W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:31 PM GMT

PDB ID	:	1PFQ
Title	:	crystal structure of human apo dipeptidyl peptidase IV / CD26
Authors	:	Oefner, C.; D'Arcy, A.; Mac Sweeney, A.; Pierau, S.; Gardiner, R.; Dale, G.E.
Deposited on	:	2003-05-27
Resolution	:	1.90 Å(reported)

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 (i)

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.
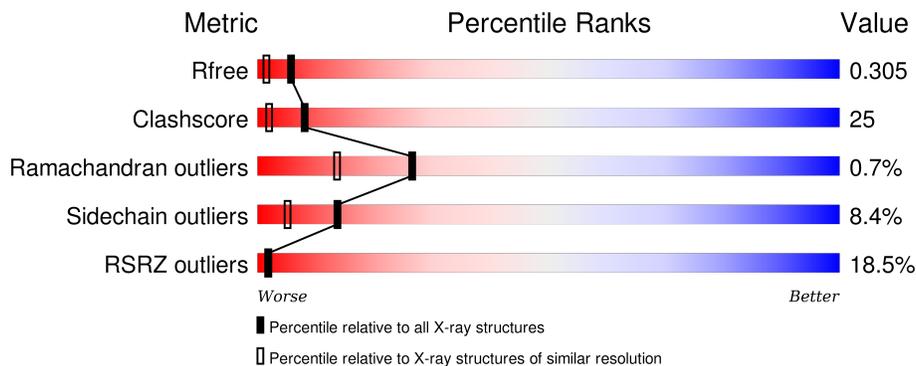
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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 >=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	731	17% / 64% / 30% / 5%
1	B	731	20% / 59% / 34% / 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12418 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 IV soluble form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5964	3827	982	1129	26			
1	B	725	Total	C	N	O	S	0	0	0
			5926	3801	977	1122	26			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
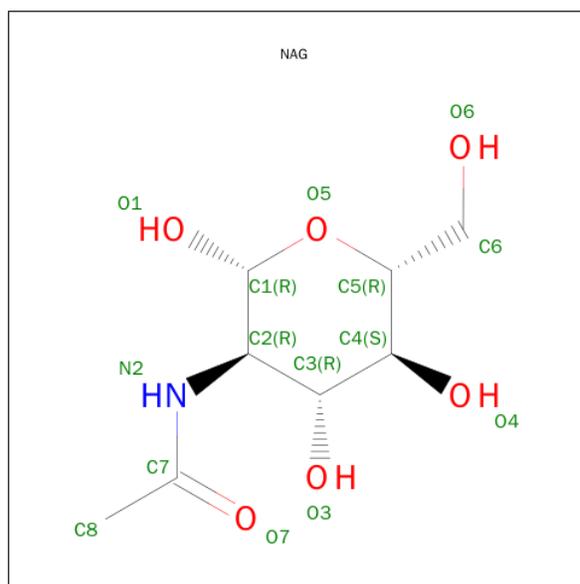
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	268	Total O 268 268	0	0
3	B	204	Total O 204 204	0	0

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 IV soluble form

Chain A:

• Molecule 1: Dipeptidyl peptidase IV soluble form

Chain B:
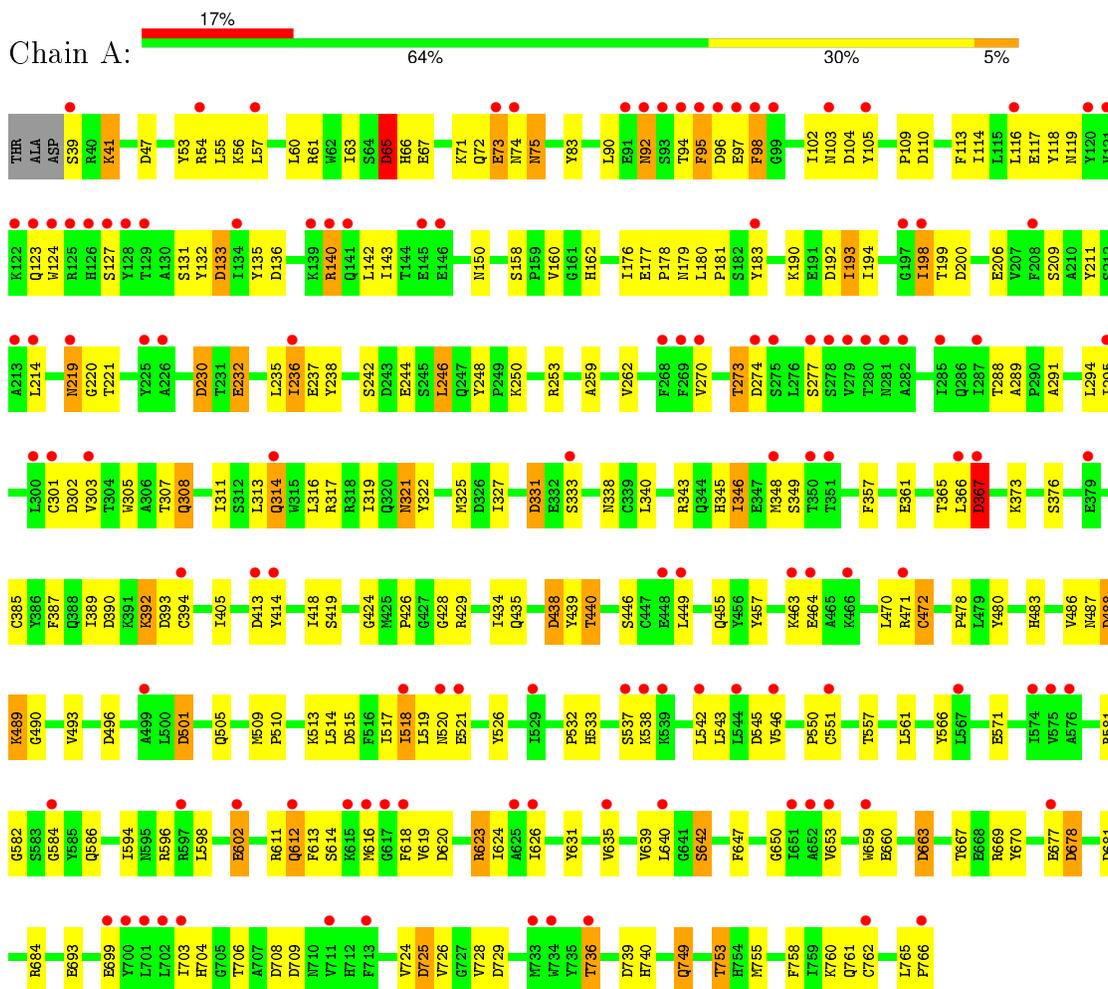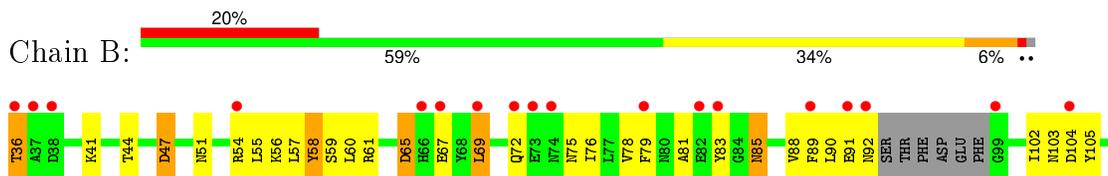
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.03Å 118.14Å 184.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 29.77 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.7 (20.00-1.90) 98.7 (29.77-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.254 , 0.298 0.264 , 0.305	Depositor DCC
R_{free} test set	6101 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	37.5	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 61.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Outliers	0 of 233277 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12418	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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 (i)

5.1 Standard geometry (i)

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

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	0.27	0/6136	0.60	27/8344 (0.3%)
1	B	0.26	0/6094	0.60	33/8287 (0.4%)
All	All	0.26	0/12230	0.60	60/16631 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	545	ASP	CB-CG-OD2	6.25	123.93	118.30
1	A	545	ASP	CB-CG-OD2	5.91	123.62	118.30
1	B	725	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	200	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	725	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	663	ASP	CB-CG-OD2	5.74	123.46	118.30
1	A	739	ASP	CB-CG-OD2	5.67	123.40	118.30
1	B	739	ASP	CB-CG-OD2	5.62	123.36	118.30
1	B	729	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	192	ASP	CB-CG-OD2	5.55	123.30	118.30
1	B	393	ASP	CB-CG-OD2	5.52	123.27	118.30
1	B	501	ASP	CB-CG-OD2	5.46	123.21	118.30
1	A	488	ASP	CB-CG-OD2	5.45	123.21	118.30
1	B	136	ASP	CB-CG-OD2	5.43	123.19	118.30

