



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:23 PM GMT

PDB ID : 3TSW
Title : crystal structure of the PDZ3-SH3-GUK core module of Human ZO-1
Authors : Nomme, J.; Lavie, A.
Deposited on : 2011-09-13
Resolution : 2.85 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

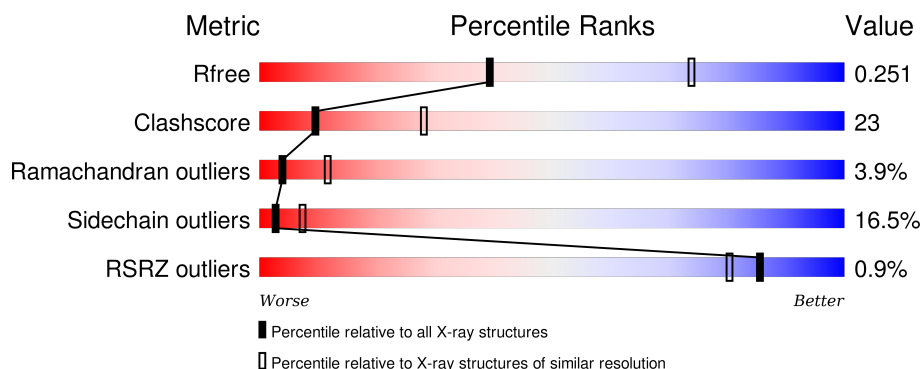
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	3170 (2.88-2.80)
Clashscore	102246	3658 (2.88-2.80)
Ramachandran outliers	100387	3591 (2.88-2.80)
Sidechain outliers	100360	3594 (2.88-2.80)
RSRZ outliers	91569	3184 (2.88-2.80)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	391	<div> <div>2%</div> <div>46% 33% 6% 15%</div> </div>
1	B	391	<div> <div>20% 25% 5% 50%</div> </div>
1	C	391	<div> <div>2%</div> <div>43% 37% 6% 14%</div> </div>
1	D	391	<div> <div>22% 24% 5% 49%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8637 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 Tight junction protein ZO-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2687	1709	481	491	6			
1	B	194	Total	C	N	O	S	0	0	0
			1552	991	270	290	1			
1	C	337	Total	C	N	O	S	0	0	0
			2703	1714	488	495	6			
1	D	199	Total	C	N	O	S	0	0	0
			1590	1011	281	297	1			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	413	GLY	-	EXPRESSION TAG	UNP Q07157
A	414	SER	-	EXPRESSION TAG	UNP Q07157
A	415	HIS	-	EXPRESSION TAG	UNP Q07157
A	416	MET	-	EXPRESSION TAG	UNP Q07157
B	413	GLY	-	EXPRESSION TAG	UNP Q07157
B	414	SER	-	EXPRESSION TAG	UNP Q07157
B	415	HIS	-	EXPRESSION TAG	UNP Q07157
B	416	MET	-	EXPRESSION TAG	UNP Q07157
C	413	GLY	-	EXPRESSION TAG	UNP Q07157
C	414	SER	-	EXPRESSION TAG	UNP Q07157
C	415	HIS	-	EXPRESSION TAG	UNP Q07157
C	416	MET	-	EXPRESSION TAG	UNP Q07157
D	413	GLY	-	EXPRESSION TAG	UNP Q07157
D	414	SER	-	EXPRESSION TAG	UNP Q07157
D	415	HIS	-	EXPRESSION TAG	UNP Q07157
D	416	MET	-	EXPRESSION TAG	UNP Q07157

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

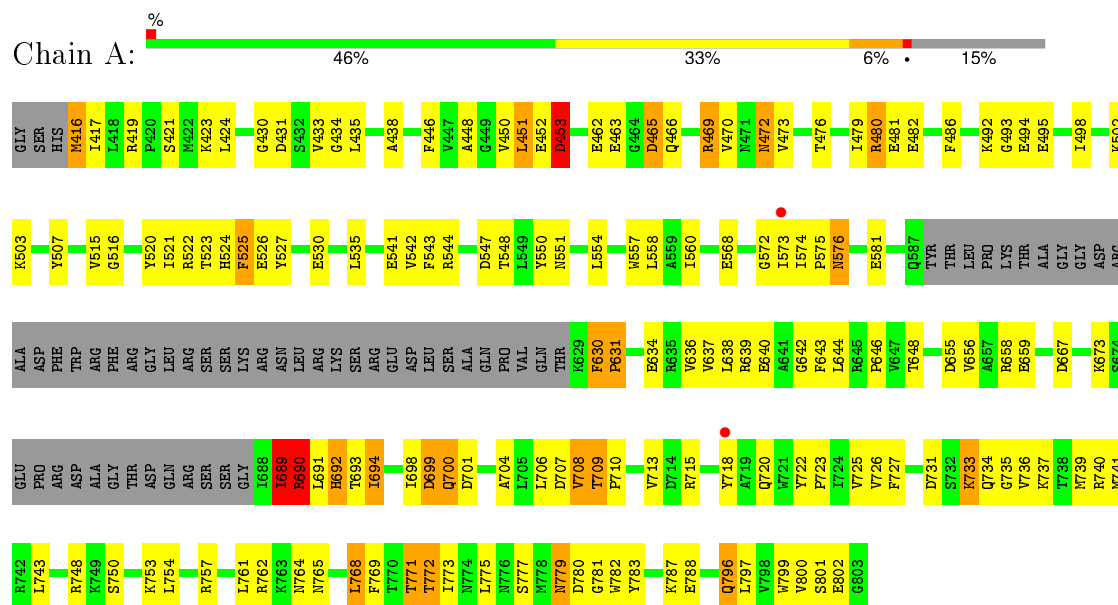
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total	O	0	0
			20	20		
3	B	13	Total	O	0	0
			13	13		
3	C	22	Total	O	0	0
			22	22		
3	D	15	Total	O	0	0
			15	15		

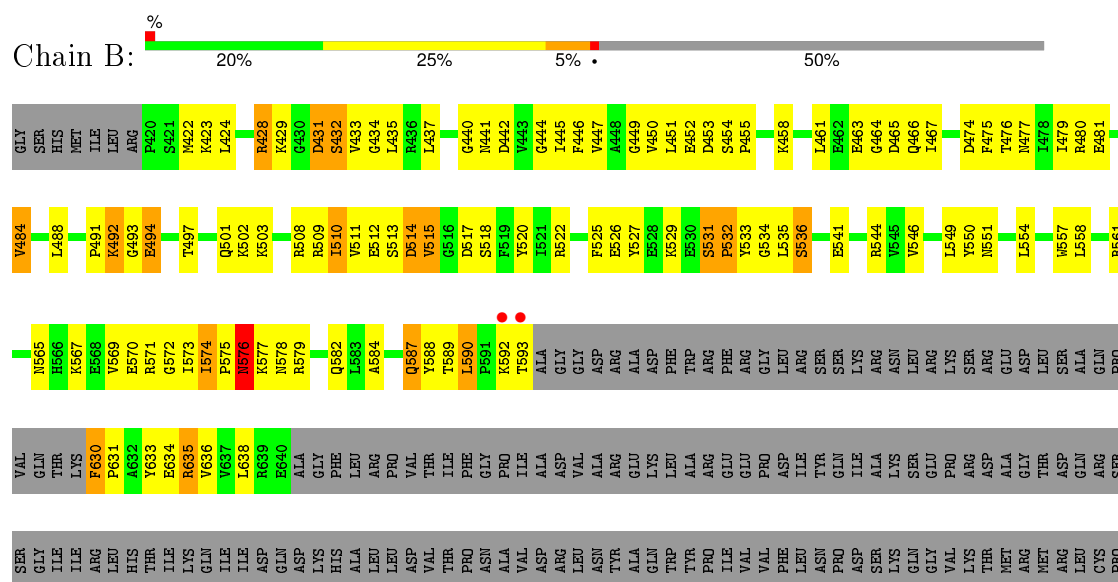
3 Residue-property plots

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.

