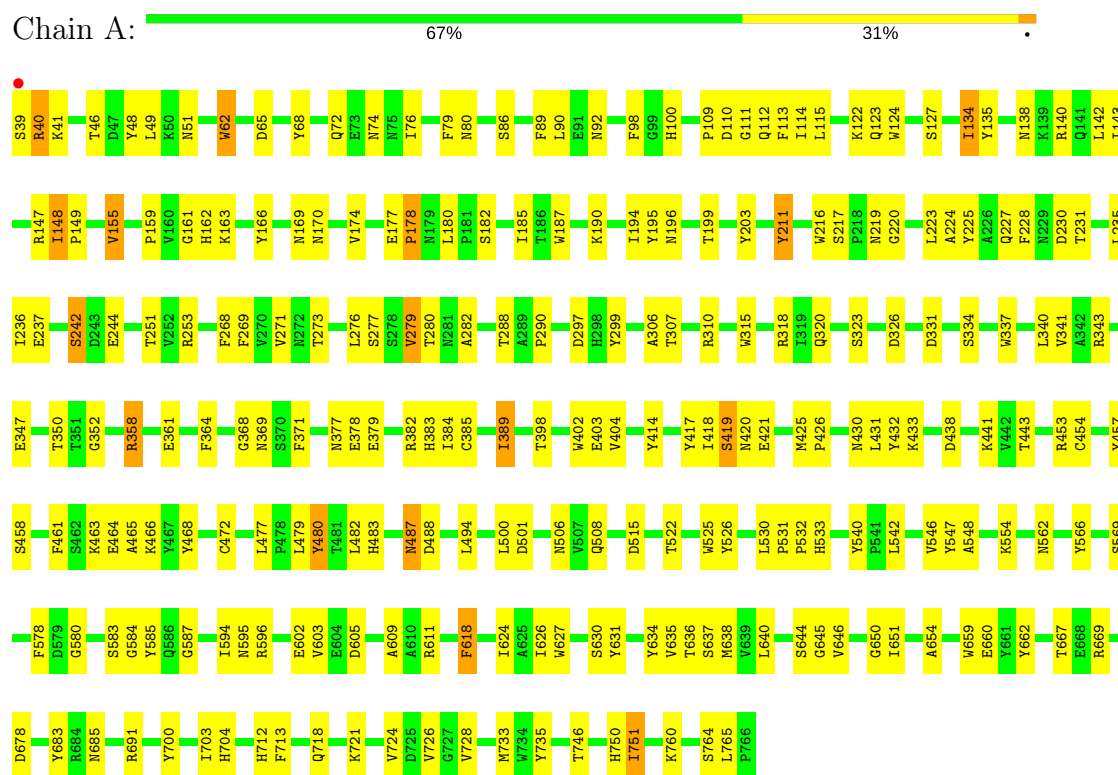


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			33	24	6	2	1		
2	B	1	Total	C	F	N	O	0	0
			33	24	6	2	1		

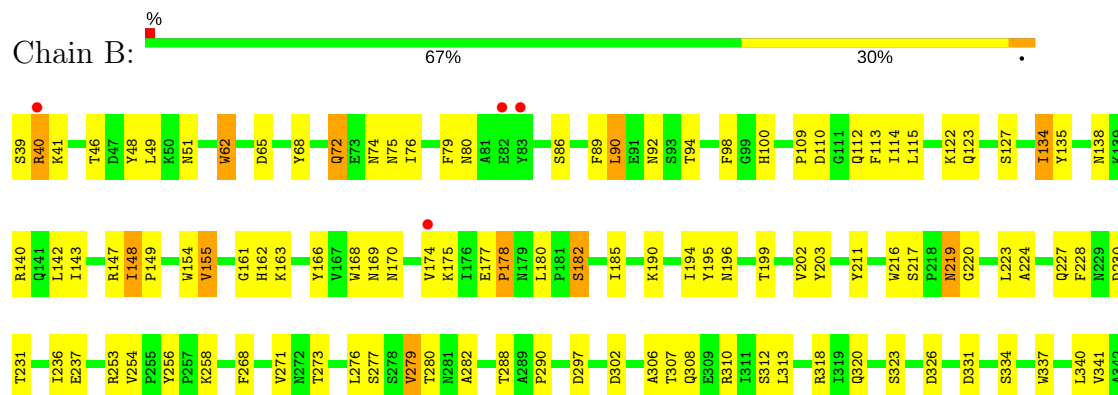
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Dipeptidyl peptidase 4