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	367	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	47	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	136	ASP	CB-CG-OD2	5.39	123.15	118.30
1	B	331	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	413	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	393	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	709	ASP	CB-CG-OD2	5.34	123.11	118.30
1	B	678	ASP	CB-CG-OD2	5.33	123.10	118.30
1	B	65	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	104	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	413	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	438	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	274	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	390	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	709	ASP	CB-CG-OD2	5.27	123.04	118.30
1	B	663	ASP	CB-CG-OD2	5.27	123.04	118.30
1	B	302	ASP	CB-CG-OD2	5.25	123.03	118.30
1	B	515	ASP	CB-CG-OD2	5.23	123.01	118.30
1	B	243	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	681	ASP	CB-CG-OD2	5.22	122.99	118.30
1	A	230	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	678	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	329	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	104	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	133	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	367	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	110	ASP	CB-CG-OD2	5.18	122.97	118.30
1	A	65	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	438	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	488	ASP	CB-CG-OD2	5.16	122.95	118.30
1	A	515	ASP	CB-CG-OD2	5.14	122.92	118.30
1	B	274	ASP	CB-CG-OD2	5.11	122.90	118.30
1	B	681	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	729	ASP	CB-CG-OD2	5.11	122.90	118.30
1	B	535	ASP	CB-CG-OD2	5.11	122.89	118.30
1	B	200	ASP	CB-CG-OD2	5.09	122.89	118.30
1	B	47	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	331	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	501	ASP	CB-CG-OD2	5.08	122.87	118.30
1	B	297	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	390	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	496	ASP	CB-CG-OD2	5.03	122.83	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	556	ASP	CB-CG-OD2	5.03	122.83	118.30
1	B	496	ASP	CB-CG-OD2	5.03	122.83	118.30
1	B	326	ASP	CB-CG-OD2	5.02	122.81	118.30
1	B	588	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	581	ARG	Peptide

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	5964	0	5683	271	3
1	B	5926	0	5650	314	3
2	A	28	0	26	1	0
2	B	28	0	26	1	0
3	A	268	0	0	26	0
3	B	204	0	0	16	2
All	All	12418	0	11385	573	5

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 25.

All (573) 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:517:ILE:HG21	1:A:612:GLN:NE2	1.28	1.45
1:A:517:ILE:CG2	1:A:612:GLN:HE22	1.37	1.36
1:A:198:ILE:HD11	1:A:211:TYR:CE2	1.73	1.22
1:B:544:LEU:HD21	1:B:606:GLN:NE2	1.56	1.20
1:A:150:ASN:ND2	3:A:1095:HOH:O	1.71	1.17
1:A:620:ASP:OD2	1:A:623:ARG:NH1	1.77	1.16

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ASN:HB3	1:A:92:ASN:ND2	1.59	1.13
1:B:81:ALA:O	1:B:492:ARG:NH2	1.81	1.13
1:B:357:PHE:CZ	1:B:551:CYS:HB2	1.86	1.10
1:A:160:VAL:CG2	1:A:219:ASN:O	2.01	1.09
1:B:484:SER:O	1:B:488:ASP:HA	1.53	1.09
1:B:83:TYR:O	1:B:492:ARG:CZ	2.00	1.08
1:B:350:THR:HG23	1:B:351:THR:HG23	1.36	1.06
1:A:74:ASN:HB3	1:A:92:ASN:CG	1.75	1.03
1:A:198:ILE:HD11	1:A:211:TYR:CZ	1.94	1.03
1:B:544:LEU:CD2	1:B:606:GLN:NE2	2.22	1.03
1:A:95:PHE:HA	1:A:98:PHE:HB2	1.40	1.01
1:A:198:ILE:CD1	1:A:211:TYR:CZ	2.46	0.99
1:B:519:LEU:HD21	1:B:612:GLN:NE2	1.77	0.99
1:A:623:ARG:HG3	1:A:623:ARG:HH11	1.26	0.98
1:A:198:ILE:CD1	1:A:211:TYR:CE2	2.46	0.98
1:A:94:THR:HG21	1:A:102:ILE:HD12	1.45	0.98
1:B:505:GLN:HE21	1:B:505:GLN:HA	1.26	0.97
1:B:749:GLN:NE2	3:B:931:HOH:O	1.97	0.96
1:A:724:VAL:HG12	1:B:746:THR:CG2	1.96	0.96
1:B:685:ASN:ND2	3:B:1022:HOH:O	1.99	0.96
1:A:103:ASN:ND2	1:A:117:GLU:OE1	1.99	0.95
1:A:71:LYS:HD2	1:A:105:TYR:OH	1.67	0.95
1:B:329:ASP:OD2	1:B:343:ARG:NH1	1.98	0.95
1:B:341:VAL:HG22	1:B:342:ALA:H	1.31	0.94
1:B:514:LEU:C	1:B:514:LEU:HD23	1.87	0.94
1:B:731:GLN:NE2	3:B:880:HOH:O	2.02	0.93
1:B:405:ILE:HD13	1:B:429:ARG:HD3	1.49	0.93
1:B:244:GLU:OE2	3:B:863:HOH:O	1.88	0.91
1:A:538:LYS:O	1:A:618:PHE:HA	1.72	0.90
1:A:135:TYR:OH	1:A:140:ARG:HA	1.70	0.90
1:A:160:VAL:HG21	1:A:219:ASN:O	1.71	0.90
1:A:237:GLU:OE1	1:B:251:THR:HG22	1.71	0.90
1:A:724:VAL:HG12	1:B:746:THR:HG22	1.54	0.89
1:A:176:ILE:HD12	1:A:183:TYR:HE2	1.36	0.89
1:A:72:GLN:O	1:A:73:GLU:HG2	1.72	0.89
1:B:492:ARG:HG2	3:B:939:HOH:O	1.70	0.89
1:B:519:LEU:HD21	1:B:612:GLN:HE21	1.35	0.88
1:A:660:GLU:HG2	3:A:959:HOH:O	1.71	0.88
1:A:74:ASN:HB3	1:A:92:ASN:HD21	1.34	0.88
1:B:514:LEU:O	1:B:514:LEU:HD23	1.73	0.88
1:B:487:ASN:HB2	1:B:489:LYS:HZ2	1.39	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:ILE:HD12	1:A:419:SER:HA	1.55	0.87
1:A:762:CYS:HB2	3:A:1115:HOH:O	1.75	0.87
1:A:160:VAL:HG22	1:A:219:ASN:O	1.73	0.87
1:B:486:VAL:HG12	1:B:487:ASN:N	1.90	0.86
1:A:726:VAL:HG12	1:A:728:VAL:HG23	1.56	0.86
