Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:54 PM 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 X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

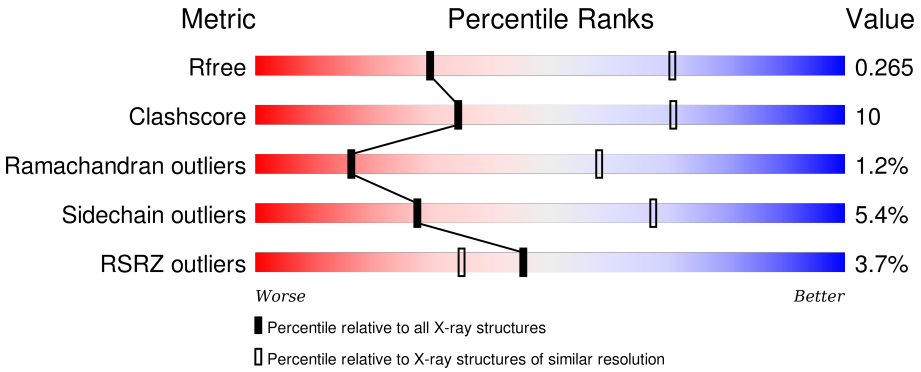
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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}	91344	1624 (3.32-3.20)
Clashscore	102246	1806 (3.32-3.20)
Ramachandran outliers	100387	1773 (3.32-3.20)
Sidechain outliers	100360	1771 (3.32-3.20)
RSRZ outliers	91569	1632 (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 >=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 <=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	3% 73% 23%
1	B	728	4% 72% 25%

2 Entry composition

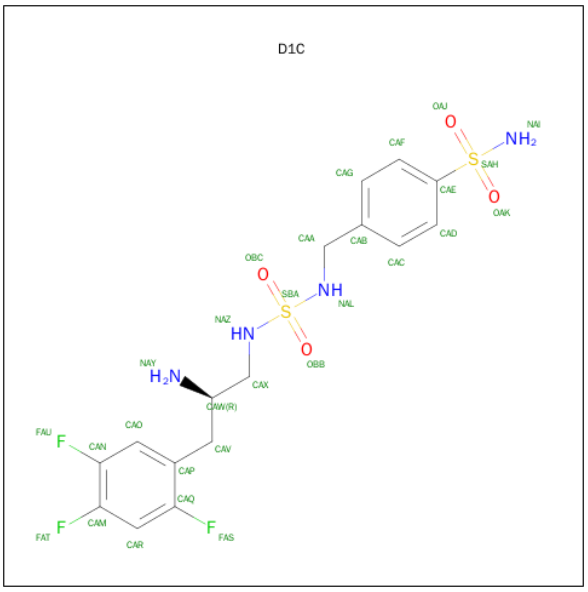
There are 2 unique types of molecules in this entry. The entry contains 11891 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	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: $C_{16}H_{19}F_3N_4O_4S_2$).



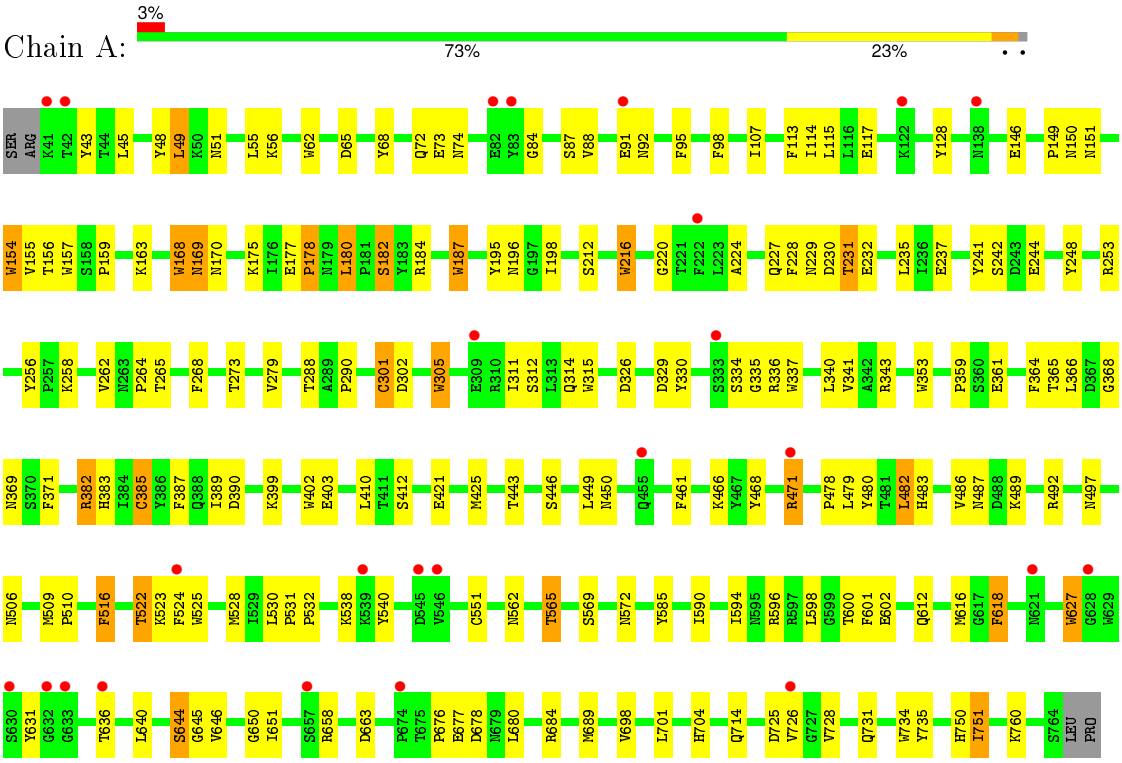
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			29	16	3	4	4	2		