#### • Molecule 1: Dipeptidyl peptidase 4



R343	M450	G584	E699
E347	P451	Y585	I703
T350	C454	Q586	H704
G352	Y457	G587	H712
W353	S458	I594	K721
R358	V459	N595	V724
E361	K463	R596	D725
F364	E464	A609	V726
S370	K466	E602	G727
F371	L477	V603	V728
E378	Y480	F618	M733
R382	T481	I624	W734
H383	L482	A625	Y735
I384	H483	I626	G741
C385	N487	W627	I742
Y386	D488	Y631	H750
T389	L494	V634	I751
T398	L500	V635	K760
N506	D501	T636	S764
D515	N506	S637	L765
Y526	D515	M638	P766
P532	Y526	V639	
L542	P532	L640	
D545	L542	S644	
V546	D545	G645	
Y547	V546	V646	
A548	Y547	C649	
G549	A548	G650	
S552	G549	A654	
Q553	S552	W659	
K554	Q553	E660	
N562	K554	Y661	
Y566	N562	Y662	
S569	Y566	Y665	
T443	S569	R669	
T442	T443	T675	
G444	D578	D678	
L445	N679	L680	
L449	L680	Y683	
	F578	R684	
	D579	N685	
	G590	R691	
	S583		

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.47Å 80.47Å 290.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.89 – 3.00 29.89 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.89-3.00) 98.4 (29.89-3.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.206 , 0.268 0.202 , 0.266	Depositor DCC
$R_{free}$ test set	2088 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	88.4	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 52.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.001 for -h,-k,l 0.099 for h,-h-k,-l 0.028 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11992	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality (i)

### 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: D5C

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	0.66	7/6135 (0.1%)	0.74	2/8344 (0.0%)
1	B	0.64	6/6135 (0.1%)	0.73	2/8344 (0.0%)
All	All	0.65	13/12270 (0.1%)	0.74	4/16688 (0.0%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	337	TRP	CD2-CE2	5.96	1.48	1.41
1	B	659	TRP	CD2-CE2	5.41	1.47	1.41
1	A	337	TRP	CD2-CE2	5.38	1.47	1.41
1	B	154	TRP	CD2-CE2	5.18	1.47	1.41
1	B	353	TRP	CD2-CE2	5.17	1.47	1.41
1	A	187	TRP	CD2-CE2	5.16	1.47	1.41
1	B	62	TRP	CD2-CE2	5.13	1.47	1.41
1	A	124	TRP	CD2-CE2	5.10	1.47	1.41
1	A	62	TRP	CD2-CE2	5.08	1.47	1.41
1	A	525	TRP	CD2-CE2	5.08	1.47	1.41
1	B	402	TRP	CD2-CE2	5.06	1.47	1.41
1	A	315	TRP	CD2-CE2	5.06	1.47	1.41
1	A	659	TRP	CD2-CE2	5.04	1.47	1.41

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	358	ARG	NE-CZ-NH2	8.11	124.35	120.30
1	B	358	ARG	NE-CZ-NH1	-7.57	116.52	120.30
1	A	358	ARG	NE-CZ-NH1	7.45	124.02	120.30
1	A	358	ARG	NE-CZ-NH2	-7.36	116.62	120.30

There are no chirality outliers.



There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5963	0	5685	149	0
1	B	5963	0	5685	149	0
2	A	33	0	20	4	0
2	B	33	0	20	2	0
All	All	11992	0	11410	292	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 12.