1:B:459:VAL:HG12	1:B:470:LEU:HD23	1.58	0.85
1:B:83:TYR:O	1:B:492:ARG:NH1	2.09	0.85
1:A:65:ASP:OD1	3:A:1097:HOH:O	1.94	0.85
1:A:94:THR:HG21	1:A:102:ILE:CD1	2.07	0.85
1:B:326:ASP:OD2	1:B:339:CYS:HB3	1.77	0.85
1:A:749:GLN:O	1:A:753:THR:HG23	1.76	0.84
1:A:74:ASN:HB3	1:A:92:ASN:OD1	1.76	0.84
1:A:387:PHE:CE2	1:A:394:CYS:HB3	2.13	0.84
1:B:65:ASP:OD1	1:B:466:LYS:HD2	1.78	0.84
1:B:505:GLN:NE2	1:B:505:GLN:HA	1.90	0.84
1:A:678:ASP:OD1	3:A:1076:HOH:O	1.97	0.83
1:A:74:ASN:CB	1:A:92:ASN:ND2	2.42	0.83
1:A:660:GLU:OE2	3:A:959:HOH:O	1.97	0.83
1:B:139:LYS:O	1:B:141:GLN:N	2.12	0.82
1:B:487:ASN:HB2	1:B:489:LYS:NZ	1.93	0.82
1:A:321:ASN:H	1:A:321:ASN:HD22	1.25	0.82
1:B:203:TYR:HA	1:B:207:VAL:HG13	1.62	0.82
1:A:765:LEU:HB2	1:A:766:PRO:HD3	1.61	0.82
1:B:243:ASP:OD2	3:B:1058:HOH:O	1.96	0.82
1:A:438:ASP:OD2	1:A:440:THR:HB	1.79	0.81
1:B:544:LEU:CD2	1:B:606:GLN:HE21	1.93	0.81
1:A:236:ILE:HD13	1:A:237:GLU:N	1.96	0.81
1:A:291:ALA:O	1:A:295:ILE:HG13	1.79	0.81
1:A:584:GLY:O	1:A:586:GLN:NE2	2.15	0.80
1:B:463:LYS:HG2	1:B:464:GLU:HG2	1.62	0.80
1:A:135:TYR:HE1	1:A:140:ARG:O	1.64	0.80
1:A:357:PHE:CZ	1:A:551:CYS:HB2	2.17	0.80
1:B:180:LEU:HB3	1:B:181:PRO:CD	2.12	0.80
1:B:544:LEU:HD21	1:B:606:GLN:HE22	1.45	0.80
1:B:414:TYR:CE1	1:B:433:LYS:HE3	2.17	0.79
1:A:455:GLN:HB2	1:A:557:THR:HG21	1.64	0.79
1:A:623:ARG:NH1	1:A:623:ARG:HG3	1.95	0.79
1:B:314:GLN:OE1	1:B:373:LYS:NZ	2.15	0.79
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.65	0.79
1:A:198:ILE:HD11	1:A:211:TYR:HE2	1.48	0.79
1:A:463:LYS:HB2	1:A:463:LYS:NZ	1.99	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:ASP:OD2	1:B:463:LYS:O	2.00	0.78
1:B:456:TYR:HB2	1:B:557:THR:HG22	1.65	0.78
1:A:736:THR:HG21	1:B:717:ALA:O	1.83	0.78
1:B:179:ASN:C	1:B:179:ASN:HD22	1.87	0.78
1:A:367:ASP:OD2	3:A:981:HOH:O	2.02	0.78
1:A:346:ILE:HD11	1:A:348:MET:CE	2.14	0.78
1:B:113:PHE:HE2	1:B:162:HIS:HD2	1.32	0.77
1:A:123:GLN:HB3	1:A:127:SER:HB3	1.65	0.77
1:B:519:LEU:HD13	1:B:608:GLU:OE1	1.84	0.77
1:B:183:TYR:HE1	1:B:279:VAL:HG12	1.50	0.77
1:A:725:ASP:HA	1:B:746:THR:HG21	1.66	0.76
1:A:596:ARG:NE	3:A:957:HOH:O	2.12	0.76
1:B:190:LYS:HD2	1:B:193:ILE:HD12	1.68	0.76
1:B:273:THR:O	1:B:276:LEU:CD2	2.33	0.76
1:A:131:SER:OG	1:A:150:ASN:OD1	2.01	0.76
1:A:653:VAL:HG21	1:A:755:MET:HE1	1.67	0.76
1:B:287:ILE:CG2	1:B:339:CYS:SG	2.75	0.75
1:A:760:LYS:HE3	1:A:766:PRO:HG3	1.65	0.75
1:A:653:VAL:CG2	1:A:755:MET:HE2	2.17	0.75
1:B:357:PHE:CZ	1:B:551:CYS:CB	2.66	0.75
1:B:519:LEU:CD2	1:B:612:GLN:NE2	2.49	0.75
1:A:653:VAL:CG2	1:A:755:MET:CE	2.65	0.75
1:B:44:THR:HG23	1:B:47:ASP:H	1.52	0.74
1:A:405:ILE:HD12	1:A:419:SER:CA	2.18	0.73
1:A:71:LYS:CD	1:A:105:TYR:OH	2.36	0.73
1:A:74:ASN:CB	1:A:92:ASN:CG	2.54	0.73
1:B:171:ASP:OD1	1:B:186:THR:CG2	2.35	0.73
1:A:198:ILE:CG1	1:A:211:TYR:CE2	2.71	0.73
1:A:135:TYR:CE1	1:A:140:ARG:O	2.41	0.73
1:B:193:ILE:HG22	1:B:194:ILE:HG12	1.69	0.73
1:B:486:VAL:HG12	1:B:487:ASN:H	1.53	0.72
1:B:411:THR:HG22	1:B:414:TYR:H	1.51	0.72
1:A:236:ILE:C	1:A:236:ILE:HD13	2.09	0.72
1:B:179:ASN:O	1:B:179:ASN:ND2	2.21	0.72
1:B:243:ASP:CG	3:B:1058:HOH:O	2.26	0.72
1:B:60:LEU:HD11	1:B:469:GLN:OE1	1.90	0.72
1:B:135:TYR:CZ	1:B:142:LEU:HD12	2.25	0.72
1:A:343:ARG:HG3	1:A:389:ILE:O	1.91	0.71
1:B:113:PHE:HE2	1:B:162:HIS:CD2	2.07	0.71
1:A:724:VAL:CG1	1:B:746:THR:HG22	2.20	0.71
1:B:613:PHE:O	1:B:616:MET:HG3	1.90	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:ILE:HD13	1:B:429:ARG:CD	2.21	0.70
1:A:434:ILE:HD11	1:A:439:TYR:O	1.91	0.70
1:A:317:ARG:NH2	3:A:875:HOH:O	2.25	0.70
1:A:73:GLU:HG3	1:A:74:ASN:N	2.07	0.70
1:A:314:GLN:HE22	1:A:373:LYS:HZ2	1.40	0.70
1:B:156:THR:HG23	1:B:216:TRP:HE1	1.57	0.70
1:B:287:ILE:HG23	1:B:339:CYS:SG	2.32	0.70
1:B:486:VAL:CG1	1:B:487:ASN:N	2.55	0.69
1:B:158:SER:OG	1:B:160:VAL:O	2.09	0.69
1:B:505:GLN:HE21	1:B:505:GLN:CA	1.98	0.69
1:A:117:GLU:HB3	1:A:132:TYR:CE1	2.28	0.69
1:B:597:ARG:HA	1:B:682:HIS:CD2	2.28	0.69
1:A:463:LYS:HB2	1:A:463:LYS:HZ2	1.57	0.69
1:A:653:VAL:HG22	1:A:755:MET:HE2	1.74	0.69
1:B:114:ILE:HG21	1:B:140:ARG:HH12	1.57	0.68
1:B:135:TYR:OH	1:B:142:LEU:HD12	1.94	0.68
1:A:74:ASN:CB	1:A:92:ASN:OD1	2.41	0.68
1:A:314:GLN:HE22	1:A:373:LYS:NZ	1.92	0.68
1:B:431:LEU:HD23	1:B:432:TYR:N	2.09	0.68
1:A:602:GLU:OE2	1:A:631:TYR:OH	2.11	0.67
1:B:180:LEU:HB3	1:B:181:PRO:HD2	1.75	0.67
1:B:663:ASP:O	1:B:667:THR:HG23	1.95	0.67
1:B:243:ASP:OD1	3:B:1058:HOH:O	2.12	0.67
1:A:760:LYS:CE	1:A:766:PRO:HG3	2.25	0.67
1:B:342:ALA:HB1	1:B:391:LYS:HE3	1.74	0.67
1:B:117:GLU:HB3	1:B:132:TYR:CE1	2.31	0.67
1:A:198:ILE:HG12	1:A:199:THR:N	2.09	0.66
1:A:244:GLU:OE2	3:A:1116:HOH:O	2.13	0.66
1:A:143:ILE:CD1	1:A:178:PRO:HB2	2.25	0.66
1:A:322:TYR:HD2	1:A:348:MET:HG2	1.59	0.66
1:B:341:VAL:HG22	1:B:342:ALA:N	2.08	0.66
1:A:493:VAL:O	3:A:997:HOH:O	2.13	0.66
1:B:65:ASP:OD1	1:B:466:LYS:CD	2.43	0.65
1:B:102:ILE:HD13	1:B:105:TYR:OH	1.96	0.65
1:A:57:LEU:O	3:A:992:HOH:O	2.13	0.65
1:B:156:THR:HG21	1:B:214:LEU:HD11	1.78	0.65
1:A:405:ILE:HD13	1:A:418:ILE:HG22	1.79	0.65
1:A:346:ILE:H	1:A:392:LYS:HZ1	1.44	0.65
1:A:518:ILE:O	1:A:518:ILE:HG13	1.94	0.65
1:A:114:ILE:CG2	1:A:135:TYR:HB3	2.27	0.65
1:A:198:ILE:CD1	1:A:211:TYR:OH	2.44	0.65

