



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:47 AM UTC

PDB ID : 3TSW / pdb_00003tsw
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

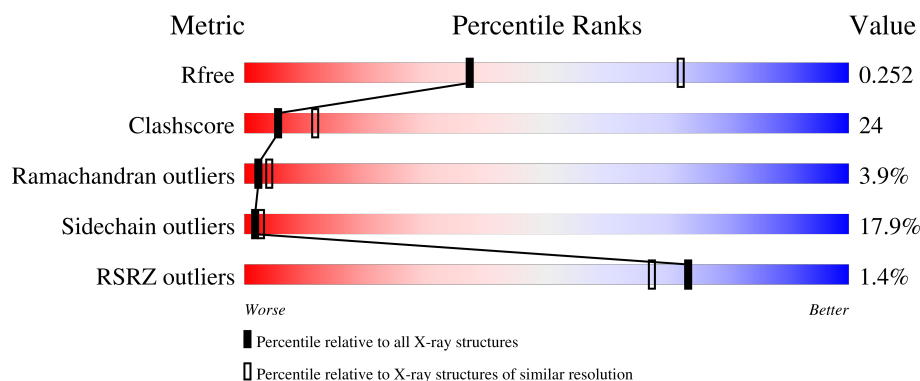
1 Overall quality at a glance

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}	180053	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	% 42% 35% 8% 15%
1	B	391	19% 24% 5% 50%
1	C	391	2% 42% 38% 6% 14%
1	D	391	% 23% 23% 5% 49%

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 (CCD ID: SO4) (formula: O₄S).

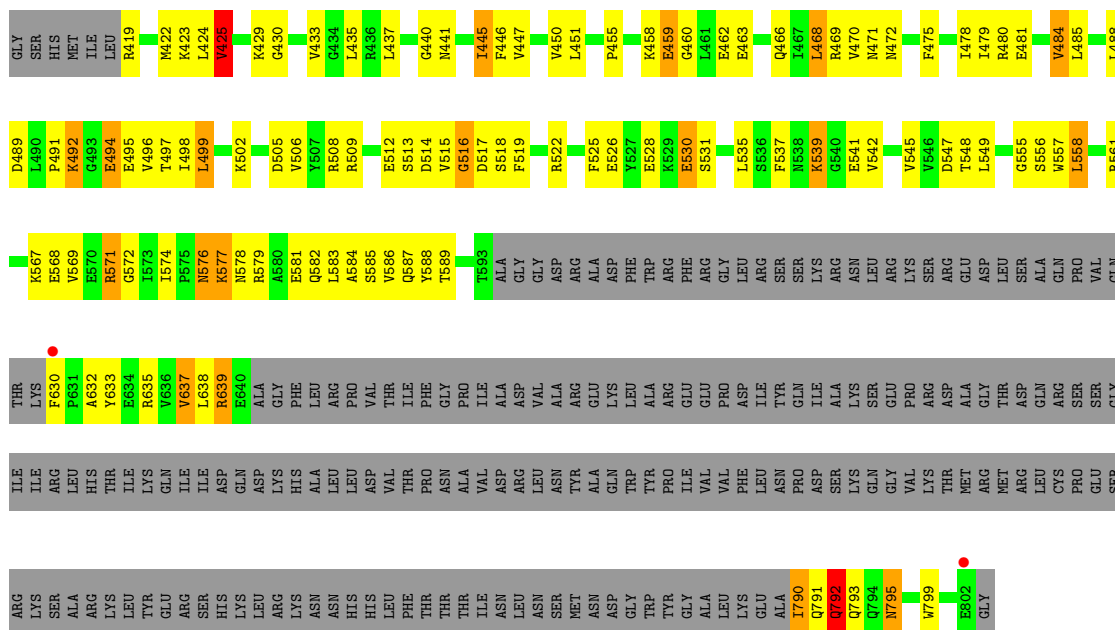


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- 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		

Chain C:



