



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 09:36 AM GMT

PDB ID : 4DSA  
Title : Crystal Structure of DPP-IV with Compound C1  
Authors : Xiong, B.; Zhu, L.R.; Chen, D.Q.; Zhao, Y.L.; Jiang, F.; Shen, J.K.  
Deposited on : 2012-02-18  
Resolution : 3.25 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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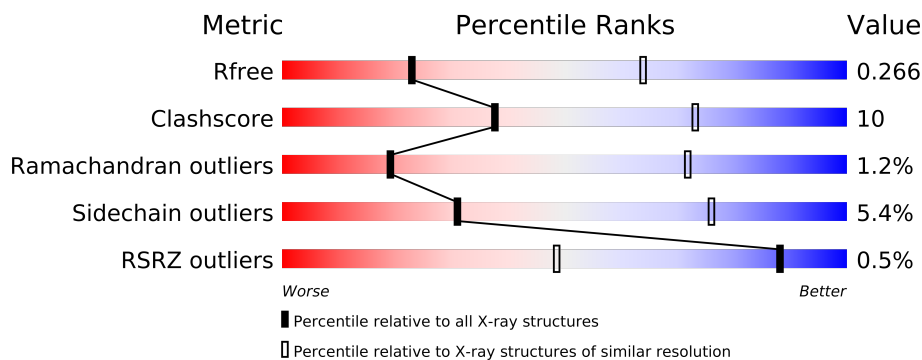
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
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) : stable22683

# 1 Overall quality at a glance



The reported resolution of this entry is 3.25 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	1085 (3.32-3.20)
Clashscore	79885	1374 (3.32-3.20)
Ramachandran outliers	78287	1348 (3.32-3.20)
Sidechain outliers	78261	1346 (3.32-3.20)
RSRZ outliers	66119	1086 (3.32-3.20)

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	728	
1	B	728	

## 2 Entry composition i

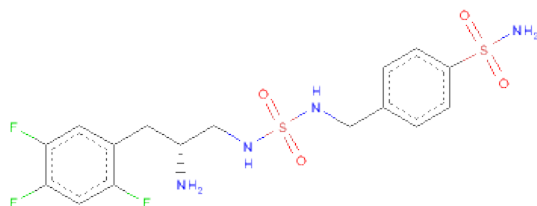
There are 2 unique types of molecules in this entry. The entry contains 11891 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	724	Total	C	N	O	S	0	0	0
			5931	3807	975	1123	26			
1	B	724	Total	C	N	O	S	0	0	0
			5931	3807	975	1123	26			

- Molecule 2 is 4-[[[(2R)-2-AMINO-3-(2,4,5-TRIFLUOROPHENYL)PROPYL]SULFAMOYL}AMINO)METHYL]BENZENESULFONAMIDE (three-letter code: D1C) (formula: C<sub>16</sub>H<sub>19</sub>F<sub>3</sub>N<sub>4</sub>O<sub>4</sub>S<sub>2</sub>).



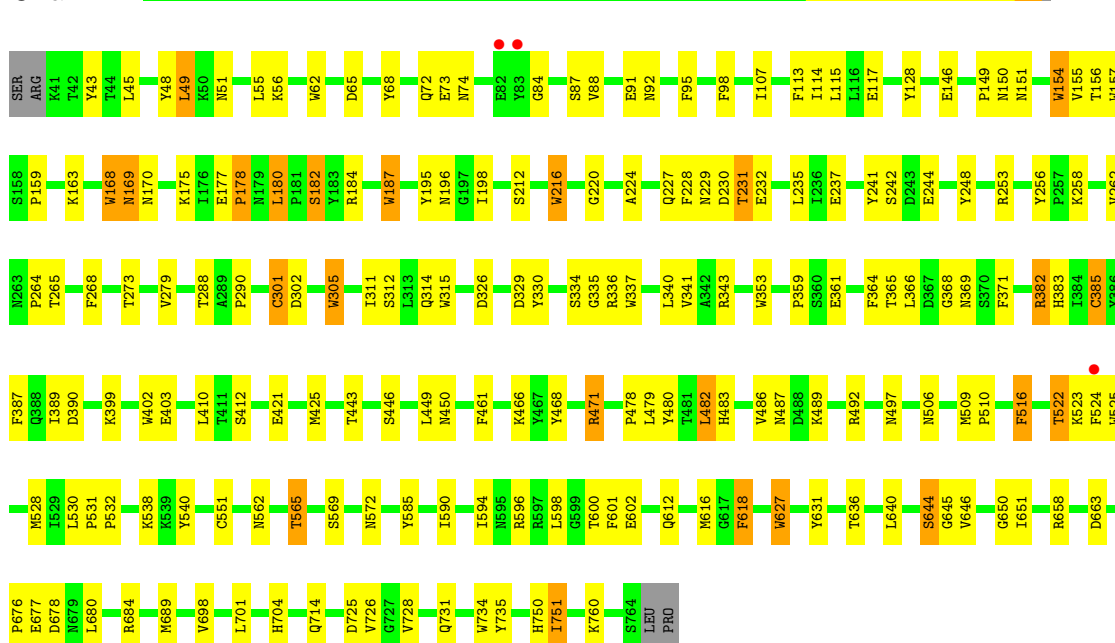
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O S	0	0
			29	16	3	4	4 2		