All (292) 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:A:74:ASN:HB2	1:A:92:ASN:HB2	1.55	0.87
1:B:74:ASN:HB2	1:B:92:ASN:HB2	1.56	0.87
1:B:352:GLY:HA2	1:B:595:ASN:ND2	1.95	0.81
1:B:352:GLY:HA2	1:B:595:ASN:HD22	1.45	0.80
1:A:420:ASN:HD22	1:A:426:PRO:HA	1.48	0.78
1:A:595:ASN:OD1	1:A:596:ARG:HG3	1.86	0.76
1:B:420:ASN:HD22	1:B:426:PRO:HA	1.49	0.76
1:A:352:GLY:HA2	1:A:595:ASN:HD22	1.50	0.76
1:B:114:ILE:HG22	1:B:135:TYR:HB3	1.66	0.76
1:B:595:ASN:OD1	1:B:596:ARG:HG3	1.86	0.76
1:A:237:GLU:HG2	1:A:253:ARG:HG2	1.67	0.74
1:A:352:GLY:HA2	1:A:595:ASN:ND2	2.04	0.73
1:A:596:ARG:NH2	1:A:678:ASP:OD1	2.23	0.71
1:B:596:ARG:NH2	1:B:678:ASP:OD1	2.23	0.71
1:B:237:GLU:HG2	1:B:253:ARG:HG2	1.73	0.70
1:A:358:ARG:HH21	2:A:801:D5C:CAZ	2.05	0.69
1:A:174:VAL:HG23	1:A:185:ILE:HD11	1.75	0.69
1:B:216:TRP:HZ3	1:B:273:THR:HG21	1.56	0.69
1:A:110:ASP:OD2	1:A:162:HIS:ND1	2.24	0.69
1:A:216:TRP:HZ3	1:A:273:THR:HG21	1.56	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:ASN:OD1	1:B:227:GLN:HG3	1.94	0.67
1:A:547:TYR:HB2	1:A:554:LYS:HE2	1.75	0.66
1:A:654:ALA:HA	1:A:704:HIS:CE1	2.30	0.66
1:A:114:ILE:HG22	1:A:135:TYR:HB3	1.77	0.66
1:B:546:VAL:HG21	1:B:626:ILE:HD11	1.79	0.65
1:B:134:ILE:HB	1:B:143:ILE:HD12	1.78	0.65
1:A:155:VAL:HG23	1:A:166:TYR:HB3	1.79	0.65
1:A:40:ARG:HB3	1:A:40:ARG:HH11	1.62	0.64
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.80	0.64
1:B:626:ILE:HG23	1:B:636:THR:HG23	1.79	0.64
1:B:276:LEU:HD21	1:B:282:ALA:HB2	1.80	0.64
1:B:547:TYR:HB2	1:B:554:LYS:HE2	1.80	0.64
1:B:123:GLN:HB3	1:B:127:SER:OG	1.99	0.63
1:B:549:GLY:O	1:B:552:SER:HB3	1.99	0.63
1:B:155:VAL:HG23	1:B:166:TYR:HB3	1.79	0.63
1:B:177:GLU:HB2	1:B:180:LEU:HD13	1.80	0.63
1:B:331:ASP:HB3	1:B:334:SER:HB3	1.79	0.63
1:A:134:ILE:HB	1:A:143:ILE:HD12	1.81	0.62
1:B:40:ARG:HH11	1:B:40:ARG:HB3	1.64	0.62
1:A:123:GLN:HB3	1:A:127:SER:OG	2.00	0.62
1:A:196:ASN:OD1	1:A:227:GLN:HG3	1.99	0.62
1:A:626:ILE:HG23	1:A:636:THR:HG23	1.82	0.62
1:B:110:ASP:OD2	1:B:162:HIS:ND1	2.25	0.62
1:A:290:PRO:HD3	1:A:326:ASP:OD2	2.00	0.61
1:B:113:PHE:CZ	1:B:178:PRO:HG2	2.35	0.61
1:B:170:ASN:O	1:B:196:ASN:HB2	2.01	0.60
2:A:801:D5C:OAQ	2:A:801:D5C:H12	2.01	0.60
1:A:79:PHE:HA	1:A:86:SER:CB	2.32	0.60
1:A:79:PHE:HA	1:A:86:SER:HB2	1.83	0.60
1:A:626:ILE:O	1:A:650:GLY:HA2	2.02	0.60
1:A:331:ASP:HB3	1:A:334:SER:HB3	1.82	0.59
1:A:163:LYS:NZ	1:A:220:GLY:O	2.29	0.59
1:A:320:GLN:OE1	1:A:669:ARG:HG3	2.02	0.58
1:B:580:GLY:O	1:B:583:SER:OG	2.18	0.58
1:B:726:VAL:HG12	1:B:726:VAL:O	2.02	0.58
1:A:340:LEU:HB2	1:A:343:ARG:HG2	1.84	0.58
1:A:420:ASN:ND2	1:A:426:PRO:HA	2.18	0.58
1:B:340:LEU:HB2	1:B:343:ARG:HG2	1.85	0.58
1:A:113:PHE:CZ	1:A:178:PRO:HG2	2.39	0.58
1:B:420:ASN:ND2	1:B:426:PRO:HA	2.18	0.58
1:B:202:VAL:HG21	1:B:665:VAL:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:ASN:O	1:B:170:ASN:HB2	2.05	0.57
1:B:358:ARG:HH21	2:B:801:D5C:CAZ	2.16	0.57
1:A:644:SER:O	1:A:646:VAL:N	2.37	0.57
1:A:177:GLU:HB2	1:A:180:LEU:HD13	1.87	0.56
1:A:735:TYR:CE2	1:A:751:ILE:HG13	2.40	0.56
1:B:482:LEU:HB2	1:B:494:LEU:HD11	1.87	0.56
1:B:79:PHE:HA	1:B:86:SER:CB	2.36	0.56
1:A:735:TYR:HE2	1:A:751:ILE:HG13	1.71	0.56
1:B:480:TYR:CD1	1:B:480:TYR:N	2.73	0.56
1:B:76:ILE:O	1:B:89:PHE:HB3	2.05	0.56
1:A:276:LEU:HD21	1:A:282:ALA:HB2	1.87	0.55