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 87.15 – 2.85	Depositor EDS
% Data completeness (in resolution range)	96.2 (87.17-2.85) 97.5 (87.15-2.85)	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 0.190 , 0.252	Depositor DCC
R_{free} test set	4762 reflections (9.83%)	wwPDB-VP
Wilson B-factor (Å ²)	75.9	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	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
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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.72	0/2736	1.03	6/3688 (0.2%)
1	B	0.76	0/1578	1.09	9/2124 (0.4%)
1	C	0.69	0/2753	1.01	1/3712 (0.0%)
1	D	0.83	0/1615	1.09	2/2175 (0.1%)
All	All	0.74	0/8682	1.04	18/11699 (0.2%)

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 (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	651	GLY	CA-C-N	8.42	128.07	119.82
1	A	651	GLY	C-N-CA	8.42	128.07	119.82
1	B	502	LYS	N-CA-C	7.70	119.31	111.07
1	B	574	ILE	CA-C-N	-6.86	112.58	119.92
1	B	574	ILE	C-N-CA	-6.86	112.58	119.92
1	B	796	GLN	N-CA-C	6.75	125.18	110.80
1	B	569	VAL	N-CA-C	6.21	116.36	110.53
1	B	460	GLY	N-CA-C	6.19	121.65	114.16
1	A	630	PHE	CA-C-N	6.02	127.36	119.84
1	A	630	PHE	C-N-CA	6.02	127.36	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	795	ASN	N-CA-C	5.98	118.05	109.14
1	B	592	LYS	N-CA-C	5.75	117.96	108.48
1	D	630	PHE	CA-C-N	-5.64	113.89	119.92
1	D	630	PHE	C-N-CA	-5.64	113.89	119.92
1	A	556	SER	N-CA-C	5.55	117.45	108.34
1	C	427	PHE	N-CA-C	5.39	117.27	109.07
1	B	441	ASN	N-CA-C	5.20	119.09	112.34
1	A	573	ILE	N-CA-C	5.12	115.86	108.48

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	123	0
1	B	1552	0	1564	93	0
1	C	2703	0	2722	111	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	406	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 24.