### 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.

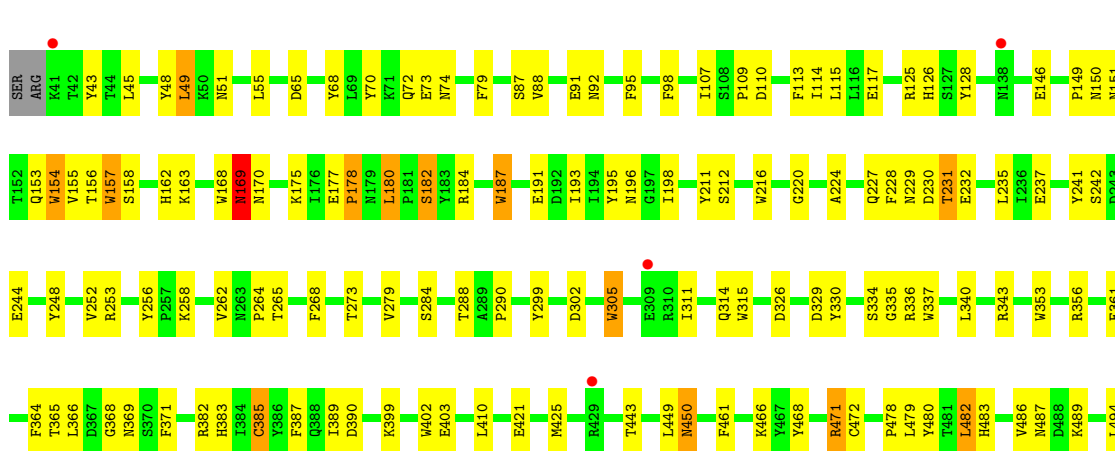
#### • Molecule 1: Dipeptidyl peptidase 4

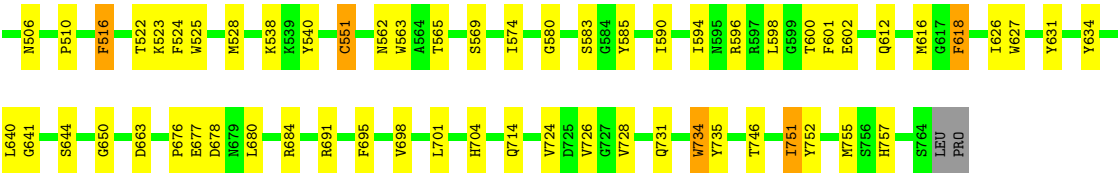
Chain A:



#### • Molecule 1: Dipeptidyl peptidase 4

Chain B:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.68Å 78.68Å 289.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.37 – 3.25 29.37 – 3.25	Depositor EDS
% Data completeness (in resolution range)	97.2 (29.37-3.25) 97.3 (29.37-3.25)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 3.24Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.198 , 0.266 0.198 , 0.266	Depositor DCC
$R_{free}$ test set	1544 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	122.7	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 91.7	EDS
Estimated twinning fraction	0.000 for -h,-k,l 0.056 for h,-h-k,-l 0.024 for -k,-h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 30700 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11891	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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: D1C

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	0.61	13/6102 (0.2%)	0.67	0/8299
1	B	0.62	10/6102 (0.2%)	0.67	0/8299
All	All	0.61	23/12204 (0.2%)	0.67	0/16598