1:B:320:GLN:OE1	1:B:669:ARG:HG3	2.07	0.55
1:A:580:GLY:O	1:A:583:SER:OG	2.14	0.55
1:B:760:LYS:HG2	1:B:765:LEU:HB2	1.88	0.54
1:A:169:ASN:O	1:A:170:ASN:HB2	2.07	0.54
1:B:638:MET:O	1:B:691:ARG:NH1	2.40	0.54
1:A:431:LEU:HD12	1:A:432:TYR:H	1.72	0.54
1:A:418:ILE:HA	1:A:430:ASN:O	2.08	0.54
1:A:358:ARG:HH21	2:A:801:D5C:CBA	2.20	0.54
1:A:540:TYR:N	1:A:618:PHE:O	2.35	0.53
1:B:435:GLN:NE2	1:B:441:LYS:HD2	2.24	0.53
1:B:39:SER:HB3	1:B:506:ASN:O	2.08	0.53
1:A:750:HIS:ND1	1:B:724:VAL:HG22	2.24	0.53
1:B:297:ASP:HB3	1:B:318:ARG:HB2	1.91	0.53
1:B:312:SER:O	1:B:313:LEU:HD23	2.08	0.53
1:B:79:PHE:HA	1:B:86:SER:HB2	1.90	0.53
1:B:48:TYR:CE1	1:B:562:ASN:HA	2.45	0.52
1:A:654:ALA:HA	1:A:704:HIS:ND1	2.23	0.52
1:B:542:LEU:HD22	1:B:624:ILE:HG23	1.92	0.52
1:A:724:VAL:HG22	1:B:750:HIS:ND1	2.24	0.52
1:A:704:HIS:HB3	1:A:713:PHE:CD1	2.45	0.52
1:A:76:ILE:O	1:A:89:PHE:HB3	2.10	0.52
1:B:431:LEU:HD12	1:B:432:TYR:N	2.25	0.52
1:B:403:GLU:OE2	1:B:587:GLY:HA2	2.09	0.51
1:A:242:SER:O	1:B:721:LYS:NZ	2.38	0.51
1:B:532:PRO:HD3	1:B:569:SER:HA	1.93	0.51
1:A:323:SER:OG	1:A:347:GLU:HB3	2.11	0.51
1:A:403:GLU:OE2	1:A:587:GLY:HA2	2.10	0.51
1:A:62:TRP:CE3	1:A:68:TYR:HB3	2.45	0.51
1:B:548:ALA:HB3	1:B:635:VAL:HG21	1.91	0.51
1:A:40:ARG:NH1	1:A:40:ARG:HB3	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:LEU:HD12	1:B:432:TYR:H	1.76	0.50
1:B:236:ILE:HG12	1:B:712:HIS:CD2	2.46	0.50
1:B:654:ALA:HA	1:B:704:HIS:CE1	2.46	0.50
1:B:98:PHE:HE2	1:B:100:HIS:HB2	1.77	0.50
1:A:48:TYR:CE1	1:A:562:ASN:HA	2.47	0.50
1:A:482:LEU:HB2	1:A:494:LEU:HD11	1.94	0.50
1:A:143:ILE:HD13	1:A:178:PRO:O	2.12	0.50
1:A:155:VAL:HG23	1:A:166:TYR:CB	2.41	0.50
1:A:159:PRO:HD3	1:A:216:TRP:CG	2.48	0.49
1:A:414:TYR:CZ	1:A:433:LYS:HE2	2.47	0.49
1:A:39:SER:HB3	1:A:506:ASN:O	2.12	0.49
1:A:190:LYS:H	1:A:194:ILE:HB	1.78	0.49
1:B:62:TRP:CE3	1:B:68:TYR:HB3	2.47	0.49
1:A:297:ASP:HB3	1:A:318:ARG:HB2	1.94	0.49
1:A:480:TYR:N	1:A:480:TYR:CD1	2.81	0.49
1:A:637:SER:HG	1:A:700:TYR:HH	1.60	0.49
1:A:631:TYR:O	1:A:634:TYR:HB3	2.13	0.49
1:A:65:ASP:O	1:A:466:LYS:HB2	2.13	0.48
1:B:454:CYS:HB3	1:B:457:TYR:CZ	2.49	0.48
1:A:112:GLN:HG2	1:A:138:ASN:OD1	2.13	0.48
1:A:199:THR:HG22	1:A:203:TYR:HB3	1.95	0.48
1:A:384:ILE:HG13	1:A:404:VAL:HG21	1.94	0.48
1:B:279:VAL:HG13	1:B:279:VAL:O	2.12	0.48
1:B:65:ASP:O	1:B:466:LYS:HB2	2.14	0.48
1:A:170:ASN:O	1:A:196:ASN:HB2	2.13	0.48
1:A:548:ALA:HB3	1:A:635:VAL:HG21	1.96	0.48
1:B:40:ARG:HB3	1:B:40:ARG:NH1	2.26	0.48
1:A:542:LEU:HD22	1:A:624:ILE:HG23	1.96	0.48
1:A:115:LEU:HD21	1:A:155:VAL:CG1	2.44	0.48
1:A:431:LEU:HD12	1:A:432:TYR:N	2.29	0.48
1:A:340:LEU:CB	1:A:343:ARG:HG2	2.44	0.48
1:B:340:LEU:HB2	1:B:343:ARG:CG	2.44	0.47
1:A:340:LEU:HB2	1:A:343:ARG:CG	2.43	0.47
1:A:546:VAL:HG21	1:A:626:ILE:HD11	1.97	0.47
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.96	0.47
1:A:704:HIS:CD2	1:A:713:PHE:HA	2.49	0.47
1:B:109:PRO:HD2	1:B:161:GLY:O	2.14	0.47
1:A:477:LEU:CD1	1:A:501:ASP:HB2	2.44	0.47
1:B:384:ILE:HG13	1:B:404:VAL:HG21	1.95	0.47
1:B:435:GLN:HE22	1:B:441:LYS:HD2	1.79	0.47
1:A:463:LYS:C	1:A:465:ALA:H	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:644:SER:O	1:B:646:VAL:N	2.47	0.47
1:B:463:LYS:C	1:B:465:ALA:H	2.17	0.47
1:A:425:MET:HA	1:A:426:PRO:HD3	1.81	0.47
1:A:726:VAL:HG12	1:A:726:VAL:O	2.14	0.47