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:520:ASN:O	1:B:521:GLU:HB2	1.95	0.65
1:A:571:GLU:OE2	3:A:917:HOH:O	2.14	0.65
1:A:73:GLU:HG3	1:A:74:ASN:H	1.62	0.64
1:A:237:GLU:OE1	1:B:251:THR:CG2	2.44	0.64
1:A:346:ILE:HD11	1:A:348:MET:HE3	1.78	0.64
1:B:597:ARG:HD3	1:B:600:THR:OG1	1.97	0.64
1:B:544:LEU:HD21	1:B:606:GLN:HE21	1.52	0.64
1:B:431:LEU:HD22	1:B:445:LEU:HD12	1.79	0.64
1:B:402:TRP:CD1	1:B:421:GLU:HG3	2.32	0.64
1:B:411:THR:HG23	1:B:413:ASP:H	1.62	0.64
1:B:663:ASP:O	1:B:667:THR:CG2	2.45	0.64
1:A:63:ILE:HD11	1:A:67:GLU:HB2	1.80	0.64
1:A:198:ILE:HD12	1:A:211:TYR:CZ	2.33	0.63
1:A:346:ILE:HD11	1:A:348:MET:HE2	1.80	0.63
1:A:124:TRP:H	1:A:127:SER:HB3	1.63	0.63
1:B:544:LEU:CD2	1:B:606:GLN:HE22	2.02	0.63
1:A:550:PRO:O	1:A:551:CYS:CB	2.47	0.63
1:A:726:VAL:O	1:A:726:VAL:CG1	2.46	0.63
1:B:610:ALA:O	1:B:614:SER:HB2	1.98	0.63
1:A:236:ILE:HD12	1:A:238:TYR:HD2	1.64	0.63
1:A:471:ARG:HG3	1:A:480:TYR:CE2	2.34	0.63
1:B:83:TYR:O	1:B:492:ARG:NH2	2.32	0.63
1:A:557:THR:HG22	1:A:557:THR:O	1.97	0.63
1:B:557:THR:CG2	1:B:557:THR:O	2.47	0.63
1:B:455:GLN:HB2	1:B:557:THR:HG21	1.79	0.63
1:A:253:ARG:HD2	3:A:960:HOH:O	1.98	0.63
1:A:557:THR:O	1:A:557:THR:CG2	2.46	0.62
1:B:116:LEU:HD12	1:B:133:ASP:O	1.98	0.62
1:A:301:CYS:SG	1:A:316:LEU:HB2	2.39	0.62
1:B:557:THR:O	1:B:557:THR:HG23	1.99	0.62
1:A:653:VAL:HG21	1:A:755:MET:CE	2.28	0.62
1:B:67:GLU:CD	1:B:78:VAL:CG1	2.68	0.62
1:A:726:VAL:HG13	1:A:726:VAL:O	2.00	0.62
1:B:88:VAL:HG11	1:B:91:GLU:HB2	1.82	0.62
1:B:519:LEU:CD1	1:B:608:GLU:OE1	2.46	0.62
1:B:498:SER:O	1:B:502:LYS:HG2	1.99	0.62
1:B:484:SER:O	1:B:488:ASP:CA	2.41	0.62
1:B:128:TYR:HE2	1:B:132:TYR:OH	1.82	0.62
1:B:350:THR:HG23	1:B:351:THR:CG2	2.24	0.61
1:A:94:THR:CG2	1:A:102:ILE:CD1	2.77	0.61
1:B:273:THR:HA	1:B:276:LEU:HD22	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.82	0.61
1:A:761:GLN:NE2	3:A:1115:HOH:O	2.33	0.61
1:B:229:ASN:HB2	3:B:1038:HOH:O	1.99	0.61
1:A:71:LYS:HD2	1:A:105:TYR:HH	1.64	0.61
1:A:236:ILE:CD1	1:A:238:TYR:HD2	2.14	0.61
1:A:198:ILE:HD11	1:A:211:TYR:OH	1.99	0.61
1:A:653:VAL:CG2	1:A:755:MET:HE1	2.30	0.61
1:B:463:LYS:HG2	1:B:464:GLU:OE2	2.01	0.61
1:B:471:ARG:HG2	1:B:480:TYR:CE2	2.35	0.61
1:B:405:ILE:CD1	1:B:429:ARG:HD3	2.26	0.60
1:B:276:LEU:HD23	1:B:276:LEU:N	2.17	0.60
1:B:128:TYR:HE2	1:B:132:TYR:HH	1.50	0.60
1:A:724:VAL:O	1:B:746:THR:HG23	2.00	0.60
1:B:342:ALA:HB1	1:B:391:LYS:CE	2.32	0.60
1:A:653:VAL:HG22	1:A:755:MET:CE	2.29	0.60
1:A:598:LEU:HD13	1:A:659:TRP:CZ2	2.36	0.60
1:B:288:THR:HG22	1:B:289:ALA:O	2.02	0.60
1:B:726:VAL:HG12	1:B:728:VAL:HG23	1.84	0.60
1:B:459:VAL:HG12	1:B:470:LEU:CD2	2.32	0.59
1:B:179:ASN:ND2	1:B:179:ASN:C	2.55	0.59
1:A:517:ILE:HG21	1:A:612:GLN:HE22	0.51	0.59
1:A:198:ILE:HG13	1:A:211:TYR:CE2	2.37	0.59
1:A:74:ASN:C	1:A:92:ASN:ND2	2.55	0.59
1:A:176:ILE:HD12	1:A:183:TYR:CE2	2.28	0.59
1:B:463:LYS:CG	1:B:464:GLU:OE2	2.50	0.59
1:A:41:LYS:HE3	1:A:53:TYR:OH	2.02	0.59
1:A:611:ARG:O	1:A:614:SER:HB2	2.02	0.59
1:A:765:LEU:CB	1:A:766:PRO:HD3	2.29	0.59
1:A:550:PRO:O	1:A:551:CYS:HB2	2.03	0.59
1:A:72:GLN:O	1:A:73:GLU:CG	2.47	0.59
1:B:83:TYR:HB2	1:B:85:ASN:OD1	2.03	0.59
1:A:71:LYS:NZ	1:A:105:TYR:OH	2.35	0.58
1:B:44:THR:HG22	1:B:47:ASP:CG	2.23	0.58
1:A:56:LYS:HD2	3:A:999:HOH:O	2.01	0.58
1:B:171:ASP:OD1	1:B:186:THR:HG23	2.02	0.58
1:B:411:THR:HG22	1:B:414:TYR:N	2.19	0.58
1:B:273:THR:O	1:B:276:LEU:HD22	2.03	0.58
1:A:703:ILE:HD12	1:A:755:MET:CE	2.34	0.58
1:B:402:TRP:NE1	1:B:421:GLU:HG3	2.17	0.58
1:A:405:ILE:CD1	1:A:419:SER:HA	2.31	0.58
1:B:463:LYS:HG2	1:B:464:GLU:CG	2.34	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ILE:HD11	1:A:67:GLU:CB	2.34	0.58
1:B:514:LEU:CD2	1:B:514:LEU:O	2.50	0.58
1:A:758:PHE:O	1:A:761:GLN:HG3	2.03	0.58
1:B:67:GLU:CD	1:B:78:VAL:HG11	2.23	0.58
1:B:498:SER:O	1:B:502:LYS:CG	2.52	0.58
1:A:63:ILE:CD1	1:A:67:GLU:HB2	2.34	0.58
1:B:171:ASP:OD1	1:B:186:THR:HG22	2.03	0.58
1:B:487:ASN:CG	1:B:489:LYS:HZ1	2.07	0.57
1:A:760:LYS:HB3	1:A:766:PRO:CG	2.34	0.57
1:B:308:GLN:OE1	1:B:308:GLN:HA	2.04	0.57
1:B:431:LEU:CD2	1:B:432:TYR:N	2.68	0.57
1:B:402:TRP:CE2	1:B:421:GLU:HG3	2.40	0.57
1:B:518:ILE:HG13	1:B:518:ILE:O	2.04	0.57
1:B:110:ASP:OD1	1:B:112:GLN:HG3	2.03	0.57
1:B:146:GLU:O	1:B:175:LYS:HE3	2.05	0.57
1:A:114:ILE:HG23	1:A:135:TYR:HB3	1.86	0.57
1:B:470:LEU:HD12	1:B:483:HIS:NE2	2.20	0.57
1:A:143:ILE:HD11	1:A:178:PRO:HB2	1.87	0.56
1:A:135:TYR:OH	1:A:140:ARG:CA	2.48	0.56
1:B:640:LEU:HD22	1:B:698:VAL:HG11	1.87	0.56
1:B:745:SER:O	1:B:749:GLN:NE2	2.39	0.56
1:A:387:PHE:CE2	1:A:394:CYS:CB	2.87	0.56
1:B:287:ILE:HG21	1:B:339:CYS:SG	2.45	0.56
1:B:103:ASN:ND2	1:B:117:GLU:OE1	2.32	0.56
1:B:128:TYR:CE2	1:B:132:TYR:OH	2.59	0.56
1:B:184:ARG:HD3	1:B:187:TRP:CZ2	2.40	0.56
1:A:235:LEU:N	1:A:235:LEU:HD22	2.21	0.56