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	337	TRP	CD2-CE2	6.13	1.48	1.41
1	A	157	TRP	CD2-CE2	5.96	1.48	1.41
1	B	337	TRP	CD2-CE2	5.92	1.48	1.41
1	B	563	TRP	CD2-CE2	5.69	1.48	1.41
1	A	187	TRP	CD2-CE2	5.65	1.48	1.41
1	A	154	TRP	CD2-CE2	5.53	1.48	1.41
1	B	157	TRP	CD2-CE2	5.52	1.48	1.41
1	B	525	TRP	CD2-CE2	5.51	1.48	1.41
1	A	315	TRP	CD2-CE2	5.50	1.48	1.41
1	A	627	TRP	CD2-CE2	5.47	1.48	1.41
1	A	62	TRP	CD2-CE2	5.44	1.47	1.41
1	B	154	TRP	CD2-CE2	5.42	1.47	1.41
1	B	187	TRP	CD2-CE2	5.38	1.47	1.41
1	B	734	TRP	CD2-CE2	5.30	1.47	1.41
1	B	305	TRP	CD2-CE2	5.27	1.47	1.41
1	B	315	TRP	CD2-CE2	5.25	1.47	1.41
1	A	734	TRP	CD2-CE2	5.21	1.47	1.41
1	B	353	TRP	CD2-CE2	5.12	1.47	1.41
1	A	353	TRP	CD2-CE2	5.10	1.47	1.41
1	A	305	TRP	CD2-CE2	5.10	1.47	1.41
1	A	525	TRP	CD2-CE2	5.06	1.47	1.41
1	A	168	TRP	CD2-CE2	5.03	1.47	1.41
1	A	216	TRP	CD2-CE2	5.00	1.47	1.41

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	5931	0	5649	118	0
1	B	5931	0	5649	121	0
2	A	29	0	19	0	0
All	All	11891	0	11317	231	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 10.