3 Residue-property plots (i)

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

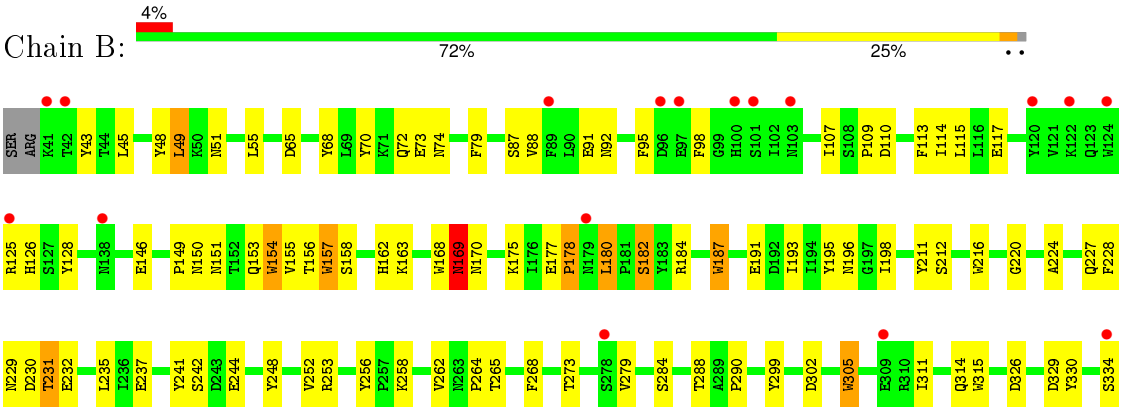
- Molecule 1: Dipeptidyl peptidase 4

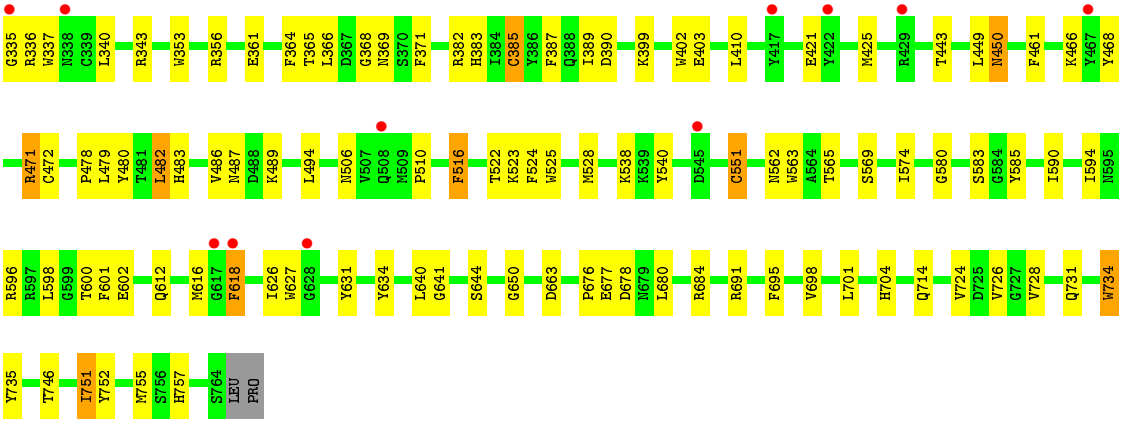
Chain A:



- Molecule 1: Dipeptidyl peptidase 4

Chain B:




G335 R336 W337 N338 G339 L340 R343 W353 R356 E361 F364 T365 L366 D367 G368 N369 S370 F371 R382 H383 I384 C385 Y386 F387 Q388 I389 D390 K399 W402 E403 L410 Y417 E421 Y422 M425 R429 T443 L449 N450 F461 K466 Y467 Y468
R471 C472 P478 L479 Y480 T481 L482 H483 V486 N487 D488 K489 L494 N506 V507 Q508 M509 P510 F516 T522 K523 F524 W525 M528 K538 K539 Y540 D545 C551 N562 W563 A564 T565 S569 I574 G580 S583 G584 Y585 I590 I594 N595
R596 R597 L598 G599 T600 F601 E602 Q612 M616 G617 F618 I626 W627 G628 Y631 Y634 L640 G641 S644 G650 D663 P676 E677 D678 N679 L680 R684 R691 F695 V698 L701 H704 Q714 V724 D725 V726 G727 V728 Q731 W734
Y735 T746 I751 Y752 M755 S756 H757 S764 LEU PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	2.09 (at 3.24Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.198 , 0.266 0.193 , 0.265	Depositor DCC
R_{free} test set	1596 reflections (5.47%)	DCC
Wilson B-factor (Å^2)	122.7	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 93.5	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[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	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^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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 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	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

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 10.