All (406) 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
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:C:576:ASN:ND2	1:C:579:ARG:H	1.80	0.79
1:D:793:GLN:HE21	1:D:795:ASN:HB2	1.47	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:422:MET:HE2	1:D:499:LEU:HD11	1.68	0.74
1:D:425:VAL:HG22	1:D:459:GLU:HB3	1.68	0.74
1:D:485:LEU:O	1:D:489:ASP:CG	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:506:VAL:HG23	3:C:64:HOH:O	1.91	0.70
1:B:576:ASN:HD21	1:B:579:ARG:N	1.90	0.69
1:B:582:GLN:HE22	1:D:478:ILE:HD12	1.56	0.69
1:B:579:ARG:CG	1:D:489:ASP:HB3	2.22	0.69
1:A:802:GLU:OE2	1:A:802:GLU:HA	1.92	0.69
1:C:466:GLN:OE1	1:C:503:LYS:HD2	1.93	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:C:634:GLU:O	1:C:635:ARG:C	2.36	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
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:464:GLY:O	1:B:502:LYS:O	2.12	0.68
1:B:491:PRO:HD2	1:B:494:GLU:HG3	1.76	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:A:524:HIS:CG	1:A:630:PHE:HB3	2.31	0.65
1:B:454:SER:HB2	1:B:455:PRO:HD2	1.79	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:440:GLY:HA3	1:D:516:GLY:C	2.23	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:B:494:GLU:OE2	1:B:494:GLU:HA	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:C:634:GLU:HG2	1.98	0.61
1:C:513:SER:O	1:C:514:ASP:C	2.42	0.61
1:B:440:GLY:N	1:B:444:GLY:O	2.34	0.61
1:C:694:ILE:C	1:C:696:GLN:H	2.08	0.61
1:D:576:ASN:N	1:D:576:ASN:HD22	1.98	0.61
1:B:529:LYS:HZ1	1:B:532:PRO:HA	1.64	0.60
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:779:ASN:C	1:A:779:ASN:HD22	2.10	0.60
1:A:643:PHE:HD1	1:A:644:LEU:O	1.85	0.60
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:B:428:ARG:HG2	1:B:429:LYS:O	2.03	0.59
1:C:694:ILE:HG13	1:C:721:TRP:HZ3	1.67	0.59
1:D:578:ASN:O	1:D:582:GLN:HG2	2.02	0.59
1:A:673:LYS:O	1:A:693:THR:HG21	2.02	0.59
1:D:429:LYS:O	1:D:492:LYS:O	2.20	0.59
1:B:531:SER:C	1:B:533:TYR:H	2.10	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:423:LYS:NZ	3:A:4:HOH:O	2.35	0.58
1:A:547:ASP:OD2	1:A:550:TYR:HA	2.03	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:A:750:SER:HB3	1:A:753:LYS:HE3	1.86	0.58
1:B:479:ILE:HD11	1:B:635:ARG:NH2	2.18	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:A:523:THR:HG23	1:A:541:GLU:O	2.04	0.57
1:B:630:PHE:N	1:B:630:PHE:CD2	2.73	0.57
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:492:LYS:O	1:D:492:LYS:HG2	2.05	0.56
1:A:655:ASP:HA	1:A:658:ARG:CZ	2.36	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:C:437:LEU:HD13	1:C:445:ILE:HG21	1.87	0.55
1:C:726:VAL:HG22	1:C:771:THR:HG23	1.87	0.55
1:B:440:GLY:O	1:B:444:GLY:N	2.38	0.55
1:D:437:LEU:HD13	1:D:445:ILE:HD12	1.88	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
1:A:646:PRO:HB3	1:A:706:LEU:HD11	1.88	0.55
1:C:478:ILE:HD13	1:C:482:GLU:OE1	2.06	0.55
1:A:473:VAL:HG21	1:A:486:PHE:CZ	2.42	0.54
1:A:438:ALA:HA	1:A:480:ARG:HH21	1.72	0.54
1:D:793:GLN:NE2	1:D:795:ASN:HB2	2.19	0.54
1:A:535:LEU:HD12	1:A:543:PHE:HE2	1.72	0.54
1:C:502:LYS:O	1:C:503:LYS:C	2.50	0.54
1:B:796:GLN:HE21	1:B:796:GLN:HA	1.73	0.54
1:D:558:LEU:HD23	1:D:572:GLY:O	2.08	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:A:780:ASP:HA	1:A:782:TRP:CD1	2.44	0.53