All (231) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:175:LYS:HG3	1:A:182:SER:HB3	1.52	0.90
1:B:175:LYS:HG3	1:B:182:SER:HB3	1.56	0.86
1:B:383:HIS:HD2	1:B:399:LYS:HA	1.41	0.85
1:A:383:HIS:HD2	1:A:399:LYS:HA	1.41	0.84
1:A:383:HIS:CD2	1:A:399:LYS:HA	2.15	0.81
1:B:383:HIS:CD2	1:B:399:LYS:HA	2.14	0.80
1:B:237:GLU:HG2	1:B:253:ARG:HG2	1.61	0.80
1:A:177:GLU:HB2	1:A:180:LEU:HD22	1.63	0.79
1:A:253:ARG:HH12	1:B:253:ARG:HH12	1.35	0.74
1:A:43:TYR:CD2	1:A:565:THR:HG22	2.21	0.74
1:B:177:GLU:HB2	1:B:180:LEU:HD22	1.70	0.72
1:B:385:CYS:HB3	1:B:387:PHE:CE1	2.26	0.71
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.73	0.70
1:A:369:ASN:HA	1:A:389:ILE:HD12	1.72	0.70
1:A:385:CYS:HB3	1:A:387:PHE:CE1	2.26	0.70
1:A:237:GLU:HG2	1:A:253:ARG:HG2	1.75	0.69
1:B:369:ASN:HA	1:B:389:ILE:HD12	1.73	0.69
1:B:516:PHE:HD1	1:B:523:LYS:HB2	1.57	0.68
1:A:149:PRO:HG2	1:A:168:TRP:CD1	2.27	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:340:LEU:HB2	1:A:343:ARG:HD2	1.76	0.68
1:B:522:THR:HG21	1:B:590:ILE:HD11	1.77	0.67
1:B:596:ARG:NH2	1:B:678:ASP:OD1	2.28	0.66
1:B:115:LEU:HD21	1:B:155:VAL:HG11	1.76	0.66
1:B:43:TYR:CD2	1:B:565:THR:HG22	2.29	0.66
1:A:516:PHE:HD1	1:A:523:LYS:HB2	1.61	0.66
1:B:149:PRO:HG2	1:B:168:TRP:CD1	2.29	0.66
1:A:382:ARG:H	1:A:403:GLU:HG2	1.61	0.65
1:B:232:GLU:HB2	1:B:262:VAL:HG11	1.78	0.65
1:B:382:ARG:H	1:B:403:GLU:HG2	1.60	0.65
1:B:195:TYR:HB2	1:B:228:PHE:HB2	1.79	0.64
1:A:290:PRO:HD3	1:A:326:ASP:OD2	1.98	0.63
1:B:487:ASN:HD21	1:B:489:LYS:HE2	1.63	0.63
1:A:403:GLU:OE1	1:A:585:TYR:HA	1.99	0.63
1:B:340:LEU:HB2	1:B:343:ARG:HD2	1.81	0.63
1:A:232:GLU:HB2	1:A:262:VAL:HG11	1.82	0.62
1:A:726:VAL:HG23	1:A:728:VAL:HG23	1.82	0.62
1:B:231:THR:HG22	1:B:232:GLU:HG3	1.82	0.61
1:A:115:LEU:HD21	1:A:155:VAL:HG11	1.83	0.61
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.83	0.60
1:A:150:ASN:O	1:A:151:ASN:HB2	2.01	0.60
1:A:55:LEU:HD22	1:A:478:PRO:HG2	1.84	0.60
1:A:487:ASN:HD21	1:A:489:LYS:HE2	1.67	0.60
1:A:195:TYR:HB2	1:A:228:PHE:HB2	1.85	0.59
1:B:146:GLU:O	1:B:175:LYS:NZ	2.34	0.59
1:A:364:PHE:CD1	1:A:371:PHE:HB3	2.37	0.59
1:B:726:VAL:HG23	1:B:728:VAL:HG23	1.85	0.59
1:B:115:LEU:HD21	1:B:155:VAL:CG1	2.33	0.59
1:A:113:PHE:CZ	1:A:178:PRO:HG2	2.38	0.59
1:A:231:THR:HG22	1:A:232:GLU:HG3	1.84	0.59
1:B:598:LEU:HD22	1:B:631:TYR:OH	2.03	0.59
1:B:170:ASN:O	1:B:196:ASN:HB2	2.04	0.58
1:B:163:LYS:NZ	1:B:220:GLY:O	2.34	0.58
1:A:482:LEU:HD23	1:A:483:HIS:H	1.69	0.58
1:B:383:HIS:HE1	1:B:402:TRP:O	1.86	0.58
1:A:107:ILE:HG13	1:A:114:ILE:HG13	1.86	0.58
1:A:383:HIS:HE1	1:A:402:TRP:O	1.87	0.57
1:B:107:ILE:HG13	1:B:114:ILE:HG13	1.86	0.57
1:A:224:ALA:HB1	1:A:268:PHE:CZ	2.39	0.57
1:A:163:LYS:NZ	1:A:220:GLY:O	2.33	0.57
1:B:196:ASN:OD1	1:B:227:GLN:HG3	2.05	0.57
1:B:482:LEU:HD23	1:B:483:HIS:H	1.70	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:600:THR:OG1	1:A:601:PHE:N	2.38	0.56
1:B:385:CYS:HB3	1:B:387:PHE:HE1	1.70	0.56
1:A:115:LEU:HD21	1:A:155:VAL:CG1	2.35	0.56
1:B:290:PRO:HD3	1:B:326:ASP:OD2	2.05	0.56
1:A:596:ARG:NH2	1:A:678:ASP:OD1	2.38	0.56
1:B:364:PHE:CD1	1:B:371:PHE:HB3	2.41	0.56
1:A:258:LYS:HD2	1:B:248:TYR:CE1	2.41	0.55
1:A:88:VAL:HG21	1:A:91:GLU:HG2	1.88	0.55
1:A:229:ASN:HB3	1:A:265:THR:OG1	2.06	0.55
1:B:516:PHE:HD2	1:B:516:PHE:H	1.54	0.55
1:A:510:PRO:HD3	1:A:569:SER:HB2	1.88	0.55
1:A:305:TRP:CE2	1:A:311:ILE:HD12	2.42	0.54
1:B:88:VAL:HG21	1:B:91:GLU:HG2	1.90	0.54
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.43	0.54
1:A:636:THR:HG21	1:A:651:ILE:O	2.08	0.53