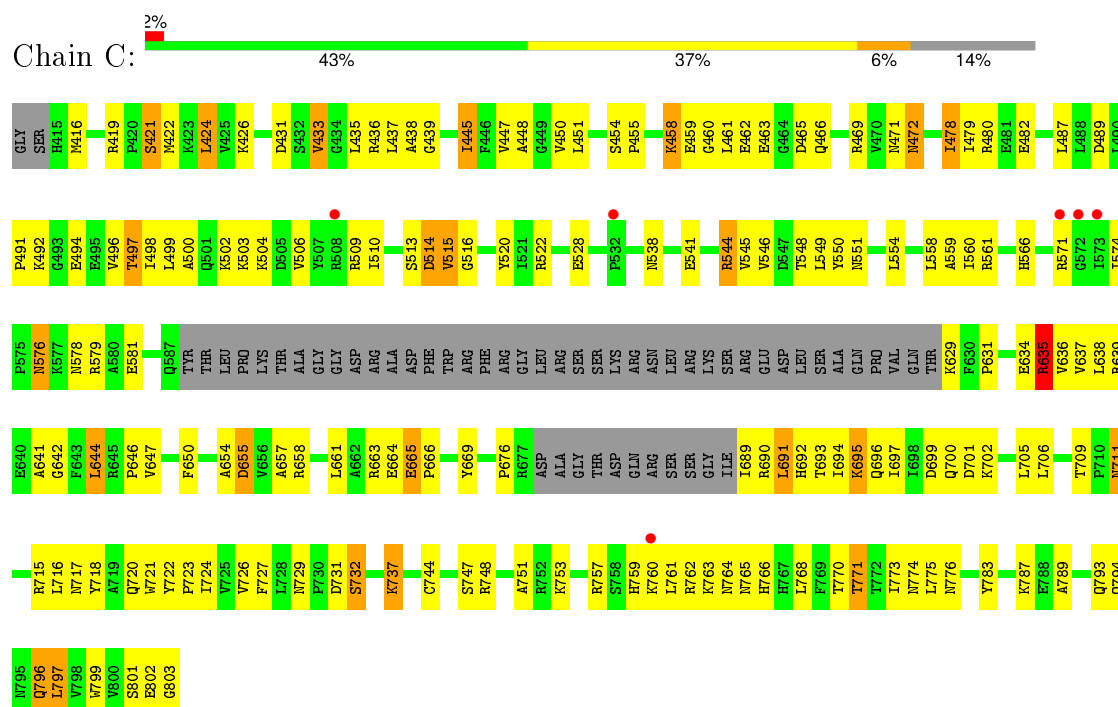
• Molecule 1: Tight junction protein ZO-1



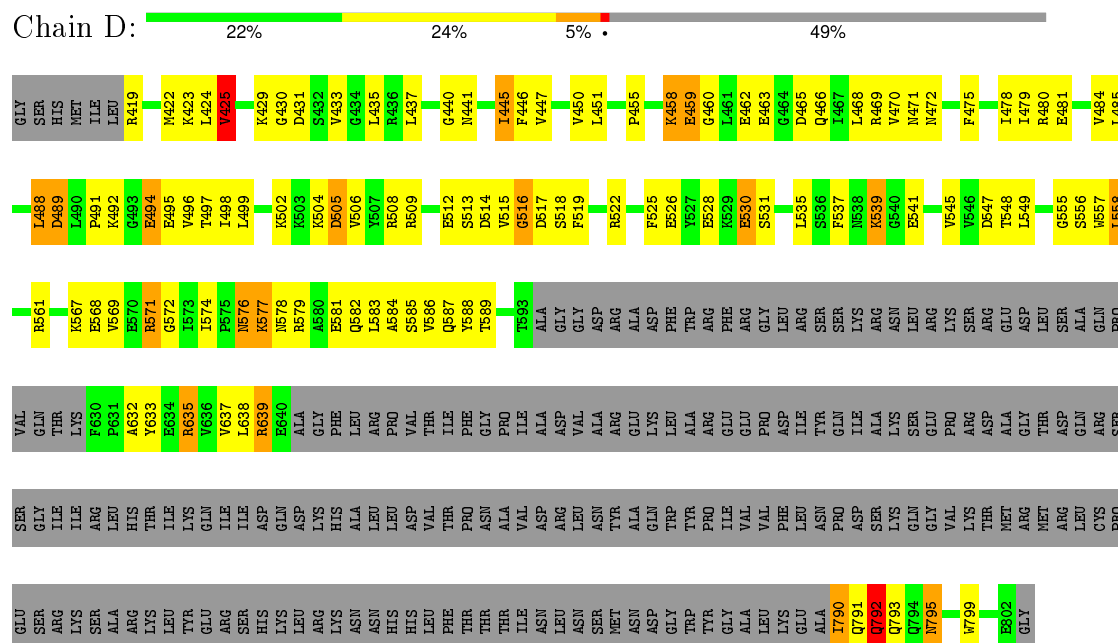
• Molecule 1: Tight junction protein ZO-1



- Molecule 1: Tight junction protein ZO-1



- Molecule 1: Tight junction protein ZO-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	100.63Å 100.63Å 182.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	87.17 – 2.85 29.55 – 2.85	Depositor EDS
% Data completeness (in resolution range)	96.2 (87.17-2.85) 97.6 (29.55-2.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.85Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.211 , 0.290 0.191 , 0.251	Depositor DCC
R_{free} test set	4762 reflections (11.23%)	DCC
Wilson B-factor (Å ²)	75.9	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.1	EDS
Estimated twinning fraction	0.508 for 1.000H, 1.000K, L 0.492 for -1.000H, 1.000H+1.000K, -L 0.000 for -h,-k,l 0.002 for h,-h-k,-l 0.139 for -k,-h,-l	Xtriage
Reported twinning fraction	0.508 for 1.000H, 1.000K, L 0.492 for -1.000H, 1.000H+1.000K, -L	Depositor
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 47162 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8637	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.57	0/2736	0.71	0/3688
1	B	0.62	0/1578	0.79	1/2124 (0.0%)
1	C	0.55	0/2753	0.72	2/3712 (0.1%)
1	D	0.68	0/1615	0.85	2/2175 (0.1%)
All	All	0.59	0/8682	0.76	5/11699 (0.0%)

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	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	488	LEU	CA-CB-CG	5.31	127.51	115.30
1	B	796	GLN	N-CA-C	5.25	125.18	111.00
1	C	424	LEU	CA-CB-CG	5.21	127.29	115.30
1	D	489	ASP	CB-CG-OD2	5.09	122.88	118.30
1	C	797	LEU	CA-CB-CG	5.08	126.98	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	482	GLU	Peptide
1	B	795	ASN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2687	0	2722	112	0
1	B	1552	0	1564	90	0
1	C	2703	0	2722	106	0
1	D	1590	0	1605	100	0
2	A	10	0	0	1	0
2	B	10	0	0	2	0
2	C	5	0	0	0	0
2	D	10	0	0	0	0
3	A	20	0	0	4	0
3	B	13	0	0	0	0
3	C	22	0	0	6	0
3	D	15	0	0	3	0
All	All	8637	0	8613	387	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 23.