1:A:724:VAL:CG1	1:B:746:THR:CG2	2.78	0.56
1:A:703:ILE:HD12	1:A:755:MET:HE3	1.88	0.55
1:B:273:THR:C	1:B:276:LEU:HD22	2.26	0.55
1:A:96:ASP:O	1:A:142:LEU:CD1	2.55	0.55
1:A:71:LYS:CD	1:A:105:TYR:HH	2.19	0.55
1:A:660:GLU:CG	3:A:959:HOH:O	2.42	0.55
1:A:463:LYS:HD2	3:A:1097:HOH:O	2.05	0.55
1:B:471:ARG:CG	1:B:480:TYR:CE2	2.90	0.55
1:B:371:PHE:CE2	1:B:387:PHE:CD1	2.95	0.55
1:B:514:LEU:CD2	1:B:514:LEU:C	2.62	0.55
1:A:365:THR:HB	3:A:981:HOH:O	2.06	0.55
1:A:435:GLN:O	1:A:439:TYR:HA	2.07	0.55
1:B:342:ALA:CB	1:B:391:LYS:HE3	2.37	0.55
1:B:487:ASN:CB	1:B:489:LYS:NZ	2.69	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:749:GLN:O	1:A:753:THR:CG2	2.53	0.54
1:A:594:ILE:HD12	1:A:598:LEU:CD2	2.37	0.54
1:A:219:ASN:N	1:A:220:GLY:HA2	2.21	0.54
1:B:453:ARG:HG3	1:B:476:GLY:HA3	1.89	0.54
1:A:325:MET:HE1	1:A:327:ILE:HD11	1.90	0.54
1:B:544:LEU:CG	1:B:606:GLN:HE22	2.20	0.54
1:B:346:ILE:HG12	3:B:899:HOH:O	2.06	0.54
1:B:519:LEU:CD2	1:B:612:GLN:HE21	2.12	0.54
1:B:544:LEU:HD23	1:B:606:GLN:HE21	1.70	0.54
1:B:563:TRP:CH2	1:B:755:MET:HE2	2.43	0.54
1:B:184:ARG:HD3	1:B:187:TRP:CE2	2.43	0.54
1:B:169:ASN:O	1:B:170:ASN:HB2	2.08	0.54
1:B:36:THR:CG2	3:B:1026:HOH:O	2.56	0.54
1:A:346:ILE:CD1	1:A:348:MET:HG3	2.38	0.53
2:B:855:NAG:O3	3:B:1017:HOH:O	2.19	0.53
1:B:391:LYS:O	1:B:392:LYS:HB2	2.08	0.53
1:B:60:LEU:CD1	1:B:469:GLN:OE1	2.57	0.53
1:A:357:PHE:CZ	1:A:551:CYS:CB	2.91	0.53
1:A:291:ALA:O	1:A:295:ILE:CG1	2.52	0.53
1:B:180:LEU:CB	1:B:181:PRO:CD	2.80	0.53
1:B:61:ARG:NH2	1:B:105:TYR:O	2.41	0.53
1:A:206:GLU:OE2	1:A:663:ASP:OD1	2.25	0.53
1:B:276:LEU:HD23	1:B:276:LEU:H	1.72	0.53
1:B:56:LYS:HD3	1:B:495:GLU:OE1	2.08	0.53
1:B:639:VAL:O	1:B:642:SER:HB2	2.09	0.53
1:A:760:LYS:HB3	1:A:766:PRO:CD	2.38	0.53
1:B:387:PHE:CE2	1:B:394:CYS:HB3	2.44	0.53
1:A:198:ILE:HD12	1:A:211:TYR:OH	2.09	0.53
1:A:322:TYR:CD2	1:A:348:MET:HG2	2.43	0.53
1:A:546:VAL:HG21	1:A:635:VAL:HG11	1.90	0.53
1:B:341:VAL:HG13	1:B:342:ALA:N	2.24	0.53
1:A:242:SER:HB3	1:A:246:LEU:HD12	1.90	0.53
1:A:75:ASN:HB2	1:A:90:LEU:O	2.09	0.52
1:A:659:TRP:CE3	1:A:667:THR:HG23	2.44	0.52
1:A:232:GLU:O	1:A:232:GLU:OE1	2.27	0.52
1:A:219:ASN:HB2	1:A:308:GLN:HG2	1.90	0.52
1:A:486:VAL:HG12	1:A:487:ASN:ND2	2.24	0.52
1:A:726:VAL:CG1	1:A:728:VAL:HG23	2.33	0.52
1:B:67:GLU:HG3	1:B:79:PHE:O	2.09	0.52
1:A:74:ASN:CB	1:A:92:ASN:HD21	2.14	0.52
1:A:236:ILE:CD1	1:A:236:ILE:C	2.78	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:THR:CG2	1:A:294:LEU:HD11	2.40	0.52
1:A:331:ASP:HB2	1:A:338:ASN:HD21	1.75	0.52
1:A:760:LYS:HB3	1:A:766:PRO:HD3	1.90	0.52
1:B:431:LEU:HD23	1:B:432:TYR:H	1.73	0.52
1:B:698:VAL:HG12	1:B:699:GLU:N	2.25	0.51
1:A:305:TRP:CZ2	1:A:311:ILE:HD12	2.46	0.51
1:B:594:ILE:CD1	1:B:602:GLU:HG3	2.41	0.51
1:B:357:PHE:O	1:B:358:ARG:HB3	2.11	0.51
1:A:177:GLU:HB2	1:A:180:LEU:HD13	1.91	0.51
1:A:760:LYS:NZ	1:A:766:PRO:HG3	2.25	0.51
1:B:273:THR:CA	1:B:276:LEU:HD22	2.40	0.51
1:B:91:GLU:HG2	1:B:92:ASN:OD1	2.11	0.51
1:A:73:GLU:CG	1:A:74:ASN:N	2.72	0.51
1:B:154:TRP:CE2	1:B:212:SER:HB2	2.46	0.51
1:A:325:MET:HE2	1:A:345:HIS:ND1	2.26	0.51
1:A:97:GLU:OE1	1:A:133:ASP:OD1	2.29	0.51
1:A:463:LYS:HG2	1:A:464:GLU:HG2	1.92	0.51
1:B:549:GLY:O	1:B:552:SER:HB3	2.11	0.51
1:A:73:GLU:CG	1:A:74:ASN:H	2.23	0.51
1:A:340:LEU:N	1:A:340:LEU:HD12	2.26	0.51
1:A:221:THR:O	1:A:273:THR:HB	2.10	0.50
1:A:519:LEU:O	1:A:520:ASN:HB2	2.11	0.50
1:B:357:PHE:CE1	1:B:551:CYS:CB	2.95	0.50
1:B:44:THR:O	1:B:47:ASP:HB2	2.11	0.50
1:B:67:GLU:HG2	1:B:78:VAL:HG13	1.93	0.50
1:A:179:ASN:O	1:A:180:LEU:HD12	2.11	0.50
1:A:198:ILE:HG13	1:A:211:TYR:CD2	2.46	0.50
1:B:696:LYS:HG3	1:B:728:VAL:HG22	1.94	0.50
1:B:276:LEU:O	1:B:276:LEU:HG	2.11	0.50
1:A:55:LEU:CD1	1:A:561:LEU:HD12	2.42	0.50
1:B:582:GLY:CA	1:B:590:ILE:O	2.60	0.50
1:A:626:ILE:O	1:A:650:GLY:HA2	2.11	0.49
1:B:626:ILE:O	1:B:650:GLY:HA2	2.12	0.49
1:A:109:PRO:HG2	1:A:158:SER:O	2.11	0.49
1:A:703:ILE:CD1	1:A:755:MET:HE3	2.43	0.49
1:A:501:ASP:O	1:A:505:GLN:HG2	2.12	0.49
1:A:232:GLU:HB3	1:A:262:VAL:HG11	1.93	0.49
1:B:330:TYR:HB2	1:B:337:TRP:CH2	2.47	0.49
1:A:113:PHE:CE1	1:A:178:PRO:HG2	2.47	0.49
1:A:331:ASP:HB2	1:A:338:ASN:ND2	2.27	0.49
1:A:405:ILE:CD1	1:A:419:SER:CA	2.90	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:664:SER:O	1:B:668:GLU:HB2	2.12	0.49
1:A:317:ARG:HG2	3:A:1019:HOH:O	2.12	0.49
1:B:176:ILE:O	1:B:177:GLU:HG3	2.13	0.49
1:B:415:LEU:C	1:B:415:LEU:HD23	2.34	0.48
1:B:550:PRO:O	1:B:551:CYS:CB	2.59	0.48
1:B:65:ASP:OD2	1:B:464:GLU:HB2	2.13	0.48
1:B:667:THR:O	1:B:671:MET:HB2	2.12	0.48
1:A:262:VAL:HA	3:A:1005:HOH:O	2.12	0.48
1:A:180:LEU:HB3	1:A:181:PRO:HD2	1.94	0.48
1:B:90:LEU:HD22	1:B:140:ARG:HH21	1.77	0.48
1:A:708:ASP:OD2	1:A:740:HIS:HD2	1.96	0.48
1:A:94:THR:O	1:A:94:THR:HG22	2.14	0.48
1:B:110:ASP:CG	1:B:112:GLN:HG3	2.34	0.48