1:B:74:ASN:HB3	1:B:92:ASN:HB2	1.90	0.53
1:B:55:LEU:HD22	1:B:478:PRO:HG2	1.91	0.53
1:A:528:MET:HE1	1:A:530:LEU:HD21	1.90	0.53
1:A:216:TRP:HZ3	1:A:273:THR:HG21	1.73	0.53
1:B:540:TYR:N	1:B:618:PHE:O	2.33	0.53
1:B:516:PHE:CD1	1:B:523:LYS:HB2	2.42	0.53
1:B:216:TRP:HZ3	1:B:273:THR:HG21	1.74	0.53
1:A:640:LEU:HB3	1:A:698:VAL:HG21	1.90	0.52
1:A:516:PHE:H	1:A:516:PHE:HD2	1.56	0.52
1:B:580:GLY:O	1:B:583:SER:OG	2.26	0.52
1:B:403:GLU:OE1	1:B:585:TYR:HA	2.09	0.52
1:A:74:ASN:HB3	1:A:92:ASN:HB2	1.92	0.52
1:B:113:PHE:CZ	1:B:178:PRO:HG2	2.45	0.52
1:B:600:THR:OG1	1:B:601:PHE:N	2.43	0.51
1:B:594:ILE:HD11	1:B:602:GLU:OE1	2.09	0.51
1:A:196:ASN:OD1	1:A:227:GLN:HG3	2.11	0.51
1:A:385:CYS:HB3	1:A:387:PHE:HE1	1.71	0.51
1:A:750:HIS:CD2	1:B:724:VAL:HG22	2.46	0.51
1:B:538:LYS:O	1:B:618:PHE:HA	2.11	0.51
1:B:334:SER:OG	1:B:336:ARG:HG2	2.11	0.51
1:B:594:ILE:HD11	1:B:602:GLU:H	1.76	0.51
1:A:154:TRP:CE2	1:A:212:SER:HB3	2.46	0.50
1:A:146:GLU:O	1:A:175:LYS:NZ	2.42	0.50
1:B:191:GLU:O	1:B:193:ILE:HG13	2.11	0.50
1:A:224:ALA:HB1	1:A:268:PHE:HZ	1.74	0.50
1:B:224:ALA:HB1	1:B:268:PHE:HZ	1.75	0.50
1:A:74:ASN:HB3	1:A:92:ASN:CB	2.42	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:154:TRP:CE2	1:B:212:SER:HB3	2.47	0.50
1:B:230:ASP:OD1	1:B:264:PRO:HB3	2.12	0.50
1:A:402:TRP:NE1	1:A:421:GLU:HG3	2.27	0.50
1:A:594:ILE:HD11	1:A:602:GLU:H	1.77	0.50
1:A:461:PHE:CD1	1:A:468:TYR:HB3	2.47	0.50
1:B:330:TYR:CE1	1:B:335:GLY:HA2	2.47	0.50
1:A:594:ILE:HD11	1:A:602:GLU:OE1	2.12	0.49
1:B:74:ASN:HB3	1:B:92:ASN:CB	2.43	0.49
1:B:229:ASN:HB3	1:B:265:THR:OG1	2.12	0.49
1:A:538:LYS:O	1:A:618:PHE:HA	2.13	0.49
1:B:402:TRP:NE1	1:B:421:GLU:HG3	2.28	0.49
1:B:68:TYR:HE2	1:B:482:LEU:HD11	1.77	0.49
1:A:258:LYS:HD2	1:B:248:TYR:CZ	2.48	0.49
1:B:640:LEU:HB3	1:B:698:VAL:HG21	1.95	0.49
1:B:305:TRP:CE2	1:B:311:ILE:HD12	2.48	0.49
1:A:195:TYR:HB3	1:A:198:ILE:O	2.13	0.48
1:B:169:ASN:O	1:B:170:ASN:HB2	2.13	0.48
1:B:235:LEU:HD13	1:B:253:ARG:HB3	1.95	0.48
1:B:516:PHE:HD1	1:B:523:LYS:CB	2.25	0.48
1:A:68:TYR:HE2	1:A:482:LEU:HD11	1.78	0.48
1:B:125:ARG:HD2	1:B:126:HIS:NE2	2.28	0.48
1:A:701:LEU:HA	1:A:731:GLN:HB2	1.95	0.48
1:A:65:ASP:O	1:A:466:LYS:HB2	2.13	0.48
1:A:235:LEU:HD13	1:A:253:ARG:HB3	1.94	0.48
1:A:334:SER:OG	1:A:336:ARG:HG2	2.13	0.48
1:A:237:GLU:HG2	1:A:253:ARG:CG	2.44	0.48
1:A:680:LEU:HD11	1:A:684:ARG:CZ	2.43	0.48
1:A:594:ILE:HA	1:A:594:ILE:HD12	1.78	0.48
1:B:184:ARG:HH21	1:B:187:TRP:HA	1.79	0.48
1:A:714:GLN:HA	1:B:241:TYR:CE1	2.48	0.48
1:B:510:PRO:HD3	1:B:569:SER:HB2	1.95	0.48
1:B:150:ASN:O	1:B:151:ASN:HB2	2.14	0.47
1:B:735:TYR:OH	1:B:751:ILE:HA	2.13	0.47
1:A:248:TYR:CE1	1:B:258:LYS:HD2	2.49	0.47
1:A:598:LEU:HD22	1:A:631:TYR:OH	2.15	0.47
1:B:365:THR:O	1:B:368:GLY:N	2.46	0.47
1:A:516:PHE:CD1	1:A:523:LYS:HB2	2.46	0.47
1:B:594:ILE:HD12	1:B:594:ILE:HA	1.82	0.47
1:A:522:THR:HG21	1:A:590:ILE:HD11	1.96	0.47
1:B:110:ASP:OD2	1:B:162:HIS:ND1	2.29	0.47
1:A:524:PHE:HE1	1:A:590:ILE:HG12	1.80	0.47
1:B:528:MET:HE2	1:B:528:MET:HB3	1.74	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:524:PHE:HE1	1:B:590:ILE:HG12	1.81	0.46
1:B:302:ASP:HB3	1:B:314:GLN:HB2	1.96	0.46
1:B:402:TRP:CD1	1:B:421:GLU:HG3	2.50	0.46
1:A:528:MET:HE2	1:A:528:MET:HB3	1.68	0.46
1:A:402:TRP:CD1	1:A:421:GLU:HG3	2.50	0.46
1:A:644:SER:O	1:A:646:VAL:N	2.49	0.46
1:A:305:TRP:CZ2	1:A:311:ILE:HD12	2.51	0.45
1:A:159:PRO:HD3	1:A:216:TRP:CG	2.51	0.45
1:A:170:ASN:O	1:A:196:ASN:HB2	2.16	0.45
1:A:184:ARG:HH21	1:A:187:TRP:HA	1.82	0.45