1:B:190:LYS:H	1:B:194:ILE:HB	1.79	0.47
1:B:438:ASP:OD2	1:B:441:LYS:HG3	2.15	0.47
1:A:98:PHE:HE2	1:A:100:HIS:HB2	1.80	0.46
1:A:383:HIS:ND1	1:A:398:THR:OG1	2.41	0.46
1:B:236:ILE:CG2	1:B:254:VAL:HB	2.46	0.46
1:A:578:PHE:CD2	1:A:609:ALA:HB2	2.51	0.46
1:A:68:TYR:CD1	1:A:68:TYR:C	2.89	0.46
1:A:216:TRP:CZ3	1:A:273:THR:HG21	2.45	0.46
1:A:704:HIS:HB3	1:A:713:PHE:HD1	1.81	0.46
1:A:148:ILE:HG22	1:A:149:PRO:HD2	1.98	0.46
1:A:482:LEU:C	1:A:483:HIS:CD2	2.89	0.46
1:A:532:PRO:HD3	1:A:569:SER:HA	1.97	0.46
1:B:127:SER:HB2	1:B:211:TYR:CD2	2.51	0.46
1:B:418:ILE:HA	1:B:430:ASN:O	2.16	0.46
1:A:279:VAL:O	1:A:279:VAL:HG13	2.16	0.46
1:B:364:PHE:CD1	1:B:371:PHE:HB3	2.51	0.46
1:A:662:TYR:HB3	1:A:667:THR:OG1	2.16	0.46
1:B:217:SER:O	1:B:219:ASN:N	2.49	0.46
1:B:477:LEU:HD22	1:B:500:LEU:HD12	1.98	0.46
1:B:660:GLU:HG3	1:B:683:TYR:CD2	2.51	0.46
1:B:149:PRO:HG2	1:B:168:TRP:CD1	2.52	0.45
1:B:163:LYS:NZ	1:B:220:GLY:O	2.36	0.45
1:A:251:THR:HB	1:A:253:ARG:NH2	2.31	0.45
1:B:175:LYS:HG3	1:B:182:SER:HB3	1.98	0.45
1:A:728:VAL:O	1:B:750:HIS:CE1	2.69	0.45
1:B:174:VAL:HG23	1:B:185:ILE:HD11	1.98	0.45
1:A:660:GLU:HG3	1:A:683:TYR:CD2	2.51	0.45
1:B:74:ASN:HB2	1:B:92:ASN:CB	2.37	0.45
1:A:515:ASP:HB3	1:A:526:TYR:CZ	2.51	0.45
1:A:236:ILE:HG12	1:A:712:HIS:CD2	2.51	0.45
1:A:369:ASN:HA	1:A:389:ILE:CD1	2.47	0.45
1:B:112:GLN:HG2	1:B:138:ASN:OD1	2.17	0.45
1:B:216:TRP:CZ3	1:B:273:THR:HG21	2.44	0.45
1:B:487:ASN:O	1:B:488:ASP:HB2	2.16	0.45
1:B:114:ILE:CG2	1:B:135:TYR:HB3	2.40	0.45
1:A:487:ASN:O	1:A:488:ASP:HB2	2.17	0.45
1:A:417:TYR:HE2	1:A:419:SER:HB3	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:ARG:HH21	1:A:479:LEU:HB2	1.82	0.44
1:B:418:ILE:HD11	1:B:459:VAL:HG12	2.00	0.44
1:B:631:TYR:O	1:B:634:TYR:HB3	2.16	0.44
1:A:225:TYR:CZ	1:A:269:PHE:HB2	2.52	0.44
1:A:358:ARG:NH2	2:A:801:D5C:CBA	2.79	0.44
1:A:728:VAL:O	1:B:750:HIS:HE1	2.01	0.44
1:B:143:ILE:HD13	1:B:178:PRO:O	2.16	0.44
1:B:306:ALA:HB3	1:B:310:ARG:HG2	1.99	0.44
1:B:340:LEU:CB	1:B:343:ARG:HG2	2.47	0.44
1:B:741:GLY:O	1:B:742:ILE:C	2.55	0.44
1:B:482:LEU:C	1:B:483:HIS:CD2	2.91	0.44
1:B:626:ILE:O	1:B:650:GLY:HA2	2.16	0.44
1:A:113:PHE:CE1	1:A:178:PRO:HG2	2.52	0.44
1:B:68:TYR:CD1	1:B:68:TYR:C	2.90	0.44
1:A:203:TYR:OH	1:A:299:TYR:HB3	2.18	0.44
1:B:199:THR:HG22	1:B:203:TYR:HB3	1.99	0.44
1:B:323:SER:OG	1:B:347:GLU:HB3	2.18	0.44
1:A:438:ASP:OD2	1:A:441:LYS:HG3	2.18	0.44
1:A:477:LEU:HD22	1:A:500:LEU:HD12	2.00	0.44
1:A:750:HIS:CE1	1:B:728:VAL:O	2.71	0.44
1:B:155:VAL:HG23	1:B:166:TYR:CB	2.46	0.44
1:B:219:ASN:HB2	1:B:308:GLN:OE1	2.18	0.44
1:B:80:ASN:H	1:B:86:SER:HB3	1.83	0.44
1:A:235:LEU:HD13	1:A:253:ARG:HB3	2.00	0.43
1:B:307:THR:OG1	1:B:310:ARG:HB3	2.18	0.43
1:B:417:TYR:HE2	1:B:419:SER:HB3	1.82	0.43
1:B:76:ILE:HD12	1:B:90:LEU:HD22	1.99	0.43
1:A:115:LEU:HD21	1:A:155:VAL:HG11	2.00	0.43
1:B:584:GLY:O	1:B:585:TYR:HB2	2.19	0.43
1:A:159:PRO:HD3	1:A:216:TRP:CB	2.48	0.43
1:A:760:LYS:HG2	1:A:765:LEU:HB2	2.00	0.43
1:B:515:ASP:HB3	1:B:526:TYR:CZ	2.53	0.43
1:B:703:ILE:HA	1:B:733:MET:O	2.18	0.43
1:B:290:PRO:HD3	1:B:326:ASP:OD2	2.19	0.43
1:B:602:GLU:HG2	1:B:603:VAL:N	2.33	0.43
1:B:675:THR:C	1:B:680:LEU:HB2	2.38	0.43
1:B:703:ILE:HG12	1:B:733:MET:HB3	2.00	0.43
1:A:377:ASN:OD1	1:A:379:GLU:N	2.51	0.43
1:A:49:LEU:HD23	1:A:49:LEU:HA	1.78	0.43