All (387) 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:D:450:VAL:HG12	1:D:451:LEU:H	1.19	1.08
1:A:558:LEU:HD12	1:A:573:ILE:HG22	1.28	1.05
1:B:582:GLN:NE2	1:D:478:ILE:HD12	1.77	0.99
1:B:518:SER:OG	2:B:7:SO4:O4	1.88	0.92
1:B:431:ASP:H	1:B:492:LYS:HG2	1.33	0.92
1:A:691:LEU:HA	1:A:694:ILE:HG23	1.52	0.90
1:D:419:ARG:HH22	1:D:505:ASP:HB2	1.34	0.89
1:A:637:VAL:HG11	3:A:1:HOH:O	1.71	0.88
1:B:491:PRO:HD2	1:B:494:GLU:CG	2.04	0.88
1:B:491:PRO:HD2	1:B:494:GLU:HG2	1.56	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:576:ASN:HD21	1:B:579:ARG:H	1.22	0.86
1:A:710:PRO:HA	1:A:768:LEU:HD11	1.56	0.85
1:D:491:PRO:HD2	1:D:494:GLU:HG3	1.58	0.85
1:D:450:VAL:HG12	1:D:451:LEU:N	1.91	0.84
1:A:800:VAL:HG11	1:B:588:TYR:CE2	2.14	0.83
1:C:709:THR:OG1	1:C:711:ASN:HB2	1.79	0.82
1:A:655:ASP:HA	1:A:658:ARG:NH1	1.94	0.81
1:B:484:VAL:HG11	1:B:549:LEU:HD11	1.62	0.81
1:D:450:VAL:CG1	1:D:451:LEU:H	1.93	0.81
1:D:419:ARG:NH2	1:D:505:ASP:HB2	1.96	0.80
1:A:558:LEU:HD12	1:A:573:ILE:CG2	2.09	0.80
1:D:793:GLN:HE21	1:D:795:ASN:HB2	1.47	0.79
1:C:576:ASN:ND2	1:C:579:ARG:H	1.80	0.79
1:A:720:GLN:HE22	1:A:801:SER:H	1.31	0.79
1:C:789:ALA:O	1:C:793:GLN:HG2	1.84	0.77
1:A:731:ASP:OD1	1:A:777:SER:HB3	1.86	0.76
1:B:579:ARG:HG3	1:D:489:ASP:HB3	1.66	0.76
1:D:425:VAL:HG22	1:D:459:GLU:HB3	1.68	0.74
1:D:519:PHE:HB3	1:D:635:ARG:HH21	1.51	0.73
1:C:634:GLU:OE2	1:C:801:SER:HB3	1.88	0.73
1:B:431:ASP:N	1:B:492:LYS:HG2	2.03	0.73
1:C:560:ILE:HG12	1:C:571:ARG:HG3	1.70	0.72
1:B:522:ARG:HD2	1:B:634:GLU:OE1	1.90	0.72
1:A:492:LYS:HG2	1:A:493:GLY:N	2.03	0.72
1:A:655:ASP:HA	1:A:658:ARG:HH12	1.54	0.72
1:A:462:GLU:O	1:A:465:ASP:OD1	2.08	0.71
1:C:433:VAL:HG21	1:C:487:LEU:HB3	1.70	0.71
1:A:720:GLN:HE22	1:A:801:SER:N	1.89	0.71
1:C:471:ASN:OD1	1:C:497:THR:HG23	1.91	0.70
1:C:506:VAL:HG23	3:C:64:HOH:O	1.91	0.70
1:B:582:GLN:HE22	1:D:478:ILE:HD12	1.56	0.69
1:B:576:ASN:HD21	1:B:579:ARG:N	1.90	0.69
1:A:802:GLU:HA	1:A:802:GLU:OE2	1.92	0.69
1:B:579:ARG:CG	1:D:489:ASP:HB3	2.22	0.69
1:C:466:GLN:OE1	1:C:503:LYS:HD2	1.93	0.69
1:D:485:LEU:O	1:D:489:ASP:CG	2.31	0.69
1:B:479:ILE:HD11	1:B:635:ARG:HH21	1.56	0.69
1:D:481:GLU:HB2	1:D:548:THR:HB	1.73	0.68
1:A:433:VAL:HG23	1:A:435:LEU:HB2	1.75	0.68
1:D:437:LEU:HD12	1:D:484:VAL:HG12	1.74	0.68
1:B:494:GLU:OE1	1:D:530:GLU:HG3	1.93	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:455:PRO:HA	1:C:458:LYS:HB2	1.74	0.68
1:B:474:ASP:OD1	1:B:477:ASN:HB2	1.94	0.68
1:B:491:PRO:HD2	1:B:494:GLU:HG3	1.76	0.68
1:B:464:GLY:O	1:B:502:LYS:O	2.12	0.68
1:B:520:TYR:OH	1:B:544:ARG:HD2	1.94	0.68
1:A:720:GLN:NE2	1:A:801:SER:H	1.92	0.67
1:B:529:LYS:NZ	1:B:532:PRO:HA	2.08	0.67
1:C:419:ARG:NH2	1:C:506:VAL:HG21	2.10	0.67
1:B:631:PRO:HB2	1:B:633:TYR:O	1.95	0.66
1:D:586:VAL:HG13	3:D:6:HOH:O	1.94	0.66
1:D:441:ASN:ND2	1:D:479:ILE:HG12	2.11	0.66
1:C:491:PRO:HB2	1:C:494:GLU:HG2	1.77	0.66
1:A:715:ARG:NH2	2:A:5:SO4:O3	2.29	0.66
1:C:762:ARG:O	1:C:766:HIS:HB3	1.95	0.66
1:D:525:PHE:HB2	1:D:587:GLN:OE1	1.95	0.66
1:A:522:ARG:HH21	1:A:799:TRP:HB2	1.61	0.65
1:B:517:ASP:O	1:B:546:VAL:HA	1.96	0.65
1:B:454:SER:HB2	1:B:455:PRO:HD2	1.79	0.65
1:A:524:HIS:CG	1:A:630:PHE:HB3	2.31	0.65
1:B:494:GLU:HA	1:B:494:GLU:OE2	1.97	0.65
1:D:484:VAL:HG11	1:D:549:LEU:HD11	1.77	0.65
1:D:508:ARG:O	1:D:512:GLU:HG3	1.97	0.64
1:C:665:GLU:HB2	1:C:669:TYR:HD2	1.63	0.64
1:D:522:ARG:NH2	1:D:799:TRP:HB2	2.13	0.64
1:A:466:GLN:OE1	1:A:503:LYS:HD2	1.98	0.63
1:A:642:GLY:HA3	1:B:588:TYR:O	1.99	0.63
1:C:634:GLU:O	1:C:635:ARG:C	2.36	0.63
1:B:525:PHE:CG	1:B:584:ALA:HB2	2.33	0.63
1:D:535:LEU:HG	1:D:572:GLY:HA3	1.81	0.63
1:B:508:ARG:O	1:B:511:VAL:HG12	1.99	0.62
1:C:433:VAL:HB	1:C:435:LEU:HD13	1.81	0.62
1:B:638:LEU:HG	1:B:799:TRP:CZ3	2.35	0.62
1:B:437:LEU:O	1:B:480:ARG:NH2	2.29	0.61
1:C:634:GLU:HG2	1:C:634:GLU:O	1.98	0.61
1:B:440:GLY:N	1:B:444:GLY:O	2.34	0.61
1:B:529:LYS:HZ1	1:B:532:PRO:HA	1.63	0.61
1:D:576:ASN:HD22	1:D:576:ASN:N	1.98	0.61
1:D:423:LYS:HE2	1:D:460:GLY:O	2.01	0.60
1:D:637:VAL:HG11	1:D:639:ARG:NH1	2.17	0.60
1:A:648:THR:HB	1:A:725:VAL:HG22	1.83	0.60
1:A:643:PHE:HD1	1:A:644:LEU:O	1.85	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:731:ASP:O	1:C:732:SER:HB3	2.02	0.60
1:D:577:LYS:O	1:D:581:GLU:HB2	2.03	0.59
1:A:715:ARG:O	1:A:718:TYR:HB3	2.01	0.59
1:C:694:ILE:HG13	1:C:721:TRP:HZ3	1.67	0.59
1:B:428:ARG:HG2	1:B:429:LYS:O	2.03	0.59
1:D:440:GLY:HA3	1:D:516:GLY:C	2.23	0.59
1:D:578:ASN:O	1:D:582:GLN:HG2	2.02	0.59
1:D:429:LYS:O	1:D:492:LYS:O	2.20	0.59
1:A:673:LYS:O	1:A:693:THR:HG21	2.02	0.59
1:B:446:PHE:CE1	1:B:466:GLN:HG3	2.38	0.58
1:C:641:ALA:HA	1:D:588:TYR:CE2	2.38	0.58
1:A:547:ASP:OD2	1:A:550:TYR:HA	2.03	0.58
1:A:423:LYS:NZ	3:A:4:HOH:O	2.35	0.58
1:C:731:ASP:O	1:C:732:SER:CB	2.51	0.58
1:C:506:VAL:HG22	1:C:509:ARG:NH1	2.18	0.58
1:B:479:ILE:HD11	1:B:635:ARG:NH2	2.18	0.58
1:A:750:SER:HB3	1:A:753:LYS:HE3	1.86	0.58
1:C:426:LYS:HA	1:C:496:VAL:O	2.04	0.58
1:C:664:GLU:O	1:C:666:PRO:HD3	2.03	0.58
1:D:429:LYS:HG2	1:D:430:GLY:N	2.19	0.57
1:C:419:ARG:HH21	1:C:506:VAL:HG21	1.67	0.57
1:C:694:ILE:C	1:C:696:GLN:H	2.08	0.57
1:B:630:PHE:CD2	1:B:630:PHE:N	2.73	0.57
1:A:523:THR:HG23	1:A:541:GLU:O	2.04	0.57
1:C:513:SER:O	1:C:514:ASP:C	2.42	0.56
1:A:643:PHE:HE2	1:B:588:TYR:CE1	2.22	0.56
1:C:576:ASN:HD21	1:C:579:ARG:H	1.53	0.56
1:D:419:ARG:HH22	1:D:505:ASP:N	2.03	0.56
1:D:492:LYS:HG2	1:D:492:LYS:O	2.05	0.56
1:A:655:ASP:HA	1:A:658:ARG:CZ	2.36	0.56
1:C:522:ARG:HH12	1:C:722:TYR:HH	1.54	0.56
1:A:779:ASN:ND2	1:A:781:GLY:H	2.03	0.56
1:C:447:VAL:HG12	1:C:463:GLU:HA	1.87	0.55
1:A:779:ASN:HD22	1:A:779:ASN:C	2.10	0.55
1:C:437:LEU:HD13	1:C:445:ILE:HG21	1.87	0.55
1:B:531:SER:C	1:B:533:TYR:H	2.10	0.55
1:C:726:VAL:HG22	1:C:771:THR:HG23	1.87	0.55
1:D:437:LEU:HD13	1:D:445:ILE:HD12	1.88	0.55