1:B:41:LYS:NZ	1:B:47:ASP:OD1	2.47	0.48
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.48	0.48
1:B:372:TYR:OH	1:B:436:LEU:HD11	2.14	0.48
1:A:463:LYS:HB2	1:A:463:LYS:HZ3	1.77	0.48
1:B:91:GLU:O	1:B:92:ASN:C	2.52	0.48
1:B:372:TYR:CZ	1:B:386:TYR:HD1	2.32	0.48
1:B:627:TRP:HB2	1:B:651:ILE:HB	1.96	0.48
1:B:55:LEU:HD23	1:B:500:LEU:CD2	2.43	0.48
1:A:110:ASP:OD2	1:A:162:HIS:ND1	2.47	0.48
1:A:618:PHE:CD1	1:A:619:VAL:HG23	2.49	0.47
1:B:698:VAL:CG1	1:B:699:GLU:N	2.77	0.47
1:B:435:GLN:HG3	1:B:441:LYS:HB3	1.95	0.47
1:B:542:LEU:HD12	1:B:619:VAL:CG1	2.44	0.47
1:B:519:LEU:HD13	1:B:608:GLU:CD	2.34	0.47
1:A:405:ILE:HD13	1:A:429:ARG:HD3	1.95	0.47
1:B:156:THR:HG21	1:B:214:LEU:CD1	2.44	0.47
1:A:96:ASP:O	1:A:142:LEU:HD11	2.15	0.47
1:A:346:ILE:HD12	1:A:346:ILE:C	2.35	0.47
1:B:145:GLU:O	1:B:147:ARG:HG3	2.13	0.47
1:A:321:ASN:H	1:A:321:ASN:ND2	2.04	0.47
1:B:411:THR:CG2	1:B:414:TYR:H	2.22	0.47
1:B:726:VAL:O	1:B:726:VAL:CG1	2.63	0.47
1:A:517:ILE:HG22	1:A:518:ILE:N	2.28	0.47
1:B:350:THR:HG21	3:B:866:HOH:O	2.15	0.47
1:B:341:VAL:HG13	1:B:343:ARG:H	1.80	0.47
1:B:171:ASP:CB	1:B:186:THR:HG22	2.43	0.47
1:B:542:LEU:HD12	1:B:619:VAL:HG11	1.97	0.47
1:B:145:GLU:HG2	1:B:145:GLU:H	1.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:VAL:O	1:A:642:SER:HB2	2.15	0.47
1:B:693:GLU:O	1:B:696:LYS:HD3	2.15	0.47
1:A:60:LEU:HD12	1:A:60:LEU:O	2.15	0.47
1:A:598:LEU:CD1	1:A:659:TRP:CZ2	2.98	0.47
1:A:236:ILE:HD12	1:A:238:TYR:CD2	2.47	0.47
1:B:556:ASP:C	1:B:556:ASP:OD1	2.54	0.47
1:B:514:LEU:HD21	1:B:525:TRP:CZ3	2.51	0.46
1:A:135:TYR:CE1	1:A:140:ARG:C	2.89	0.46
1:A:179:ASN:C	1:A:180:LEU:HD12	2.35	0.46
1:A:505:GLN:HE21	1:A:505:GLN:HA	1.79	0.46
1:B:219:ASN:HB3	1:B:221:THR:OG1	2.16	0.46
1:B:357:PHE:CE2	1:B:551:CYS:HB2	2.46	0.46
1:A:405:ILE:CD1	1:A:418:ILE:HG22	2.44	0.46
1:B:518:ILE:HA	1:B:522:THR:O	2.15	0.46
1:B:36:THR:HG22	3:B:1026:HOH:O	2.15	0.46
1:A:449:LEU:HA	1:A:449:LEU:HD23	1.82	0.46
1:A:346:ILE:H	1:A:392:LYS:NZ	2.12	0.46
1:A:288:THR:HG22	1:A:289:ALA:O	2.15	0.46
1:A:340:LEU:H	1:A:340:LEU:HD12	1.81	0.46
1:B:759:ILE:HA	1:B:759:ILE:HD13	1.80	0.46
1:B:431:LEU:C	1:B:431:LEU:CD2	2.83	0.46
1:A:602:GLU:CD	1:A:631:TYR:HH	2.18	0.46
1:A:325:MET:CE	1:A:345:HIS:ND1	2.78	0.46
1:B:563:TRP:CH2	1:B:755:MET:CE	2.99	0.46
1:B:292:SER:OG	1:B:322:TYR:HE1	1.98	0.46
1:A:446:SER:HB2	1:A:457:TYR:CE1	2.49	0.46
1:B:463:LYS:HG3	1:B:464:GLU:OE2	2.15	0.46
1:B:113:PHE:CE2	1:B:162:HIS:CD2	2.96	0.46
1:B:582:GLY:HA2	1:B:590:ILE:O	2.16	0.46
1:A:317:ARG:CZ	3:A:875:HOH:O	2.62	0.46
1:B:518:ILE:O	1:B:518:ILE:CG1	2.64	0.46
1:B:411:THR:HG23	1:B:413:ASP:N	2.29	0.45
1:B:90:LEU:CD2	1:B:140:ARG:HH21	2.30	0.45
1:B:302:ASP:N	1:B:302:ASP:OD1	2.49	0.45
1:A:113:PHE:CZ	1:A:178:PRO:HG2	2.49	0.45
1:B:44:THR:HG22	1:B:47:ASP:OD1	2.16	0.45
1:B:664:SER:HB2	1:B:668:GLU:OE2	2.16	0.45
1:A:532:PRO:O	1:A:533:HIS:HB2	2.17	0.45
1:B:357:PHE:CE1	1:B:551:CYS:HB3	2.51	0.45
1:B:372:TYR:OH	1:B:436:LEU:CD1	2.64	0.45
1:B:78:VAL:HG23	1:B:89:PHE:HB2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ASP:OD2	1:A:66:HIS:HD2	2.00	0.45
1:A:319:ILE:O	1:A:321:ASN:ND2	2.47	0.45
1:B:330:TYR:HB2	1:B:337:TRP:CZ3	2.52	0.45
1:A:74:ASN:O	1:A:92:ASN:ND2	2.50	0.45
1:A:659:TRP:HE3	1:A:667:THR:HG23	1.82	0.45
1:A:71:LYS:CE	1:A:105:TYR:OH	2.65	0.45
1:B:471:ARG:HG3	1:B:480:TYR:HE2	1.81	0.45
1:B:487:ASN:OD1	1:B:489:LYS:NZ	2.42	0.44
1:B:306:ALA:O	1:B:307:THR:HG22	2.17	0.44
1:B:110:ASP:C	1:B:110:ASP:OD1	2.56	0.44
1:B:435:GLN:HG3	1:B:441:LYS:CB	2.47	0.44
1:A:194:ILE:HD12	2:A:853:NAG:H82	1.99	0.44
1:B:350:THR:HG23	1:B:351:THR:N	2.31	0.44
1:A:301:CYS:SG	1:A:316:LEU:CB	3.05	0.44
1:B:492:ARG:CG	3:B:939:HOH:O	2.46	0.44
1:A:96:ASP:O	1:A:142:LEU:HD12	2.18	0.44
1:A:118:TYR:O	1:A:119:ASN:HB2	2.18	0.44
1:A:94:THR:CG2	1:A:102:ILE:HD11	2.45	0.44
1:B:75:ASN:OD1	1:B:91:GLU:HG3	2.17	0.44
1:B:219:ASN:HB3	1:B:221:THR:H	1.82	0.44
1:B:369:ASN:HB3	1:B:389:ILE:CD1	2.48	0.44
1:B:608:GLU:HA	1:B:611:ARG:HB2	2.00	0.44
1:A:623:ARG:CG	1:A:623:ARG:NH1	2.71	0.44
1:B:550:PRO:O	1:B:551:CYS:HB2	2.17	0.44
1:B:350:THR:CG2	1:B:351:THR:HG23	2.27	0.44
1:B:136:ASP:HB2	1:B:139:LYS:O	2.18	0.44
1:B:165:ALA:HB2	1:B:216:TRP:CZ2	2.52	0.44
1:B:111:GLY:C	1:B:137:LEU:HD12	2.37	0.44
1:A:463:LYS:CB	1:A:463:LYS:NZ	2.69	0.44
1:B:44:THR:CG2	1:B:47:ASP:H	2.26	0.43
1:B:614:SER:OG	1:B:624:ILE:HD11	2.17	0.43
1:B:214:LEU:HD12	1:B:214:LEU:C	2.38	0.43
1:A:143:ILE:CD1	1:A:178:PRO:CB	2.96	0.43
1:A:60:LEU:HD12	1:A:60:LEU:C	2.38	0.43
1:A:724:VAL:HG12	1:B:746:THR:HG21	1.95	0.43
1:B:434:ILE:HA	1:B:441:LYS:O	2.19	0.43
1:A:624:ILE:HG22	1:A:647:PHE:CD1	2.53	0.43
1:A:623:ARG:CG	1:A:623:ARG:HH11	2.09	0.43
1:A:703:ILE:HD12	1:A:755:MET:HE2	2.01	0.43
1:A:532:PRO:O	1:A:533:HIS:CB	2.67	0.43
1:B:466:LYS:HG2	1:B:467:TYR:CE2	2.53	0.43