1:B:148:ILE:HG22	1:B:149:PRO:HD2	2.00	0.43
1:B:594:ILE:HD12	1:B:594:ILE:HA	1.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:ARG:NH1	1:A:368:GLY:O	2.49	0.43
1:A:630:SER:O	1:A:631:TYR:C	2.57	0.43
1:A:508:GLN:OE1	1:A:533:HIS:NE2	2.52	0.43
1:A:636:THR:HG21	1:A:651:ILE:O	2.19	0.43
1:B:237:GLU:HG2	1:B:253:ARG:CG	2.47	0.43
1:A:217:SER:O	1:A:219:ASN:N	2.52	0.42
1:B:402:TRP:CD1	1:B:421:GLU:HG3	2.54	0.42
1:B:195:TYR:HB2	1:B:228:PHE:HB2	2.00	0.42
1:B:258:LYS:HA	1:B:662:TYR:O	2.20	0.42
1:A:369:ASN:HA	1:A:389:ILE:HD12	2.01	0.42
1:A:602:GLU:HG2	1:A:603:VAL:N	2.34	0.42
1:A:718:GLN:OE1	1:A:721:LYS:HE2	2.18	0.42
1:B:98:PHE:CE2	1:B:100:HIS:HB2	2.54	0.42
1:B:382:ARG:HG2	1:B:382:ARG:HH11	1.84	0.42
1:A:109:PRO:HD2	1:A:161:GLY:O	2.19	0.42
1:A:703:ILE:HG12	1:A:733:MET:HB3	2.00	0.42
1:B:649:CYS:HB3	1:B:699:GLU:HB2	2.02	0.42
1:B:463:LYS:C	1:B:465:ALA:N	2.73	0.42
1:A:306:ALA:HB3	1:A:310:ARG:HG2	2.01	0.42
1:A:80:ASN:H	1:A:86:SER:HB3	1.84	0.42
1:B:223:LEU:HD12	1:B:223:LEU:HA	1.79	0.42
1:B:618:PHE:N	1:B:618:PHE:CD2	2.87	0.42
1:A:224:ALA:HB1	1:A:268:PHE:CZ	2.54	0.41
1:A:611:ARG:HH11	1:A:611:ARG:HG2	1.85	0.41
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.55	0.41
1:A:638:MET:O	1:A:691:ARG:NH1	2.53	0.41
1:B:127:SER:HB2	1:B:211:TYR:CG	2.56	0.41
1:B:450:ASN:O	1:B:451:PRO:C	2.59	0.41
1:A:584:GLY:O	1:A:585:TYR:HB2	2.20	0.41
1:A:718:GLN:HA	1:A:718:GLN:OE1	2.21	0.41
1:B:626:ILE:HD13	1:B:639:VAL:HG11	2.02	0.41
1:A:223:LEU:HD12	1:A:223:LEU:HA	1.77	0.41
1:B:115:LEU:HD21	1:B:155:VAL:CG1	2.51	0.41
1:B:477:LEU:CD1	1:B:501:ASP:HB2	2.50	0.41
1:A:454:CYS:HB3	1:A:457:TYR:CZ	2.56	0.41
1:B:256:TYR:CE1	1:B:712:HIS:HE1	2.37	0.41
1:B:735:TYR:CE2	1:B:751:ILE:HG13	2.56	0.41
1:A:127:SER:HB2	1:A:211:TYR:CD2	2.56	0.41
1:B:49:LEU:HA	1:B:49:LEU:HD23	1.82	0.41
1:A:746:THR:HG21	1:B:725:ASP:HA	2.02	0.41
1:B:735:TYR:HE2	1:B:751:ILE:HG13	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:PHE:HA	1:B:86:SER:HB3	2.02	0.41
1:A:364:PHE:CD1	1:A:371:PHE:HB3	2.56	0.41
1:A:644:SER:C	1:A:646:VAL:H	2.23	0.41
1:A:79:PHE:HA	1:A:86:SER:HB3	2.03	0.41
1:B:302:ASP:HA	1:B:358:ARG:NH1	2.35	0.41
1:B:68:TYR:CE1	1:B:79:PHE:HB2	2.55	0.41
1:B:302:ASP:HA	1:B:358:ARG:HH11	1.85	0.41
1:A:195:TYR:HB2	1:A:228:PHE:HB2	2.02	0.41
1:A:417:TYR:CE2	1:A:419:SER:HB3	2.56	0.41
1:A:402:TRP:CD1	1:A:421:GLU:HG3	2.55	0.41
1:A:594:ILE:HA	1:A:594:ILE:HD12	1.92	0.41
1:B:420:ASN:HB2	1:B:426:PRO:HA	2.02	0.41
1:A:174:VAL:CG2	1:A:185:ILE:HD11	2.48	0.40
1:A:461:PHE:CD1	1:A:468:TYR:HB3	2.56	0.40
1:B:382:ARG:CG	1:B:382:ARG:HH11	2.34	0.40
1:A:530:LEU:HA	1:A:531:PRO:HD3	1.97	0.40
1:B:384:ILE:HD12	1:B:398:THR:HG21	2.04	0.40
1:A:74:ASN:HB2	1:A:92:ASN:CB	2.39	0.40
1:B:370:SER:HB2	1:B:386:TYR:CE1	2.57	0.40
1:B:433:LYS:HD2	1:B:445:LEU:HD21	2.03	0.40
1:B:578:PHE:CD2	1:B:609:ALA:HB2	2.56	0.40
1:B:72:GLN:O	1:B:75:ASN:HB2	2.21	0.40
1:A:307:THR:CG2	1:A:368:GLY:HA3	2.51	0.40
1:A:578:PHE:HE2	1:A:605:ASP:HB3	1.86	0.40
1:B:113:PHE:CE1	1:B:178:PRO:HG2	2.56	0.40
1:B:358:ARG:NH2	2:B:801:D5C:CBA	2.84	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	726/728 (100%)	642 (88%)	75 (10%)	9 (1%)	15	53
1	B	726/728 (100%)	650 (90%)	68 (9%)	8 (1%)	17	56
All	All	1452/1456 (100%)	1292 (89%)	143 (10%)	17 (1%)	15	53