1:B:440:GLY:O	1:B:444:GLY:N	2.38	0.55
1:C:701:ASP:O	1:C:702:LYS:HG3	2.07	0.55
1:B:429:LYS:HG3	1:B:433:VAL:HG13	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:478:ILE:HD13	1:C:482:GLU:OE1	2.06	0.55
1:A:646:PRO:HB3	1:A:706:LEU:HD11	1.88	0.55
1:A:473:VAL:HG21	1:A:486:PHE:CZ	2.42	0.54
1:D:793:GLN:NE2	1:D:795:ASN:HB2	2.19	0.54
1:A:438:ALA:HA	1:A:480:ARG:HH21	1.72	0.54
1:A:535:LEU:HD12	1:A:543:PHE:HE2	1.72	0.54
1:D:558:LEU:HD23	1:D:572:GLY:O	2.08	0.54
1:B:796:GLN:HA	1:B:796:GLN:HE21	1.73	0.54
1:D:569:VAL:O	1:D:569:VAL:CG1	2.56	0.53
1:B:452:GLU:O	1:B:453:ASP:HB2	2.08	0.53
1:D:441:ASN:HD22	1:D:479:ILE:HG12	1.72	0.53
1:B:431:ASP:O	1:B:432:SER:HB2	2.07	0.53
1:A:780:ASP:HA	1:A:782:TRP:CD1	2.44	0.53
1:C:550:TYR:O	1:C:551:ASN:HB2	2.08	0.53
1:D:425:VAL:O	1:D:425:VAL:HG12	2.07	0.52
1:B:447:VAL:HG12	1:B:449:GLY:H	1.74	0.52
1:A:548:THR:HA	1:A:557:TRP:CD1	2.43	0.52
1:D:419:ARG:HH22	1:D:505:ASP:H	1.57	0.52
1:B:630:PHE:HD2	1:B:630:PHE:N	2.08	0.52
1:C:737:LYS:HD2	1:C:751:ALA:HB3	1.92	0.52
1:A:526:GLU:HG2	1:A:527:TYR:N	2.24	0.52
1:D:505:ASP:HA	1:D:508:ARG:HH21	1.74	0.52
1:B:491:PRO:CD	1:B:494:GLU:HG2	2.34	0.52
1:B:533:TYR:HD2	1:B:573:ILE:HG23	1.74	0.52
1:D:632:ALA:O	1:D:633:TYR:HD1	1.93	0.52
1:A:802:GLU:CA	1:A:802:GLU:OE2	2.58	0.52
1:B:535:LEU:HD21	1:B:571:ARG:O	2.09	0.52
1:C:646:PRO:HG2	1:C:723:PRO:HB3	1.92	0.52
1:B:567:LYS:HG3	1:C:421:SER:HB3	1.92	0.52
1:D:790:ILE:O	1:D:792:GLN:N	2.43	0.52
1:C:559:ALA:HB3	1:C:574:ILE:HG12	1.91	0.52
1:D:585:SER:OG	3:D:6:HOH:O	1.91	0.51
1:A:535:LEU:HG	1:A:572:GLY:HA3	1.93	0.51
1:A:638:LEU:O	1:A:639:ARG:HD3	2.11	0.51
1:B:557:TRP:CH2	1:B:577:LYS:HB3	2.45	0.51
1:A:639:ARG:NH2	3:A:1:HOH:O	2.23	0.51
1:A:434:GLY:HA3	1:A:451:LEU:HB2	1.92	0.51
1:C:695:LYS:HB2	1:C:721:TRP:HH2	1.76	0.51
1:A:560:ILE:HG21	1:A:568:GLU:HB3	1.93	0.51
1:C:465:ASP:HB3	1:C:500:ALA:HB1	1.93	0.51
1:A:689:ILE:CD1	1:A:715:ARG:HH12	2.24	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:655:ASP:OD2	1:C:655:ASP:N	2.44	0.50
1:D:419:ARG:HH12	1:D:505:ASP:HB2	1.76	0.50
1:A:636:VAL:HG12	1:A:801:SER:HA	1.92	0.50
1:C:697:ILE:HA	1:C:700:GLN:HB3	1.93	0.50
1:D:419:ARG:HH22	1:D:505:ASP:CB	2.14	0.50
1:A:448:ALA:HA	1:A:507:TYR:OH	2.10	0.50
1:C:502:LYS:O	1:C:503:LYS:C	2.50	0.50
1:C:436:ARG:N	1:C:436:ARG:HD2	2.27	0.50
1:D:419:ARG:NH1	1:D:505:ASP:HB2	2.26	0.50
1:D:480:ARG:HD3	1:D:549:LEU:HB2	1.92	0.50
1:B:636:VAL:HA	1:B:800:VAL:O	2.11	0.50
1:A:462:GLU:HG3	1:A:502:LYS:HE3	1.92	0.50
1:C:510:ILE:HA	1:C:515:VAL:HG23	1.94	0.50
1:C:717:ASN:O	1:C:720:GLN:N	2.42	0.50
1:A:547:ASP:HB3	1:A:558:LEU:HB2	1.94	0.50
1:D:445:ILE:HD11	1:D:480:ARG:HA	1.92	0.50
1:C:647:VAL:HG22	1:C:724:ILE:HD12	1.93	0.50
1:D:470:VAL:HG22	1:D:498:ILE:HG12	1.94	0.50
1:D:491:PRO:CD	1:D:494:GLU:HG3	2.38	0.50
1:D:450:VAL:CG1	1:D:451:LEU:N	2.61	0.49
1:B:567:LYS:HG3	1:C:421:SER:CB	2.41	0.49
1:A:765:ASN:O	1:A:765:ASN:OD1	2.29	0.49
1:C:635:ARG:HG2	1:C:803:GLY:HA2	1.94	0.49
1:D:638:LEU:HG	1:D:799:TRP:CH2	2.47	0.49
1:C:695:LYS:HB2	1:C:721:TRP:CH2	2.47	0.49
1:D:419:ARG:CZ	1:D:505:ASP:HB2	2.40	0.49
1:A:521:ILE:HA	1:A:634:GLU:O	2.12	0.49
1:D:495:GLU:HA	1:D:495:GLU:OE2	2.13	0.49
1:A:452:GLU:O	1:A:453:ASP:HB3	2.12	0.49
1:D:455:PRO:HA	1:D:458:LYS:HB3	1.93	0.49
1:D:567:LYS:NZ	3:D:31:HOH:O	2.43	0.49
1:A:638:LEU:HD22	1:A:797:LEU:HB3	1.95	0.49
1:C:419:ARG:HH21	1:C:506:VAL:CG2	2.25	0.49
1:C:637:VAL:HB	1:C:802:GLU:HB3	1.95	0.48
1:A:469:ARG:HG2	1:A:472:ASN:HA	1.94	0.48
1:D:541:GLU:OE1	1:D:561:ARG:NH1	2.45	0.48
1:B:445:ILE:O	1:B:467:ILE:HB	2.13	0.48
1:D:513:SER:O	1:D:515:VAL:N	2.46	0.48
1:B:461:LEU:HA	1:B:465:ASP:OD2	2.13	0.48
1:D:579:ARG:O	1:D:583:LEU:HG	2.14	0.48
1:B:796:GLN:CA	1:B:796:GLN:HE21	2.27	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:547:ASP:HB3	1:D:558:LEU:HB3	1.95	0.48
1:C:644:LEU:HD21	3:C:23:HOH:O	2.14	0.48
1:B:422:MET:HG3	1:B:501:GLN:HG3	1.94	0.48
1:B:526:GLU:HB3	1:B:587:GLN:OE1	2.14	0.48
1:C:638:LEU:HD22	1:C:797:LEU:HB3	1.96	0.48
1:C:638:LEU:HG	1:C:799:TRP:CZ3	2.49	0.48
1:D:478:ILE:HG12	1:D:479:ILE:O	2.14	0.48
1:B:576:ASN:C	1:B:576:ASN:HD22	2.17	0.47
1:A:470:VAL:HG22	1:A:498:ILE:HG12	1.96	0.47
1:C:699:ASP:C	1:C:701:ASP:H	2.18	0.47
1:A:743:LEU:HD11	1:A:782:TRP:HZ2	1.79	0.47
1:A:434:GLY:CA	1:A:451:LEU:HB2	2.44	0.47
1:B:569:VAL:HG12	1:B:570:GLU:HG2	1.96	0.47
1:B:578:ASN:O	1:B:579:ARG:C	2.52	0.47
1:A:535:LEU:CG	1:A:572:GLY:HA3	2.44	0.47
1:A:710:PRO:HG3	1:A:761:LEU:HD11	1.96	0.47
1:C:794:GLN:HG3	1:D:528:GLU:OE1	2.14	0.47
1:A:640:GLU:O	1:B:587:GLN:HA	2.15	0.47
1:A:643:PHE:HA	1:B:526:GLU:OE1	2.15	0.47
1:C:664:GLU:O	1:C:666:PRO:CD	2.63	0.47
1:C:650:PHE:O	1:C:727:PHE:HA	2.15	0.47
1:B:533:TYR:CE2	1:B:572:GLY:HA2	2.49	0.47
1:C:520:TYR:O	1:C:636:VAL:N	2.34	0.47
1:C:479:ILE:HG22	1:C:480:ARG:N	2.30	0.47
1:B:536:SER:O	1:B:561:ARG:NH2	2.40	0.47
1:B:480:ARG:HD3	1:B:549:LEU:HB2	1.96	0.46
1:A:630:PHE:HA	1:A:631:PRO:HD2	1.59	0.46
1:C:694:ILE:C	1:C:696:GLN:N	2.67	0.46
1:C:447:VAL:O	1:C:463:GLU:HA	2.15	0.46
1:C:469:ARG:HD3	1:C:472:ASN:HA	1.97	0.46
1:A:637:VAL:HG12	1:A:638:LEU:H	1.79	0.46
1:B:592:LYS:O	1:B:593:THR:C	2.52	0.46
1:A:757:ARG:HB2	3:A:38:HOH:O	2.14	0.46
1:A:634:GLU:HG2	1:A:636:VAL:HG13	1.97	0.46
1:D:548:THR:HA	1:D:557:TRP:CD1	2.51	0.46
1:D:638:LEU:C	1:D:639:ARG:HG2	2.36	0.46
1:C:663:ARG:HD2	3:C:50:HOH:O	2.14	0.46
1:A:708:VAL:HG23	1:A:709:THR:N	2.29	0.46
1:C:638:LEU:HG	1:C:799:TRP:CH2	2.51	0.46
1:B:428:ARG:NH2	2:B:1:SO4:O4	2.49	0.46
1:D:475:PHE:HA	1:D:478:ILE:HG22	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:HIS:CD2	1:A:630:PHE:HB3	2.50	0.46
1:A:727:PHE:HB3	1:A:772:THR:HB	1.98	0.46
1:C:642:GLY:O	1:D:539:LYS:HE3	2.15	0.46
1:B:435:LEU:HD12	1:B:450:VAL:HG13	1.97	0.46
1:B:795:ASN:HB3	1:B:796:GLN:HB2	1.98	0.45