1:B:431:ASP:O	1:B:432:SER:HB2	2.07	0.53
1:D:441:ASN:HD22	1:D:479:ILE:HG12	1.72	0.53
1:C:550:TYR:O	1:C:551:ASN:HB2	2.08	0.53
1:A:575:PRO:O	1:A:633:TYR:OH	2.20	0.53
1:B:576:ASN:C	1:B:576:ASN:HD22	2.17	0.53
1:A:548:THR:HA	1:A:557:TRP:CD1	2.43	0.52
1:B:447:VAL:HG12	1:B:449:GLY:H	1.74	0.52
1:D:425:VAL:HG12	1:D:425:VAL:O	2.07	0.52
1:B:630:PHE:N	1:B:630:PHE:HD2	2.08	0.52
1:D:419:ARG:HH22	1:D:505:ASP:H	1.57	0.52
1:A:526:GLU:HG2	1:A:527:TYR:N	2.24	0.52
1:C:737:LYS:HD2	1:C:751:ALA:HB3	1.92	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:C:699:ASP:C	1:C:701:ASP:H	2.18	0.52
1:D:505:ASP:HA	1:D:508:ARG:HH21	1.74	0.52
1:D:632:ALA:O	1:D:633:TYR:HD1	1.93	0.52
1:A:802:GLU:OE2	1:A:802:GLU:CA	2.58	0.52
1:B:535:LEU:HD21	1:B:571:ARG:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:ASN:O	1:B:579:ARG:C	2.52	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:C:559:ALA:HB3	1:C:574:ILE:HG12	1.91	0.52
1:D:790:ILE:O	1:D:792:GLN:N	2.43	0.52
1:A:535:LEU:HG	1:A:572:GLY:HA3	1.93	0.51
1:D:585:SER:OG	3:D:6:HOH:O	1.91	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:B:592:LYS:O	1:B:593:THR:C	2.52	0.51
1:C:694:ILE:C	1:C:696:GLN:N	2.67	0.51
1:D:638:LEU:C	1:D:639:ARG:HG2	2.36	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:D:567:LYS:NZ	3:D:31:HOH:O	2.43	0.51
1:A:689:ILE:CD1	1:A:715:ARG:HH12	2.24	0.51
1:C:655:ASP:OD2	1:C:655:ASP:N	2.44	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:HH12	1:D:505:ASP:HB2	1.76	0.50
1:A:448:ALA:HA	1:A:507:TYR:OH	2.10	0.50
1:D:419:ARG:HH22	1:D:505:ASP:CB	2.14	0.50
1:C:436:ARG:HD2	1:C:436:ARG:N	2.27	0.50
1:B:636:VAL:HA	1:B:800:VAL:O	2.11	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: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:C:647:VAL:HG22	1:C:724:ILE:HD12	1.93	0.50
1:D:445:ILE:HD11	1:D:480:ARG:HA	1.92	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:A:765:ASN:OD1	1:A:765:ASN:O	2.29	0.49
1:B:567:LYS:HG3	1:C:421:SER:CB	2.41	0.49
1:D:450:VAL:CG1	1:D:451:LEU:N	2.61	0.49
1:C:635:ARG:HG2	1:C:803:GLY:HA2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:584:ALA:O	1:D:585:SER:C	2.54	0.49
1:B:514:ASP:OD2	1:B:514:ASP:C	2.55	0.49
1:C:776:ASN:OD1	1:C:776:ASN:C	2.56	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:422:MET:HE3	1:D:468:LEU:HD13	1.94	0.49
1:B:549:LEU:O	1:B:550:TYR:C	2.54	0.49
1:D:462:GLU:O	1:D:463:GLU:C	2.56	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: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:716:LEU:O	1:C:717:ASN:C	2.55	0.49
1:A:469:ARG:HG2	1:A:472:ASN:HA	1.94	0.48
1:C:637:VAL:HB	1:C:802:GLU:HB3	1.95	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:B:461:LEU:HA	1:B:465:ASP:OD2	2.13	0.48
1:D:513:SER:O	1:D:515:VAL:N	2.46	0.48
1:D:579:ARG:O	1:D:583:LEU:HG	2.14	0.48
1:B:796:GLN:HE21	1:B:796:GLN:CA	2.27	0.48
1:B:422:MET:HG3	1:B:501:GLN:HG3	1.94	0.48
1:B:514:ASP:O	1:B:515:VAL:C	2.56	0.48
1:C:644:LEU:HD21	3:C:23:HOH:O	2.14	0.48
1:D:547:ASP:HB3	1:D:558:LEU:HB3	1.95	0.48
1:B:475:PHE:C	1:B:477:ASN:H	2.21	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:A:644:LEU:HD22	1:A:701:ASP:C	2.39	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:A:707:ASP:O	1:A:707:ASP:CG	2.57	0.47