1:A:461:PHE:CE1	1:A:468:TYR:HB3	2.52	0.45
1:A:509:MET:O	1:A:532:PRO:HB3	2.17	0.45
1:B:680:LEU:HD11	1:B:684:ARG:CZ	2.46	0.45
1:B:383:HIS:CE1	1:B:402:TRP:O	2.69	0.45
1:B:153:GLN:OE1	1:B:198:ILE:HD13	2.17	0.45
1:A:528:MET:CE	1:A:530:LEU:HD21	2.46	0.45
1:A:735:TYR:OH	1:A:751:ILE:HA	2.17	0.45
1:B:471:ARG:HD3	1:B:480:TYR:CE2	2.52	0.44
1:A:72:GLN:O	1:A:74:ASN:N	2.50	0.44
1:B:117:GLU:OE1	1:B:128:TYR:HE1	2.00	0.44
1:A:725:ASP:HA	1:B:746:THR:HG21	1.99	0.44
1:A:383:HIS:CE1	1:A:402:TRP:O	2.69	0.44
1:A:56:LYS:HB2	1:A:497:ASN:OD1	2.17	0.44
1:B:45:LEU:HG	1:B:49:LEU:HD22	1.99	0.44
1:B:48:TYR:CE1	1:B:562:ASN:HA	2.53	0.44
1:A:241:TYR:CE1	1:B:714:GLN:HA	2.52	0.44
1:A:330:TYR:CE1	1:A:335:GLY:HA2	2.53	0.44
1:A:531:PRO:HB3	1:A:572:ASN:HA	2.00	0.44
1:A:43:TYR:CD2	1:A:565:THR:CG2	2.97	0.44
1:B:676:PRO:HD2	1:B:677:GLU:OE1	2.18	0.44
1:B:70:TYR:HB3	1:B:79:PHE:HE1	1.84	0.43
1:B:482:LEU:HD12	1:B:494:LEU:HD21	2.00	0.43
1:A:369:ASN:HA	1:A:389:ILE:CD1	2.44	0.43
1:B:594:ILE:CD1	1:B:601:PHE:HB2	2.48	0.43
1:A:516:PHE:HD1	1:A:523:LYS:CB	2.30	0.43
1:A:113:PHE:CE2	1:A:178:PRO:HG2	2.53	0.43
1:B:95:PHE:HB3	1:B:98:PHE:HB2	2.00	0.43
1:B:162:HIS:NE2	1:B:177:GLU:OE1	2.51	0.43
1:B:237:GLU:HG2	1:B:253:ARG:CG	2.41	0.43
1:A:658:ARG:HB2	1:A:689:MET:CE	2.49	0.43
1:A:84:GLY:HA3	1:A:492:ARG:HH22	1.83	0.43
1:B:734:TRP:C	1:B:734:TRP:CD1	2.90	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:48:TYR:CE1	1:A:562:ASN:HA	2.54	0.42
1:A:169:ASN:O	1:A:170:ASN:HB2	2.19	0.42
1:B:701:LEU:HA	1:B:731:GLN:HB2	2.00	0.42
1:B:65:ASP:O	1:B:466:LYS:HB2	2.19	0.42
1:B:468:TYR:CE2	1:B:483:HIS:HB2	2.54	0.42
1:B:72:GLN:O	1:B:74:ASN:N	2.51	0.42
1:A:446:SER:HA	1:A:449:LEU:HG	2.01	0.42
1:B:528:MET:CE	1:B:574:ILE:HG21	2.50	0.42
1:A:301:CYS:SG	1:A:359:PRO:HD2	2.59	0.42
1:A:45:LEU:HG	1:A:49:LEU:HD22	2.01	0.42
1:A:677:GLU:N	1:A:677:GLU:OE1	2.51	0.42
1:B:256:TYR:CZ	1:B:663:ASP:HB3	2.54	0.42
1:B:195:TYR:HB3	1:B:198:ILE:O	2.19	0.42
1:A:471:ARG:HD3	1:A:480:TYR:CE2	2.55	0.42
1:B:109:PRO:HG2	1:B:158:SER:O	2.18	0.42
1:B:461:PHE:CD1	1:B:468:TYR:HB3	2.55	0.42
1:B:735:TYR:CE2	1:B:751:ILE:HG13	2.55	0.41
1:A:612:GLN:O	1:A:616:MET:HG3	2.20	0.41
1:A:540:TYR:N	1:A:618:PHE:O	2.36	0.41
1:A:256:TYR:CZ	1:A:663:ASP:HB3	2.55	0.41
1:A:159:PRO:HD3	1:A:216:TRP:CB	2.50	0.41
1:A:95:PHE:HB3	1:A:98:PHE:HB2	2.02	0.41
1:A:365:THR:O	1:A:368:GLY:N	2.53	0.41
1:A:676:PRO:HD2	1:A:677:GLU:OE1	2.21	0.41
1:A:230:ASP:OD1	1:A:264:PRO:HB3	2.19	0.41
1:A:562:ASN:O	1:A:565:THR:HB	2.20	0.41
1:B:369:ASN:HA	1:B:389:ILE:CD1	2.46	0.41
1:B:157:TRP:HA	1:B:163:LYS:O	2.21	0.41
1:A:383:HIS:CD2	1:A:399:LYS:CA	2.98	0.41
1:B:191:GLU:C	1:B:193:ILE:H	2.24	0.41
1:B:641:GLY:O	1:B:691:ARG:HB3	2.21	0.41
1:B:612:GLN:O	1:B:616:MET:HG3	2.21	0.41
1:A:530:LEU:HA	1:A:531:PRO:HD3	1.99	0.41
1:B:626:ILE:O	1:B:650:GLY:HA2	2.20	0.40
1:A:509:MET:HB3	1:A:509:MET:HE2	1.98	0.40
1:A:302:ASP:HB3	1:A:314:GLN:HB2	2.03	0.40
1:B:237:GLU:HA	1:B:252:VAL:O	2.21	0.40
1:B:695:PHE:HB3	1:B:728:VAL:HG11	2.04	0.40
1:B:461:PHE:CE1	1:B:468:TYR:HB3	2.57	0.40
1:A:117:GLU:OE1	1:A:128:TYR:HE1	2.05	0.40
1:B:752:TYR:HA	1:B:755:MET:HE2	2.02	0.40
1:B:631:TYR:O	1:B:634:TYR:HB3	2.20	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:113:PHE:CE2	1:B:178:PRO:HG2	2.56	0.40
1:B:356:ARG:HD3	1:B:551:CYS:SG	2.61	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	722/728 (99%)	643 (89%)	69 (10%)	10 (1%)	16	68
1	B	722/728 (99%)	640 (89%)	75 (10%)	7 (1%)	22	75
All	All	1444/1456 (99%)	1283 (89%)	144 (10%)	17 (1%)	19	72