1:D:447:VAL:HG12	1:D:447:VAL:O	2.16	0.45
1:D:419:ARG:NH2	1:D:505:ASP:H	2.15	0.45
1:C:637:VAL:HG12	1:C:639:ARG:HG2	1.98	0.45
1:D:519:PHE:CB	1:D:635:ARG:HH21	2.26	0.45
1:C:461:LEU:HA	1:C:461:LEU:HD23	1.86	0.45
1:A:720:GLN:NE2	1:A:801:SER:HB3	2.32	0.45
1:D:537:PHE:HA	1:D:541:GLU:OE2	2.16	0.45
1:C:438:ALA:HB2	1:C:448:ALA:HB2	1.98	0.45
1:D:440:GLY:HA3	1:D:517:ASP:N	2.32	0.45
1:A:764:ASN:O	1:A:765:ASN:OD1	2.35	0.45
1:D:441:ASN:H	1:D:517:ASP:HA	1.82	0.45
1:D:584:ALA:O	1:D:585:SER:C	2.54	0.45
1:C:545:VAL:HG11	1:C:548:THR:HG22	1.98	0.45
1:C:776:ASN:OD1	1:C:776:ASN:C	2.56	0.45
1:C:729:ASN:HB3	1:C:773:ILE:O	2.17	0.45
1:B:514:ASP:OD2	1:B:514:ASP:C	2.55	0.45
1:B:549:LEU:O	1:B:550:TYR:C	2.54	0.44
1:A:542:VAL:HG11	1:A:799:TRP:CH2	2.52	0.44
1:D:462:GLU:O	1:D:463:GLU:C	2.56	0.44
1:A:574:ILE:HB	1:A:575:PRO:HD2	1.99	0.44
1:C:757:ARG:NH2	1:C:760:LYS:HD3	2.32	0.44
1:C:783:TYR:HE2	1:C:787:LYS:HZ3	1.66	0.44
1:D:441:ASN:HD22	1:D:479:ILE:CG1	2.30	0.44
1:C:502:LYS:HD2	1:C:502:LYS:HA	1.82	0.44
1:A:690:ARG:HG3	1:A:692:HIS:CD2	2.53	0.44
1:C:566:HIS:HE1	3:C:9:HOH:O	2.00	0.44
1:B:554:LEU:HD12	1:D:488:LEU:CD1	2.48	0.44
1:C:716:LEU:O	1:C:717:ASN:C	2.55	0.44
1:A:646:PRO:HB2	1:A:723:PRO:HB3	1.99	0.44
1:A:470:VAL:O	1:A:473:VAL:N	2.51	0.44
1:D:446:PHE:CE1	1:D:466:GLN:HB2	2.53	0.44
1:C:447:VAL:HG12	1:C:447:VAL:O	2.18	0.44
1:A:643:PHE:CD1	1:A:644:LEU:O	2.68	0.44
1:D:518:SER:HA	1:D:545:VAL:O	2.18	0.44
1:D:469:ARG:HB3	1:D:499:LEU:HB3	2.00	0.44
1:D:445:ILE:CG2	1:D:446:PHE:N	2.81	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:422:MET:HE2	1:D:499:LEU:HD11	2.00	0.43
1:B:475:PHE:C	1:B:477:ASN:H	2.21	0.43
1:B:447:VAL:HG22	1:B:467:ILE:HD11	1.99	0.43
1:D:496:VAL:HG12	1:D:498:ILE:HG13	1.99	0.43
1:B:514:ASP:O	1:B:515:VAL:C	2.56	0.43
1:C:693:THR:O	1:C:693:THR:HG22	2.19	0.43
1:B:527:TYR:CE2	1:B:575:PRO:HD3	2.53	0.43
1:C:576:ASN:HD21	1:C:578:ASN:HB3	1.84	0.43
1:A:783:TYR:O	1:A:787:LYS:HG3	2.18	0.43
1:D:505:ASP:O	1:D:509:ARG:NH1	2.52	0.43
1:D:506:VAL:HA	1:D:509:ARG:CZ	2.49	0.43
1:A:644:LEU:HD22	1:A:701:ASP:C	2.39	0.43
1:C:419:ARG:HD3	1:C:503:LYS:HG2	1.99	0.43
1:D:423:LYS:HE2	1:D:460:GLY:HA3	1.99	0.43
1:A:733:LYS:H	1:A:733:LYS:NZ	2.17	0.43
1:B:491:PRO:O	1:B:493:GLY:N	2.51	0.43
1:A:465:ASP:N	1:A:465:ASP:OD1	2.52	0.43
1:C:479:ILE:HG22	1:C:480:ARG:H	1.82	0.43
1:C:520:TYR:CE2	1:C:544:ARG:HG3	2.54	0.43
1:B:576:ASN:ND2	1:B:579:ARG:H	2.04	0.43
1:A:707:ASP:O	1:A:707:ASP:CG	2.57	0.43
1:A:698:ILE:O	1:A:700:GLN:N	2.52	0.43
1:A:481:GLU:HB2	1:A:548:THR:HB	2.00	0.43
1:D:576:ASN:ND2	1:D:576:ASN:N	2.65	0.43
1:C:654:ALA:CB	1:C:658:ARG:NH2	2.82	0.43
1:A:446:PHE:CE1	1:A:466:GLN:HB2	2.54	0.42
1:B:576:ASN:ND2	1:B:579:ARG:N	2.64	0.42
1:C:744:CYS:SG	1:C:744:CYS:O	2.76	0.42
1:B:510:ILE:HD13	1:B:510:ILE:HA	1.89	0.42
1:D:522:ARG:HH22	1:D:799:TRP:HB2	1.81	0.42
1:B:531:SER:O	1:B:533:TYR:N	2.52	0.42
1:D:792:GLN:HG3	1:D:792:GLN:H	1.70	0.42
1:C:541:GLU:OE1	1:C:561:ARG:NH1	2.52	0.42
1:A:739:MET:SD	1:A:777:SER:HA	2.58	0.42
1:C:471:ASN:OD1	1:C:497:THR:CG2	2.63	0.42
1:D:574:ILE:HD12	1:D:633:TYR:OH	2.20	0.42
1:B:567:LYS:NZ	1:C:421:SER:OG	2.43	0.42
1:B:576:ASN:ND2	1:B:576:ASN:C	2.71	0.42
1:C:638:LEU:O	1:C:639:ARG:HD3	2.19	0.42
1:A:416:MET:HE2	1:D:571:ARG:HE	1.85	0.42
1:A:800:VAL:HG11	1:B:588:TYR:CD2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:GLN:OE1	1:B:503:LYS:HD3	2.20	0.42
1:A:434:GLY:HA2	1:A:451:LEU:CD1	2.49	0.42
1:A:448:ALA:O	1:A:463:GLU:HG3	2.19	0.42
1:D:422:MET:CE	1:D:499:LEU:HD11	2.49	0.42
1:A:740:ARG:HD2	1:A:754:LEU:CD1	2.49	0.42
1:C:657:ALA:O	1:C:661:LEU:HG	2.19	0.42
1:C:498:ILE:HG22	1:C:499:LEU:N	2.35	0.42
1:A:656:VAL:HG11	1:A:743:LEU:HD13	2.02	0.42
1:C:794:GLN:CG	1:C:794:GLN:O	2.67	0.42
1:A:722:TYR:HE1	1:A:800:VAL:HG12	1.84	0.42
1:A:646:PRO:HA	1:A:704:ALA:HB3	2.02	0.42
1:A:520:TYR:CZ	1:A:544:ARG:HG3	2.55	0.42
1:A:494:GLU:HG3	1:A:495:GLU:N	2.35	0.42
1:C:721:TRP:O	1:C:722:TYR:C	2.59	0.41
1:A:743:LEU:HD11	1:A:782:TRP:CZ2	2.54	0.41
1:A:473:VAL:HG21	1:A:486:PHE:HZ	1.85	0.41
1:D:471:ASN:O	1:D:472:ASN:HB2	2.20	0.41
1:C:793:GLN:NE2	3:C:12:HOH:O	2.52	0.41
1:A:452:GLU:O	1:A:453:ASP:CB	2.68	0.41
1:A:713:VAL:CG1	1:A:768:LEU:HD22	2.51	0.41
1:C:793:GLN:O	1:C:796:GLN:HB3	2.21	0.41
1:C:766:HIS:N	3:C:19:HOH:O	2.52	0.41
1:B:541:GLU:OE1	1:B:561:ARG:NH1	2.44	0.41
1:A:726:VAL:HG22	1:A:771:THR:HG22	2.03	0.41
1:A:796:GLN:HA	1:A:796:GLN:HE21	1.83	0.41
1:A:576:ASN:N	1:A:576:ASN:HD22	2.18	0.41
1:A:419:ARG:HB2	1:D:568:GLU:HG3	2.02	0.41
1:D:519:PHE:HB2	1:D:635:ARG:HE	1.86	0.41
1:C:560:ILE:HD11	1:C:571:ARG:HE	1.85	0.41
1:A:524:HIS:O	1:A:525:PHE:HB3	2.21	0.41
1:C:691:LEU:HB2	1:C:721:TRP:CH2	2.55	0.41
1:A:639:ARG:CB	1:B:588:TYR:HD2	2.33	0.41
1:D:576:ASN:O	1:D:578:ASN:N	2.54	0.41
1:B:557:TRP:O	1:B:573:ILE:HA	2.20	0.41
1:B:535:LEU:HB2	1:B:574:ILE:HG23	2.02	0.41
1:A:726:VAL:CG1	1:A:773:ILE:HD12	2.51	0.41
1:C:439:GLY:O	1:C:516:GLY:HA2	2.21	0.41
1:C:796:GLN:HG3	1:C:797:LEU:N	2.36	0.41
1:A:731:ASP:N	1:A:731:ASP:OD2	2.46	0.41
1:D:526:GLU:O	1:D:587:GLN:NE2	2.46	0.41
1:A:704:ALA:O	1:A:706:LEU:HG	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:455:PRO:HA	1:D:458:LYS:CB	2.50	0.41
1:C:629:LYS:O	1:C:718:TYR:OH	2.38	0.41
1:B:534:GLY:HA2	1:B:573:ILE:O	2.21	0.41
1:C:459:GLU:O	1:C:461:LEU:N	2.52	0.40
1:C:647:VAL:HB	1:C:705:LEU:HD23	2.02	0.40
1:A:720:GLN:CD	1:A:801:SER:H	2.24	0.40
1:A:690:ARG:HB3	1:A:693:THR:HG1	1.86	0.40
1:C:689:ILE:N	1:C:715:ARG:HH11	2.19	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	328/391 (84%)	266 (81%)	48 (15%)	14 (4%)	3	10
1	B	188/391 (48%)	153 (81%)	29 (15%)	6 (3%)	5	16
1	C	331/391 (85%)	265 (80%)	53 (16%)	13 (4%)	4	12
1	D	193/391 (49%)	150 (78%)	35 (18%)	8 (4%)	3	10
All	All	1040/1564 (66%)	834 (80%)	165 (16%)	41 (4%)	4	12