Continued on next page...

Full wwPDB X-ray Structure Validation Report

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ILE:HG12	1:B:712:HIS:CE1	2.54	0.43
1:A:725:ASP:HA	1:B:746:THR:CG2	2.44	0.43
1:A:669:ARG:HD2	1:A:670:TYR:CZ	2.53	0.43
1:B:69:LEU:HD21	1:B:76:ILE:HG21	2.01	0.43
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.53	0.43
1:B:391:LYS:O	1:B:392:LYS:CB	2.67	0.43
1:B:369:ASN:O	1:B:389:ILE:HG12	2.19	0.43
1:A:303:VAL:HB	1:A:313:LEU:HD23	2.01	0.43
1:A:307:THR:HB	3:A:982:HOH:O	2.18	0.43
1:B:341:VAL:HG13	1:B:343:ARG:N	2.34	0.43
1:B:190:LYS:HD2	1:B:193:ILE:CD1	2.45	0.43
1:B:411:THR:C	1:B:413:ASP:H	2.23	0.42
1:A:706:THR:OG1	1:A:736:THR:HA	2.19	0.42
1:A:424:GLY:O	1:A:426:PRO:HD3	2.18	0.42
1:B:278:SER:HB3	1:B:281:ASN:O	2.19	0.42
1:B:422:TYR:CE1	1:B:423:LYS:HG3	2.54	0.42
1:A:472:CYS:O	1:A:478:PRO:HA	2.19	0.42
1:A:489:LYS:HD3	1:A:489:LYS:HA	1.84	0.42
1:B:669:ARG:HD2	1:B:670:TYR:CZ	2.55	0.42
1:B:180:LEU:CB	1:B:181:PRO:HD3	2.49	0.42
1:A:244:GLU:OE2	1:B:658:ARG:NH2	2.49	0.42
1:B:375:ILE:HD11	1:B:387:PHE:HZ	1.85	0.42
1:B:485:SER:O	1:B:486:VAL:C	2.58	0.42
1:B:60:LEU:CG	1:B:469:GLN:OE1	2.68	0.42
1:B:114:ILE:CG2	1:B:140:ARG:HH12	2.29	0.42
1:B:594:ILE:CD1	1:B:601:PHE:HB2	2.49	0.42
1:B:541:PRO:HG3	1:B:623:ARG:CZ	2.49	0.42
1:A:514:LEU:HD12	1:A:526:TYR:O	2.20	0.42
1:B:563:TRP:CZ3	1:B:755:MET:CE	3.03	0.42
1:A:366:LEU:HD23	1:A:366:LEU:C	2.40	0.42
1:B:88:VAL:CG1	1:B:91:GLU:HB2	2.49	0.42
1:B:341:VAL:CG2	1:B:342:ALA:N	2.77	0.42
1:B:109:PRO:HG2	1:B:158:SER:O	2.20	0.42
1:B:582:GLY:HA3	1:B:591:MET:HA	2.02	0.41
1:A:581:ARG:HA	1:A:582:GLY:HA2	1.75	0.41
1:A:509:MET:HA	1:A:510:PRO:HD3	1.90	0.41
1:B:431:LEU:CD2	1:B:445:LEU:HD12	2.48	0.41
1:B:382:ARG:HH21	1:B:591:MET:HE2	1.85	0.41
1:B:60:LEU:HD12	1:B:60:LEU:O	2.20	0.41
1:B:306:ALA:O	1:B:307:THR:CG2	2.68	0.41
1:B:422:TYR:CD1	1:B:423:LYS:HG3	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:GLY:C	1:A:429:ARG:HG2	2.40	0.41
1:A:317:ARG:NE	3:A:875:HOH:O	2.53	0.41
1:B:594:ILE:HD12	1:B:594:ILE:HA	1.94	0.41
1:B:369:ASN:HB2	1:B:389:ILE:HG12	2.02	0.41
1:B:269:PHE:CE2	1:B:286:GLN:HB2	2.55	0.41
1:B:375:ILE:HD11	1:B:387:PHE:CZ	2.56	0.41
1:A:470:LEU:HD12	1:A:483:HIS:NE2	2.36	0.41
1:B:57:LEU:O	1:B:58:TYR:C	2.58	0.41
1:A:219:ASN:CB	1:A:220:GLY:HA2	2.51	0.41
1:B:156:THR:HG23	1:B:156:THR:O	2.19	0.41
1:B:471:ARG:HG3	1:B:480:TYR:CE2	2.56	0.41
1:A:483:HIS:HD1	1:A:490:GLY:HA2	1.86	0.41
1:B:498:SER:O	1:B:502:LYS:HG3	2.21	0.41
1:B:693:GLU:HA	1:B:726:VAL:HG11	2.03	0.41
1:B:330:TYR:HE2	1:B:332:GLU:HG2	1.86	0.41
1:B:449:LEU:HD23	1:B:449:LEU:HA	1.85	0.41
1:B:237:GLU:HA	1:B:252:VAL:O	2.21	0.41
1:B:158:SER:HB3	1:B:163:LYS:HB3	2.02	0.41
1:A:41:LYS:CE	1:A:53:TYR:OH	2.67	0.41
1:B:422:TYR:O	1:B:423:LYS:HB2	2.20	0.41
1:A:613:PHE:O	1:A:616:MET:HG2	2.21	0.41
1:B:157:TRP:CE3	1:B:164:LEU:HG	2.55	0.41
1:B:369:ASN:HB3	1:B:389:ILE:HD11	2.02	0.41
1:A:259:ALA:HB3	1:A:660:GLU:HA	2.02	0.40
1:B:741:GLY:O	1:B:742:ILE:C	2.60	0.40
1:B:492:ARG:HD3	3:B:939:HOH:O	2.20	0.40
1:B:597:ARG:HA	1:B:682:HIS:NE2	2.35	0.40
1:A:193:ILE:HD12	3:A:1071:HOH:O	2.20	0.40
1:B:452:GLU:H	1:B:452:GLU:HG3	1.71	0.40
1:B:680:LEU:O	1:B:683:TYR:HB2	2.22	0.40
1:A:765:LEU:HA	1:A:765:LEU:HD23	1.79	0.40
1:A:361:GLU:OE1	3:A:855:HOH:O	2.22	0.40
1:A:760:LYS:HE3	1:A:766:PRO:CG	2.45	0.40
1:B:214:LEU:HD12	1:B:214:LEU:O	2.22	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1043:HOH:O	3:B:1054:HOH:O[3_555]	1.53	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:PHE:CZ	1:B:168:TRP:CZ3[1_455]	1.81	0.39
1:A:83:TYR:CD1	1:A:677:GLU:OE1[1_455]	1.89	0.31
1:B:642:SER:O	3:B:1017:HOH:O[1_455]	1.91	0.29
1:A:98:PHE:CZ	1:B:168:TRP:CH2[1_455]	2.12	0.08

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	726/731 (99%)	678 (93%)	45 (6%)	3 (0%)	39	27
1	B	721/731 (99%)	667 (92%)	47 (6%)	7 (1%)	19	7
All	All	1447/1462 (99%)	1345 (93%)	92 (6%)	10 (1%)	26	14

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	ARG
1	B	140	ARG
1	B	341	VAL
1	A	98	PHE
1	B	274	ASP
1	A	73	GLU
1	B	58	TYR
1	B	145	GLU
1	B	520	ASN
1	B	486	VAL

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	653/655 (100%)	596 (91%)	57 (9%)	13	5
1	B	647/655 (99%)	595 (92%)	52 (8%)	15	6
All	All	1300/1310 (99%)	1191 (92%)	109 (8%)	14	5

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	SER
1	A	41	LYS
1	A	54	ARG
1	A	61	ARG
1	A	65	ASP
1	A	75	ASN
1	A	92	ASN
1	A	95	PHE
1	A	116	LEU
1	A	190	LYS
1	A	193	ILE
1	A	198	ILE
1	A	209	SER
1	A	214	LEU
1	A	219	ASN
1	A	230	ASP
1	A	232	GLU
1	A	236	ILE
1	A	246	LEU
1	A	250	LYS
1	A	270	VAL
1	A	273	THR
1	A	277	SER
1	A	302	ASP
1	A	308	GLN
1	A	314	GLN
1	A	321	ASN
1	A	333	SER
1	A	346	ILE
1	A	349	SER
1	A	367	ASP
1	A	376	SER
1	A	385	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	392	LYS
1	A	414	TYR
1	A	440	THR
1	A	472	CYS
1	A	488	ASP
1	A	489	LYS
1	A	513	LYS
1	A	518	ILE
1	A	521	GLU
1	A	537	SER
1	A	542	LEU
1	A	543	LEU
1	A	566	TYR
1	A	602	GLU
1	A	612	GLN
1	A	623	ARG
1	A	642	SER
1	A	684	ARG
1	A	693	GLU
1	A	699	GLU
1	A	704	HIS
1	A	736	THR
1	A	749	GLN
1	A	753	THR
1	B	36	THR
1	B	51	ASN
1	B	54	ARG
1	B	59	SER
1	B	69	LEU
1	B	72	GLN
1	B	85	ASN
1	B	116	LEU
1	B	145	GLU
1	B	162	HIS
1	B	179	ASN
1	B	186	THR
1	B	207	VAL
1	B	237	GLU
1	B	251	THR
1	B	263	ASN
1	B	266	VAL
1	B	270	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	274	ASP
1	B	319	ILE
1	B	326	ASP
1	B	334	SER
1	B	358	ARG
1	B	360	SER
1	B	361	GLU
1	B	385	CYS
1	B	399	LYS
1	B	431	LEU
1	B	472	CYS
1	B	484	SER
1	B	485	SER
1	B	488	ASP
1	B	502	LYS
1	B	505	GLN
1	B	506	ASN
1	B	514	LEU
1	B	517	ILE
1	B	543	LEU
1	B	554	LYS
1	B	557	THR
1	B	597	ARG
1	B	602	GLU
1	B	608	GLU
1	B	614	SER
1	B	616	MET
1	B	642	SER
1	B	667	THR
1	B	677	GLU
1	B	701	LEU
1	B	746	THR
1	B	749	GLN
1	B	759	ILE

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	66	HIS
1	A	92	ASN
1	A	112	GLN
1	A	179	ASN

Continued from previous page...

Mol	Chain	Res	Type
1	A	263	ASN
1	A	314	GLN
1	A	321	ASN
1	A	338	ASN
1	A	383	HIS
1	A	388	GLN
1	A	435	GLN
1	A	487	ASN
1	A	505	GLN
1	A	572	ASN
1	A	595	ASN
1	A	612	GLN
1	A	740	HIS
1	B	51	ASN
1	B	112	GLN
1	B	119	ASN
1	B	179	ASN
1	B	263	ASN
1	B	298	HIS
1	B	320	GLN
1	B	338	ASN
1	B	383	HIS
1	B	435	GLN
1	B	455	GLN
1	B	505	GLN
1	B	606	GLN
1	B	612	GLN
1	B	712	HIS
1	B	749	GLN

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)

4 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	NAG	A	851	1	14,14,15	0.58	0	15,19,21	0.77	0
2	NAG	A	853	1	14,14,15	0.52	0	15,19,21	0.82	1 (6%)
2	NAG	B	852	1	14,14,15	0.54	0	15,19,21	0.67	0
2	NAG	B	855	1	14,14,15	0.54	0	15,19,21	0.66	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	851	1	-	0/6/23/26	0/1/1/1
2	NAG	A	853	1	-	0/6/23/26	0/1/1/1
2	NAG	B	852	1	-	0/6/23/26	0/1/1/1
2	NAG	B	855	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	853	NAG	C2-N2-C7	-2.11	120.32	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	853	NAG	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	855	NAG	1	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, 95th 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	728/731 (99%)	1.09	122 (16%)	2	2	14, 40, 55, 60	0
1	B	725/731 (99%)	1.31	147 (20%)	1	1	17, 43, 64, 72	0
All	All	1453/1462 (99%)	1.20	269 (18%)	2	2	14, 41, 59, 72	0