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	PRO
1	A	644	SER
1	A	645	GLY
1	B	169	ASN
1	B	178	PRO
1	B	644	SER
1	A	73	GLU
1	A	169	ASN
1	A	341	VAL
1	A	551	CYS
1	A	760	LYS
1	B	73	GLU
1	A	565	THR
1	B	551	CYS
1	A	279	VAL
1	B	279	VAL
1	B	450	ASN

### 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	649/653 (99%)	615 (95%)	34 (5%)	32	76
1	B	649/653 (99%)	613 (94%)	36 (6%)	30	75
All	All	1298/1306 (99%)	1228 (95%)	70 (5%)	31	76

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	LEU
1	A	51	ASN
1	A	87	SER
1	A	156	THR
1	A	180	LEU
1	A	182	SER
1	A	231	THR
1	A	242	SER
1	A	244	GLU
1	A	288	THR
1	A	301	CYS
1	A	312	SER
1	A	329	ASP
1	A	361	GLU
1	A	366	LEU
1	A	382	ARG
1	A	385	CYS
1	A	390	ASP
1	A	410	LEU
1	A	412	SER
1	A	425	MET
1	A	443	THR
1	A	450	ASN
1	A	471	ARG
1	A	479	LEU
1	A	482	LEU
1	A	486	VAL
1	A	506	ASN
1	A	516	PHE