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	515	VAL
1	A	631	PRO
1	A	689	ILE
1	C	454	SER
1	C	676	PRO
1	C	732	SER
1	C	765	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	514	ASP
1	D	791	GLN
1	D	792	GLN
1	A	699	ASP
1	B	515	VAL
1	C	514	ASP
1	C	635	ARG
1	D	502	LYS
1	A	430	GLY
1	A	453	ASP
1	A	551	ASN
1	A	630	PHE
1	A	708	VAL
1	B	576	ASN
1	C	460	GLY
1	C	549	LEU
1	A	735	GLY
1	B	432	SER
1	C	472	ASN
1	C	631	PRO
1	C	644	LEU
1	D	516	GLY
1	B	532	PRO
1	B	590	LEU
1	C	695	LYS
1	D	795	ASN
1	A	525	PHE
1	A	690	ARG
1	C	489	ASP
1	B	434	GLY
1	D	555	GLY
1	D	425	VAL
1	A	736	VAL
1	A	516	GLY

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	289/338 (86%)	248 (86%)	41 (14%)	4	11
1	B	167/338 (49%)	130 (78%)	37 (22%)	1	2
1	C	289/338 (86%)	243 (84%)	46 (16%)	3	8
1	D	171/338 (51%)	144 (84%)	27 (16%)	3	8
All	All	916/1352 (68%)	765 (84%)	151 (16%)	3	7