1:A:470:VAL:HG22	1:A:498:ILE:HG12	1.96	0.47
1:A:434:GLY:CA	1:A:451:LEU:HB2	2.44	0.47
1:A:743:LEU:HD11	1:A:782:TRP:HZ2	1.79	0.47
1:B:569:VAL:HG12	1:B:570:GLU:HG2	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:650:PHE:O	1:C:727:PHE:HA	2.15	0.47
1:C:664:GLU:O	1:C:666:PRO:CD	2.63	0.47
1:B:533:TYR:CE2	1:B:572:GLY:HA2	2.49	0.47
1:B:576:ASN:C	1:B:576:ASN:ND2	2.71	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:A:630:PHE:HA	1:A:631:PRO:HD2	1.59	0.46
1:B:480:ARG:HD3	1:B:549:LEU:HB2	1.96	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:C:721:TRP:O	1:C:722:TYR:C	2.59	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:A:708:VAL:HG23	1:A:709:THR:N	2.29	0.46
1:C:663:ARG:HD2	3:C:50:HOH:O	2.14	0.46
1:D:548:THR:HA	1:D:557:TRP:CD1	2.51	0.46
1:B:428:ARG:NH2	2:B:1:SO4:O4	2.49	0.46
1:C:638:LEU:HG	1:C:799:TRP:CH2	2.51	0.46
1:D:475:PHE:HA	1:D:478:ILE:HG22	1.97	0.46
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:A:416:MET:HE2	1:D:571:ARG:HE	1.81	0.45
1:C:637:VAL:HG12	1:C:639:ARG:HG2	1.98	0.45
1:D:419:ARG:NH2	1:D:505:ASP:H	2.15	0.45
1:D:519:PHE:CB	1:D:635:ARG:HH21	2.26	0.45
1:C:461:LEU:HD23	1:C:461:LEU:HA	1.86	0.45
1:A:720:GLN:NE2	1:A:801:SER:HB3	2.32	0.45
1:A:720:GLN:CD	1:A:801:SER:H	2.24	0.45
1:C:438:ALA:HB2	1:C:448:ALA:HB2	1.98	0.45
1:D:537:PHE:HA	1:D:541:GLU:OE2	2.16	0.45
1:A:764:ASN:O	1:A:765:ASN:OD1	2.35	0.45
1:C:545:VAL:HG11	1:C:548:THR:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:729:ASN:HB3	1:C:773:ILE:O	2.17	0.45
1:D:441:ASN:H	1:D:517:ASP:HA	1.82	0.45
1:A:695:LYS:C	1:A:697:ILE:H	2.25	0.44
1:D:440:GLY:HA3	1:D:517:ASP:N	2.32	0.44
1:A:542:VAL:HG11	1:A:799:TRP:CH2	2.52	0.44
1:A:574:ILE:HB	1:A:575:PRO:HD2	1.99	0.44
1:A:645:ARG:O	1:A:646:PRO:C	2.59	0.44
1:C:757:ARG:NH2	1:C:760:LYS:HD3	2.32	0.44
1:A:690:ARG:HG3	1:A:692:HIS:CD2	2.53	0.44
1:B:554:LEU:HD12	1:D:488:LEU:CD1	2.48	0.44
1:C:502:LYS:HD2	1:C:502:LYS:HA	1.82	0.44
1:C:566:HIS:HE1	3:C:9:HOH:O	2.00	0.44
1:D:441:ASN:HD22	1:D:479:ILE:CG1	2.30	0.44
1:A:470:VAL:O	1:A:473:VAL:N	2.51	0.44
1:A:646:PRO:HB2	1:A:723:PRO:HB3	1.99	0.44
1:C:447:VAL:HG12	1:C:447:VAL:O	2.18	0.44
1:D:446:PHE:CE1	1:D:466:GLN:HB2	2.53	0.44
1:A:643:PHE:CD1	1:A:644:LEU:O	2.68	0.44
1:D:469:ARG:HB3	1:D:499:LEU:HB3	2.00	0.44
1:D:518:SER:HA	1:D:545:VAL:O	2.18	0.44
1:D:445:ILE:CG2	1:D:446:PHE:N	2.81	0.43
1:B:447:VAL:HG22	1:B:467:ILE:HD11	1.99	0.43
1:B:527:TYR:CE2	1:B:575:PRO:HD3	2.53	0.43
1:C:699:ASP:C	1:C:701:ASP:N	2.75	0.43
1:D:496:VAL:HG12	1:D:498:ILE:HG13	1.99	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:A:733:LYS:NZ	1:A:733:LYS:H	2.17	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: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:465:ASP:OD1	1:A:465:ASP:N	2.52	0.43
1:B:491:PRO:O	1:B:493:GLY:N	2.51	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:A:698:ILE:O	1:A:700:GLN:N	2.52	0.43
1:B:576:ASN:ND2	1:B:579:ARG:H	2.04	0.43
1:A:481:GLU:HB2	1:A:548:THR:HB	2.00	0.43
1:C:693:THR:O	1:C:693:THR:HG22	2.19	0.43
1:C:654:ALA:CB	1:C:658:ARG:NH2	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:712:ALA:O	1:C:713:VAL:C	2.62	0.43
1:D:576:ASN:N	1:D:576:ASN:ND2	2.65	0.43
1:A:446:PHE:CE1	1:A:466:GLN:HB2	2.54	0.42
1:B:510:ILE:HD13	1:B:510:ILE:HA	1.89	0.42