All (231) 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: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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:482:LEU:HD23	1:B:483:HIS:H	1.70	0.56
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 (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	722/728 (99%)	643 (89%)	69 (10%)	10 (1%)	14	54
1	B	722/728 (99%)	640 (89%)	75 (10%)	7 (1%)	19	62
All	All	1444/1456 (99%)	1283 (89%)	144 (10%)	17 (1%)	16	58

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

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Mol	Chain	Res	Type
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%)	29 68
1	B	649/653 (99%)	613 (94%)	36 (6%)	27 67
All	All	1298/1306 (99%)	1228 (95%)	70 (5%)	27 67

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 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

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	6.13	11 (36%)	36,44,44	2.44	9 (25%)

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	-	-	0/21/22/22	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	-21.19	1.40	1.61
2	A	800	D1C	CAV-CAP	-9.83	1.37	1.51
2	A	800	D1C	CAE-SAH	-4.62	1.70	1.77
2	A	800	D1C	CAA-CAB	-4.41	1.41	1.51
2	A	800	D1C	FAU-CAN	-2.90	1.28	1.35
2	A	800	D1C	FAS-CAQ	2.33	1.41	1.35
2	A	800	D1C	OAK-SAH	5.82	1.53	1.43
2	A	800	D1C	OAJ-SAH	5.95	1.54	1.43
2	A	800	D1C	OBB-SBA	8.95	1.53	1.43
2	A	800	D1C	OBC-SBA	9.51	1.54	1.43
2	A	800	D1C	SBA-NAL	16.64	1.78	1.61

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	800	D1C	OBC-SBA-OBB	-7.99	107.01	120.04
2	A	800	D1C	OAJ-SAH-OAK	-5.48	111.09	118.80
2	A	800	D1C	CAR-CAQ-CAP	-3.65	119.48	124.13
2	A	800	D1C	CAW-CAX-NAZ	-2.79	104.47	111.50
2	A	800	D1C	OBC-SBA-NAL	2.19	111.27	106.83
2	A	800	D1C	FAU-CAN-CAO	2.38	123.07	118.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	800	D1C	FAT-CAM-CAR	2.64	123.55	118.59
2	A	800	D1C	OBB-SBA-NAL	3.47	113.89	106.83
2	A	800	D1C	CAO-CAP-CAQ	6.93	121.91	116.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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^{th} 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^2)	Q<0.9
1	A	724/728 (99%)	0.07	25 (3%)	48	38	87, 141, 186, 246	0
1	B	724/728 (99%)	0.09	28 (3%)	43	33	86, 144, 192, 229	0
All	All	1448/1456 (99%)	0.08	53 (3%)	45	35	86, 143, 189, 246	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	524	PHE	5.7
1	A	82	GLU	5.0
1	B	309	GLU	4.8
1	A	83	TYR	4.8
1	A	455	GLN	3.8
1	B	138	ASN	3.8
1	A	628	GLY	3.5
1	B	467	TYR	3.3
1	A	632	GLY	3.3
1	A	545	ASP	3.2
1	B	100	HIS	3.1
1	A	42	THR	3.1
1	B	618	PHE	3.0
1	A	633	GLY	2.9
1	B	628	GLY	2.9
1	B	97	GLU	2.9
1	B	101	SER	2.8
1	B	103	ASN	2.8
1	B	429	ARG	2.7
1	B	334	SER	2.7
1	B	179	ASN	2.7
1	A	471	ARG	2.6
1	A	630	SER	2.6
1	B	96	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	636	THR	2.5
1	B	42	THR	2.5
1	B	545	ASP	2.5
1	A	674	PRO	2.4
1	A	138	ASN	2.4
1	B	617	GLY	2.4
1	A	657	SER	2.4
1	A	309	GLU	2.4
1	A	122	LYS	2.3
1	A	91	GLU	2.3
1	B	122	LYS	2.2
1	B	125	ARG	2.2
1	A	222	PHE	2.2
1	B	338	ASN	2.2
1	A	41	LYS	2.1
1	A	726	VAL	2.1
1	B	41	LYS	2.1
1	B	422	TYR	2.1
1	A	539	LYS	2.1
1	B	120	TYR	2.1
1	B	508	GLN	2.1
1	B	89	PHE	2.1
1	B	417	TYR	2.1
1	A	333	SER	2.1
1	B	124	TRP	2.1
1	B	335	GLY	2.1
1	A	546	VAL	2.0
1	A	621	ASN	2.0
1	B	278	SER	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

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^{th} 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^2)	Q<0.9
2	D1C	A	800	29/29	0.90	0.27	-0.15	98,148,204,207	0

6.5 Other polymers

There are no such residues in this entry.