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	416	MET
1	A	417	ILE
1	A	421	SER
1	A	424	LEU
1	A	431	ASP
1	A	450	VAL
1	A	451	LEU
1	A	453	ASP
1	A	465	ASP
1	A	469	ARG
1	A	472	ASN
1	A	476	THR
1	A	479	ILE
1	A	480	ARG
1	A	530	GLU
1	A	554	LEU
1	A	576	ASN
1	A	581	GLU
1	A	659	GLU
1	A	667	ASP
1	A	689	ILE
1	A	690	ARG
1	A	692	HIS
1	A	694	ILE
1	A	699	ASP
1	A	700	GLN
1	A	709	THR
1	A	733	LYS
1	A	734	GLN
1	A	737	LYS
1	A	741	MET
1	A	748	ARG
1	A	762	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	768	LEU
1	A	769	PHE
1	A	771	THR
1	A	772	THR
1	A	775	LEU
1	A	779	ASN
1	A	788	GLU
1	A	796	GLN
1	B	423	LYS
1	B	424	LEU
1	B	428	ARG
1	B	431	ASP
1	B	441	ASN
1	B	442	ASP
1	B	451	LEU
1	B	458	LYS
1	B	463	GLU
1	B	476	THR
1	B	481	GLU
1	B	484	VAL
1	B	488	LEU
1	B	492	LYS
1	B	494	GLU
1	B	497	THR
1	B	509	ARG
1	B	510	ILE
1	B	512	GLU
1	B	513	SER
1	B	514	ASP
1	B	531	SER
1	B	536	SER
1	B	551	ASN
1	B	558	LEU
1	B	565	ASN
1	B	574	ILE
1	B	576	ASN
1	B	587	GLN
1	B	589	THR
1	B	590	LEU
1	B	630	PHE
1	B	635	ARG
1	B	794	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	796	GLN
1	B	798	VAL
1	B	801	SER
1	C	416	MET
1	C	421	SER
1	C	422	MET
1	C	424	LEU
1	C	431	ASP
1	C	433	VAL
1	C	445	ILE
1	C	450	VAL
1	C	451	LEU
1	C	458	LYS
1	C	462	GLU
1	C	478	ILE
1	C	492	LYS
1	C	497	THR
1	C	504	LYS
1	C	515	VAL
1	C	528	GLU
1	C	538	ASN
1	C	544	ARG
1	C	546	VAL
1	C	554	LEU
1	C	558	LEU
1	C	576	ASN
1	C	581	GLU
1	C	635	ARG
1	C	655	ASP
1	C	665	GLU
1	C	690	ARG
1	C	691	LEU
1	C	692	HIS
1	C	706	LEU
1	C	711	ASN
1	C	737	LYS
1	C	747	SER
1	C	748	ARG
1	C	753	LYS
1	C	759	HIS
1	C	761	LEU
1	C	763	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	764	ASN
1	C	768	LEU
1	C	770	THR
1	C	771	THR
1	C	774	ASN
1	C	775	LEU
1	C	796	GLN
1	D	424	LEU
1	D	425	VAL
1	D	431	ASP
1	D	433	VAL
1	D	435	LEU
1	D	445	ILE
1	D	458	LYS
1	D	459	GLU
1	D	465	ASP
1	D	468	LEU
1	D	494	GLU
1	D	497	THR
1	D	504	LYS
1	D	505	ASP
1	D	530	GLU
1	D	531	SER
1	D	539	LYS
1	D	556	SER
1	D	558	LEU
1	D	571	ARG
1	D	576	ASN
1	D	577	LYS
1	D	589	THR
1	D	635	ARG
1	D	639	ARG
1	D	790	ILE
1	D	792	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	472	ASN
1	A	576	ASN
1	A	670	GLN
1	A	720	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	774	ASN
1	A	779	ASN
1	A	796	GLN
1	B	576	ASN
1	B	582	GLN
1	B	796	GLN
1	C	501	GLN
1	C	576	ASN
1	C	720	GLN
1	C	793	GLN
1	C	796	GLN
1	D	576	ASN
1	D	582	GLN
1	D	793	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](#)