1:B:576:ASN:ND2	1:B:579:ARG:N	2.64	0.42
1:C:744:CYS:O	1:C:744:CYS:SG	2.76	0.42
1:B:531:SER:O	1:B:533:TYR:N	2.52	0.42
1:C:541:GLU:OE1	1:C:561:ARG:NH1	2.52	0.42
1:D:522:ARG:HH22	1:D:799:TRP:HB2	1.81	0.42
1:D:792:GLN:H	1:D:792:GLN:HG3	1.70	0.42
1:A:739:MET:SD	1:A:777:SER:HA	2.58	0.42
1:A:781:GLY:O	1:A:782:TRP:C	2.63	0.42
1:B:567:LYS:NZ	1:C:421:SER:OG	2.43	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:C:638:LEU:O	1:C:639:ARG:HD3	2.19	0.42
1:C:664:GLU:C	1:C:666:PRO:HD3	2.43	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:A:740:ARG:HD2	1:A:754:LEU:CD1	2.49	0.42
1:A:800:VAL:HG11	1:B:588:TYR:CD2	2.54	0.42
1:B:466:GLN:OE1	1:B:503:LYS:HD3	2.20	0.42
1:C:498:ILE:HG22	1:C:499:LEU:N	2.35	0.42
1:C:657:ALA:O	1:C:661:LEU:HG	2.19	0.42
1:A:656:VAL:HG11	1:A:743:LEU:HD13	2.02	0.42
1:A:735:GLY:O	1:A:736:VAL:C	2.63	0.42
1:C:667:ASP:C	1:C:668:ILE:HG13	2.45	0.42
1:C:794:GLN:O	1:C:794:GLN:CG	2.67	0.42
1:A:698:ILE:C	1:A:700:GLN:H	2.27	0.42
1:A:722:TYR:HE1	1:A:800:VAL:HG12	1.84	0.42
1:A:520:TYR:CZ	1:A:544:ARG:HG3	2.55	0.42
1:A:646:PRO:HA	1:A:704:ALA:HB3	2.02	0.42
1:A:732:SER:HA	1:A:733:LYS:HZ3	1.84	0.42
1:A:494:GLU:HG3	1:A:495:GLU:N	2.35	0.42
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:A:734:GLN:O	1:A:735:GLY:C	2.63	0.41
1:D:471:ASN:O	1:D:472:ASN:HB2	2.20	0.41
1:A:452:GLU:O	1:A:453:ASP:CB	2.68	0.41
1:C:793:GLN:NE2	3:C:12:HOH:O	2.52	0.41
1:A:713:VAL:CG1	1:A:768:LEU:HD22	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:726:VAL:HG22	1:A:771:THR:HG22	2.03	0.41
1:A:796:GLN:HE21	1:A:796:GLN:HA	1.83	0.41
1:B:541:GLU:OE1	1:B:561:ARG:NH1	2.44	0.41
1:C:766:HIS:N	3:C:19:HOH:O	2.52	0.41
1:C:793:GLN:O	1:C:796:GLN:HB3	2.21	0.41
1:A:419:ARG:HB2	1:D:568:GLU:HG3	2.02	0.41
1:A:576:ASN:N	1:A:576:ASN:HD22	2.18	0.41
1:A:698:ILE:C	1:A:700:GLN:N	2.78	0.41
1:B:531:SER:C	1:B:533:TYR:N	2.75	0.41
1:C:560:ILE:HD11	1:C:571:ARG:HE	1.85	0.41
1:D:519:PHE:HB2	1:D:635:ARG:HE	1.86	0.41
1:A:524:HIS:O	1:A:525:PHE:HB3	2.21	0.41
1:B:475:PHE:C	1:B:477:ASN:N	2.79	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:A:726:VAL:CG1	1:A:773:ILE:HD12	2.51	0.41
1:B:535:LEU:HB2	1:B:574:ILE:HG23	2.02	0.41
1:B:557:TRP:O	1:B:573:ILE:HA	2.20	0.41
1:C:439:GLY:O	1:C:516:GLY:HA2	2.21	0.41
1:D:576:ASN:O	1:D:578:ASN:N	2.54	0.41
1:A:704:ALA:O	1:A:706:LEU:HG	2.20	0.41
1:A:731:ASP:OD2	1:A:731:ASP:N	2.46	0.41
1:A:746:GLU:O	1:A:747:SER:C	2.64	0.41
1:C:629:LYS:O	1:C:718:TYR:OH	2.38	0.41
1:C:794:GLN:O	1:C:794:GLN:CD	2.63	0.41
1:C:796:GLN:HG3	1:C:797:LEU:N	2.36	0.41
1:D:455:PRO:HA	1:D:458:LYS:CB	2.50	0.41
1:D:526:GLU:O	1:D:587:GLN:NE2	2.46	0.41
1:B:534:GLY:HA2	1:B:573:ILE:O	2.21	0.41
1:A:585:SER:C	1:A:587:GLN:H	2.29	0.40
1:B:451:LEU:O	1:B:454:SER:OG	2.36	0.40
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:C:689:ILE:N	1:C:715:ARG:HH11	2.19	0.40
1:C:718:TYR:C	1:C:720:GLN:H	2.29	0.40
1:A:641:ALA:C	1:A:643:PHE:H	2.29	0.40
1:C:709:THR:HG1	1:C:711:ASN:HB2	1.82	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%)	2	3
1	B	188/391 (48%)	153 (81%)	29 (15%)	6 (3%)	3	6
1	C	331/391 (85%)	265 (80%)	53 (16%)	13 (4%)	2	4
1	D	193/391 (49%)	150 (78%)	35 (18%)	8 (4%)	2	3
All	All	1040/1564 (66%)	834 (80%)	165 (16%)	41 (4%)	2	4