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Mol	Chain	Res	Type
1	A	522	THR
1	A	618	PHE
1	A	627	TRP
1	A	704	HIS
1	A	751	ILE
1	B	49	LEU
1	B	51	ASN
1	B	87	SER
1	B	156	THR
1	B	169	ASN
1	B	180	LEU
1	B	182	SER
1	B	211	TYR
1	B	231	THR
1	B	242	SER
1	B	244	GLU
1	B	284	SER
1	B	288	THR
1	B	299	TYR
1	B	329	ASP
1	B	361	GLU
1	B	366	LEU
1	B	385	CYS
1	B	390	ASP
1	B	410	LEU
1	B	425	MET
1	B	443	THR
1	B	449	LEU
1	B	450	ASN
1	B	471	ARG
1	B	472	CYS
1	B	479	LEU
1	B	482	LEU
1	B	486	VAL
1	B	506	ASN
1	B	516	PHE
1	B	618	PHE
1	B	627	TRP
1	B	704	HIS
1	B	751	ILE
1	B	757	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such



sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	ASN
1	A	247	GLN
1	A	430	ASN
1	A	748	HIS
1	B	66	HIS
1	B	138	ASN
1	B	247	GLN

### 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 ⓘ

1 ligand is 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	D1C	A	800	-	30,30,30	6.51	11 (36%)	44,44,44	2.62	15 (34%)

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	D1C	A	800	-	-	0/22/22/22	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	800	D1C	SBA-NAZ	-23.63	1.40	1.61
2	A	800	D1C	SBA-NAL	18.21	1.78	1.61
2	A	800	D1C	CAV-CAP	-9.65	1.37	1.51
2	A	800	D1C	OBC-SBA	9.13	1.54	1.43
2	A	800	D1C	OBB-SBA	8.60	1.53	1.43
2	A	800	D1C	OAJ-SAH	6.06	1.54	1.43
2	A	800	D1C	OAK-SAH	5.93	1.53	1.43
2	A	800	D1C	CAE-SAH	-4.27	1.70	1.77
2	A	800	D1C	CAA-CAB	-4.09	1.41	1.51
2	A	800	D1C	FAU-CAN	-2.77	1.28	1.35
2	A	800	D1C	FAS-CAQ	2.23	1.41	1.35

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	D1C	OBC-SBA-OBB	-8.65	107.01	120.12
2	A	800	D1C	CAO-CAP-CAQ	6.30	121.91	116.48
2	A	800	D1C	CAX-NAZ-SBA	-5.45	108.98	119.14
2	A	800	D1C	OBB-SBA-NAL	4.57	113.89	106.35
2	A	800	D1C	OAJ-SAH-OAK	-4.42	111.09	118.78
2	A	800	D1C	CAA-NAL-SBA	-4.34	111.98	119.05
2	A	800	D1C	CAX-CAW-CAV	-3.97	105.15	111.06
2	A	800	D1C	CAR-CAQ-CAP	-3.29	119.48	124.16
2	A	800	D1C	CAW-CAX-NAZ	-3.21	104.47	113.03
2	A	800	D1C	OBC-SBA-NAL	2.99	111.27	106.35
2	A	800	D1C	CAV-CAP-CAQ	-2.66	119.09	122.22
2	A	800	D1C	FAT-CAM-CAR	2.60	123.55	118.54
2	A	800	D1C	NAZ-SBA-NAL	-2.38	109.39	111.83
2	A	800	D1C	FAU-CAN-CAO	2.35	123.07	118.54
2	A	800	D1C	CAP-CAO-CAN	-2.24	117.94	119.97

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	724/728 (99%)	-0.04	3 (0%)	90 54	87, 141, 186, 246	0
1	B	724/728 (99%)	-0.02	4 (0%)	86 44	86, 144, 192, 229	0
All	All	1448/1456 (99%)	-0.03	7 (0%)	88 48	86, 143, 189, 246	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	82	GLU	3.6
1	A	83	TYR	2.9
1	A	524	PHE	2.7
1	B	309	GLU	2.1
1	B	41	LYS	2.1
1	B	138	ASN	2.1
1	B	429	ARG	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( $\text{\AA}^2$ )	Q<0.9
2	D1C	A	800	29/29	0.29	0.50	98,148,204,207	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.