7 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	SO4	A	5	-	4,4,4	0.13	0	6,6,6	0.19	0
2	SO4	A	6	-	4,4,4	0.17	0	6,6,6	0.18	0
2	SO4	B	1	-	4,4,4	0.19	0	6,6,6	0.25	0
2	SO4	B	7	-	4,4,4	0.22	0	6,6,6	0.28	0
2	SO4	C	3	-	4,4,4	0.12	0	6,6,6	0.21	0
2	SO4	D	2	-	4,4,4	0.22	0	6,6,6	0.40	0
2	SO4	D	4	-	4,4,4	0.09	0	6,6,6	0.35	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	SO4	A	5	-	-	0/0/0/0	0/0/0/0
2	SO4	A	6	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1	-	-	0/0/0/0	0/0/0/0
2	SO4	B	7	-	-	0/0/0/0	0/0/0/0
2	SO4	C	3	-	-	0/0/0/0	0/0/0/0
2	SO4	D	2	-	-	0/0/0/0	0/0/0/0
2	SO4	D	4	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5	SO4	1	0
2	B	1	SO4	1	0
2	B	7	SO4	1	0

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 [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	334/391 (85%)	-0.19	2 (0%) 90 87	53, 74, 86, 89	0
1	B	194/391 (49%)	-0.17	2 (1%) 84 78	52, 65, 82, 85	0
1	C	337/391 (86%)	-0.09	6 (1%) 71 63	52, 76, 92, 100	0
1	D	199/391 (50%)	-0.28	0 100 100	47, 62, 85, 91	0
All	All	1064/1564 (68%)	-0.18	10 (0%) 85 80	47, 71, 89, 100	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	572	GLY	3.3
1	B	593	THR	3.2
1	A	718	TYR	3.0
1	C	573	ILE	2.6
1	A	573	ILE	2.4
1	C	760	LYS	2.4
1	C	571	ARG	2.3
1	B	592	LYS	2.3
1	C	508	ARG	2.2
1	C	532	PRO	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	SO4	D	4	5/5	0.98	0.18	1.22	72,73,74,74	0
2	SO4	B	7	5/5	0.95	0.16	-0.21	70,70,71,71	0
2	SO4	D	2	5/5	0.98	0.11	-0.89	55,57,60,61	0
2	SO4	B	1	5/5	0.98	0.09	-1.44	64,65,66,67	0
2	SO4	A	6	5/5	0.92	0.10	-	109,110,111,111	0
2	SO4	A	5	5/5	0.96	0.08	-	97,97,98,98	0
2	SO4	C	3	5/5	0.98	0.12	-	67,67,69,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.