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	ARG
1	B	140	ARG
1	A	178	PRO
1	A	279	VAL
1	A	645	GLY
1	B	178	PRO
1	B	279	VAL
1	B	645	GLY
1	B	341	VAL
1	B	389	ILE
1	A	244	GLU
1	B	423	LYS
1	B	464	GLU
1	A	464	GLU
1	A	389	ILE
1	A	111	GLY
1	A	341	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	653/653 (100%)	614 (94%)	39 (6%)	22	60
1	B	653/653 (100%)	611 (94%)	42 (6%)	20	57
All	All	1306/1306 (100%)	1225 (94%)	81 (6%)	21	58

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	41	LYS
1	A	46	THR
1	A	51	ASN
1	A	72	GLN
1	A	90	LEU
1	A	122	LYS
1	A	134	ILE
1	A	142	LEU
1	A	147	ARG
1	A	148	ILE
1	A	155	VAL
1	A	182	SER
1	A	211	TYR
1	A	230	ASP
1	A	231	THR
1	A	242	SER
1	A	271	VAL
1	A	277	SER
1	A	280	THR
1	A	288	THR
1	A	350	THR
1	A	361	GLU
1	A	378	GLU
1	A	382	ARG
1	A	385	CYS
1	A	419	SER
1	A	443	THR
1	A	458	SER
1	A	472	CYS
1	A	480	TYR
1	A	487	ASN
1	A	522	THR
1	A	566	TYR
1	A	618	PHE
1	A	627	TRP
1	A	685	ASN
1	A	751	ILE
1	A	764	SER
1	B	40	ARG
1	B	41	LYS
1	B	46	THR
1	B	51	ASN