All (269) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	96	ASP	11.4
1	A	95	PHE	11.0
1	B	340	LEU	10.9
1	B	279	VAL	9.3
1	A	766	PRO	9.1
1	B	278	SER	8.8
1	B	436	LEU	7.9
1	A	94	THR	7.4
1	A	98	PHE	6.7
1	B	766	PRO	6.5
1	B	99	GLY	6.4
1	A	280	THR	6.2
1	B	137	LEU	6.1
1	B	342	ALA	5.9
1	A	74	ASN	5.9
1	B	334	SER	5.8
1	B	138	ASN	5.3
1	A	279	VAL	5.3
1	B	517	ILE	5.3
1	A	278	SER	5.3
1	B	367	ASP	5.2
1	A	414	TYR	5.2
1	B	74	ASN	5.2
1	B	140	ARG	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	336	ARG	5.1
1	B	734	TRP	5.0
1	B	713	PHE	4.9
1	B	392	LYS	4.8
1	B	393	ASP	4.8
1	A	734	TRP	4.7
1	B	391	LYS	4.7
1	B	378	GLU	4.7
1	B	339	CYS	4.7
1	B	521	GLU	4.6
1	B	341	VAL	4.6
1	A	125	ARG	4.6
1	A	127	SER	4.6
1	A	140	ARG	4.6
1	A	97	GLU	4.5
1	A	584	GLY	4.4
1	B	142	LEU	4.4
1	B	394	CYS	4.4
1	B	449	LEU	4.4
1	B	183	TYR	4.2
1	B	280	THR	4.2
1	B	519	LEU	4.2
1	B	36	THR	4.2
1	B	83	TYR	4.2
1	A	626	ILE	4.1
1	A	333	SER	4.1
1	B	520	ASN	4.1
1	B	92	ASN	4.1
1	B	176	ILE	4.1
1	A	105	TYR	4.0
1	A	449	LEU	4.0
1	B	66	HIS	4.0
1	A	73	GLU	3.9
1	B	276	LEU	3.9
1	A	99	GLY	3.8
1	A	520	ASN	3.8
1	B	274	ASP	3.8
1	A	301	CYS	3.8
1	A	128	TYR	3.8
1	A	551	CYS	3.8
1	B	703	ILE	3.7
1	B	366	LEU	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	703	ILE	3.7
1	B	114	ILE	3.7
1	B	717	ALA	3.7
1	B	37	ALA	3.6
1	A	274	ASP	3.6
1	B	702	LEU	3.6
1	A	518	ILE	3.6
1	B	91	GLU	3.6
1	A	277	SER	3.5
1	B	134	ILE	3.5
1	A	126	HIS	3.5
1	B	608	GLU	3.5
1	B	67	GLU	3.5
1	A	122	LYS	3.5
1	B	667	THR	3.5
1	B	488	ASP	3.5
1	B	452	GLU	3.4
1	B	301	CYS	3.4
1	B	463	LYS	3.4
1	B	701	LEU	3.4
1	A	123	GLN	3.4
1	A	120	TYR	3.4
1	B	471	ARG	3.3
1	B	115	LEU	3.3
1	B	136	ASP	3.3
1	B	523	LYS	3.3
1	B	180	LEU	3.3
1	B	350	THR	3.3
1	A	146	GLU	3.3
1	A	350	THR	3.2
1	A	124	TRP	3.2
1	B	82	GLU	3.2
1	B	145	GLU	3.2
1	A	537	SER	3.2
1	B	302	ASP	3.1
1	A	198	ILE	3.1
1	A	275	SER	3.1
1	A	701	LEU	3.1
1	B	438	ASP	3.1
1	B	120	TYR	3.0
1	A	281	ASN	3.0
1	A	539	LYS	3.0

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	367	ASP	3.0
1	A	659	TRP	3.0
1	B	652	ALA	3.0
1	A	702	LEU	3.0
1	B	172	ILE	3.0
1	B	177	GLU	3.0
1	B	73	GLU	3.0
1	A	640	LEU	3.0
1	B	522	THR	2.9
1	A	268	PHE	2.9
1	A	92	ASN	2.9
1	B	338	ASN	2.9
1	B	551	CYS	2.9
1	A	713	PHE	2.9
1	A	576	ALA	2.9
1	A	270	VAL	2.9
1	A	145	GLU	2.9
1	B	487	ASN	2.8
1	B	437	SER	2.8
1	B	445	LEU	2.8
1	A	544	LEU	2.8
1	A	466	LYS	2.8
1	B	144	THR	2.8
1	A	226	ALA	2.8
1	A	521	GLU	2.8
1	B	629	TRP	2.8
1	B	518	ILE	2.7
1	B	155	VAL	2.7
1	A	615	LYS	2.7
1	B	270	VAL	2.7
1	A	542	LEU	2.7
1	A	39	SER	2.7
1	A	463	LYS	2.7
1	B	712	HIS	2.7
1	A	103	ASN	2.7
1	A	300	LEU	2.7
1	B	448	GLU	2.7
1	A	546	VAL	2.7
1	B	516	PHE	2.7
1	B	706	THR	2.6
1	A	612	GLN	2.6
1	B	162	HIS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	538	LYS	2.6
1	B	122	LYS	2.6
1	B	489	LYS	2.6
1	A	134	ILE	2.6
1	A	575	VAL	2.6
1	B	309	GLU	2.6
1	B	179	ASN	2.6
1	B	277	SER	2.6
1	A	91	GLU	2.6
1	A	116	LEU	2.6
1	B	213	ALA	2.6
1	A	677	GLU	2.6
1	B	719	ILE	2.6
1	B	385	CYS	2.5
1	B	528	MET	2.5
1	A	214	LEU	2.5
1	A	651	ILE	2.5
1	A	464	GLU	2.5
1	B	214	LEU	2.5
1	A	121	VAL	2.5
1	B	705	GLY	2.5
1	A	652	ALA	2.5
1	B	716	SER	2.5
1	A	602	GLU	2.5
1	B	108	SER	2.5
1	B	333	SER	2.5
1	A	183	TYR	2.5
1	A	236	ILE	2.4
1	B	346	ILE	2.4
1	B	651	ILE	2.4
1	B	715	GLN	2.4
1	A	379	GLU	2.4
1	B	281	ASN	2.4
1	A	616	MET	2.4
1	A	618	PHE	2.4
1	A	213	ALA	2.4
1	A	625	ALA	2.4
1	B	351	THR	2.4
1	A	448	GLU	2.4
1	A	711	VAL	2.4
1	A	529	ILE	2.4
1	A	471	ARG	2.4

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	343	ARG	2.4
1	A	197	GLY	2.4
1	A	141	GLN	2.4
1	B	139	LYS	2.4
1	B	319	ILE	2.4
1	A	139	LYS	2.4
1	A	129	THR	2.4
1	B	151	ASN	2.3
1	B	266	VAL	2.3
1	A	762	CYS	2.3
1	A	567	LEU	2.3
1	B	141	GLN	2.3
1	B	165	ALA	2.3
1	B	653	VAL	2.3
1	B	698	VAL	2.3
1	B	104	ASP	2.3
1	B	133	ASP	2.3
1	B	681	ASP	2.3
1	B	413	ASP	2.3
1	B	733	MET	2.3
1	B	72	GLN	2.3
1	A	617	GLY	2.3
1	B	69	LEU	2.3
1	B	743	ALA	2.3
1	A	54	ARG	2.2
1	A	219	ASN	2.2
1	B	38	ASP	2.2
1	B	331	ASP	2.2
1	B	181	PRO	2.2
1	B	220	GLY	2.2
1	B	711	VAL	2.2
1	A	394	CYS	2.2
1	B	228	PHE	2.2
1	A	574	ILE	2.2
1	A	93	SER	2.2
1	A	269	PHE	2.2
1	B	720	SER	2.2
1	B	529	ILE	2.2
1	A	653	VAL	2.2
1	A	348	MET	2.2
1	B	576	ALA	2.2
1	A	413	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	700	TYR	2.2
1	B	635	VAL	2.2
1	B	442	VAL	2.1
1	B	688	VAL	2.1
1	A	225	TYR	2.1
1	B	542	LEU	2.1
1	A	208	PHE	2.1
1	A	287	ILE	2.1
1	B	111	GLY	2.1
1	B	389	ILE	2.1
1	A	57	LEU	2.1
1	A	314	GLN	2.1
1	B	655	PRO	2.1
1	A	285	ILE	2.1
1	A	295	ILE	2.1
1	B	216	TRP	2.1
1	B	666	TYR	2.1
1	B	762	CYS	2.1
1	A	597	ARG	2.1
1	A	635	VAL	2.1
1	B	558	VAL	2.1
1	A	736	THR	2.1
1	A	366	LEU	2.0
1	A	303	VAL	2.0
1	B	736	THR	2.0
1	A	699	GLU	2.0
1	A	733	MET	2.0
1	A	282	ALA	2.0
1	A	499	ALA	2.0
1	B	79	PHE	2.0
1	B	89	PHE	2.0
1	B	514	LEU	2.0
1	A	351	THR	2.0
1	B	54	ARG	2.0
1	B	761	GLN	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 (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, 95th 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	NAG	B	855	14/15	0.63	0.26	1.01	68,69,69,69	0
2	NAG	A	853	14/15	0.89	0.15	-0.30	42,43,43,44	0
2	NAG	B	852	14/15	0.87	0.14	-0.34	42,42,44,45	0
2	NAG	A	851	14/15	0.90	0.10	-1.06	48,48,49,49	0

6.5 Other polymers (i)

There are no such residues in this entry.