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Mol	Chain	Res	Type
1	B	72	GLN
1	B	90	LEU
1	B	94	THR
1	B	122	LYS
1	B	134	ILE
1	B	142	LEU
1	B	147	ARG
1	B	148	ILE
1	B	155	VAL
1	B	182	SER
1	B	219	ASN
1	B	230	ASP
1	B	231	THR
1	B	271	VAL
1	B	277	SER
1	B	280	THR
1	B	288	THR
1	B	350	THR
1	B	358	ARG
1	B	361	GLU
1	B	378	GLU
1	B	382	ARG
1	B	385	CYS
1	B	419	SER
1	B	426	PRO
1	B	433	LYS
1	B	443	THR
1	B	449	LEU
1	B	458	SER
1	B	480	TYR
1	B	487	ASN
1	B	545	ASP
1	B	566	TYR
1	B	618	PHE
1	B	627	TRP
1	B	685	ASN
1	B	751	ILE
1	B	764	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	B	74	ASN
1	B	750	HIS

### 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](#)

2 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	D5C	A	801	-	35,35,35	2.18	9 (25%)	46,50,50	1.37	5 (10%)
2	D5C	B	801	-	35,35,35	2.15	9 (25%)	46,50,50	1.05	5 (10%)

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	D5C	A	801	-	-	0/24/24/24	0/3/3/3
2	D5C	B	801	-	-	0/24/24/24	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	D5C	CAJ-CAD	-7.22	1.41	1.51
2	B	801	D5C	CAJ-CAD	-7.04	1.41	1.51
2	A	801	D5C	FAG-CAE	-5.45	1.22	1.35
2	A	801	D5C	CAR-CAP	-4.07	1.41	1.50
2	B	801	D5C	FAG-CAE	-3.82	1.26	1.35
2	B	801	D5C	CAR-CAP	-3.75	1.42	1.50
2	B	801	D5C	CBD-CBB	-3.66	1.41	1.49
2	B	801	D5C	CAU-CAX	-3.61	1.39	1.49
2	B	801	D5C	FAH-CAA	-3.55	1.26	1.35
2	B	801	D5C	FAI-CAB	-3.42	1.27	1.35
2	A	801	D5C	CAU-CAX	-3.17	1.40	1.49
2	A	801	D5C	CBD-CBB	-2.89	1.43	1.49
2	A	801	D5C	CAV-CAU	2.02	1.43	1.39
2	A	801	D5C	FBE-CBD	2.10	1.40	1.32
2	A	801	D5C	CAW-CAR	2.30	1.43	1.39
2	A	801	D5C	CAL-CAK	2.49	1.56	1.53
2	B	801	D5C	CAS-CAR	2.66	1.43	1.39
2	B	801	D5C	CAW-CAR	2.70	1.43	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	D5C	CAT-CAU-CAX	-3.11	115.88	121.38
2	A	801	D5C	CAF-CAA-CAB	-3.00	118.37	121.09
2	A	801	D5C	CAS-CAR-CAP	-2.35	113.06	120.61
2	A	801	D5C	CAF-CAE-CAD	-2.32	121.19	124.09
2	B	801	D5C	CAV-CAW-CAR	-2.18	118.35	120.79
2	B	801	D5C	CAF-CAE-CAD	-2.16	121.39	124.09
2	B	801	D5C	CAS-CAT-CAU	-2.05	118.12	121.10
2	B	801	D5C	FAH-CAA-CAF	2.01	122.42	118.63
2	B	801	D5C	CAC-CAD-CAE	2.04	118.44	116.63
2	A	801	D5C	CAW-CAR-CAP	2.34	128.14	120.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	D5C	4	0

*Continued on next page...*

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	D5C	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	728/728 (100%)	-0.23	1 (0%) 95 88	60, 102, 151, 200	0
1	B	728/728 (100%)	-0.24	4 (0%) 90 74	57, 106, 156, 228	0
All	All	1456/1456 (100%)	-0.23	5 (0%) 93 82	57, 104, 155, 228	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	83	TYR	6.2
1	B	82	GLU	2.9
1	A	39	SER	2.8
1	B	40	ARG	2.8
1	B	174	VAL	2.2

### 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( $\text{\AA}^2$ )	Q<0.9
2	D5C	A	801	33/33	0.92	0.30	2.12	74,105,139,143	0
2	D5C	B	801	33/33	0.93	0.24	0.35	80,110,147,151	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.