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
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

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Mol	Chain	Res	Type
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 [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	289/338 (86%)	237 (82%)	52 (18%)	2	3
1	B	167/338 (49%)	128 (77%)	39 (23%)	1	0
1	C	289/338 (86%)	242 (84%)	47 (16%)	2	4
1	D	171/338 (51%)	145 (85%)	26 (15%)	3	5
All	All	916/1352 (68%)	752 (82%)	164 (18%)	2	3

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	416	MET
1	A	417	ILE

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Mol	Chain	Res	Type
1	A	421	SER
1	A	424	LEU
1	A	425	VAL
1	A	426	LYS
1	A	431	ASP
1	A	450	VAL
1	A	451	LEU
1	A	452	GLU
1	A	453	ASP
1	A	465	ASP
1	A	469	ARG
1	A	472	ASN
1	A	476	THR
1	A	478	ILE
1	A	479	ILE
1	A	484	VAL
1	A	492	LYS
1	A	494	GLU
1	A	495	GLU
1	A	521	ILE
1	A	526	GLU
1	A	530	GLU
1	A	554	LEU
1	A	576	ASN
1	A	581	GLU
1	A	637	VAL
1	A	659	GLU
1	A	660	LYS
1	A	689	ILE
1	A	690	ARG
1	A	694	ILE
1	A	699	ASP
1	A	700	GLN
1	A	708	VAL
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	753	LYS
1	A	762	ARG

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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	450	VAL
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	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	528	GLU
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	583	LEU
1	B	587	GLN
1	B	589	THR
1	B	590	LEU
1	B	592	LYS
1	B	630	PHE

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Mol	Chain	Res	Type
1	B	635	ARG
1	B	794	GLN
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	461	LEU
1	C	462	GLU
1	C	476	THR
1	C	478	ILE
1	C	484	VAL
1	C	485	LEU
1	C	492	LYS
1	C	497	THR
1	C	504	LYS
1	C	515	VAL
1	C	528	GLU
1	C	546	VAL
1	C	554	LEU
1	C	558	LEU
1	C	576	ASN
1	C	581	GLU
1	C	637	VAL
1	C	655	ASP
1	C	665	GLU
1	C	690	ARG
1	C	691	LEU
1	C	694	ILE
1	C	706	LEU
1	C	711	ASN
1	C	733	LYS
1	C	747	SER
1	C	748	ARG

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Mol	Chain	Res	Type
1	C	753	LYS
1	C	759	HIS
1	C	761	LEU
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	433	VAL
1	D	435	LEU
1	D	445	ILE
1	D	459	GLU
1	D	468	LEU
1	D	484	VAL
1	D	492	LYS
1	D	494	GLU
1	D	497	THR
1	D	499	LEU
1	D	530	GLU
1	D	531	SER
1	D	539	LYS
1	D	542	VAL
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	637	VAL
1	D	639	ARG
1	D	790	ILE
1	D	792	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	472	ASN
1	A	524	HIS

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Mol	Chain	Res	Type
1	A	576	ASN
1	A	670	GLN
1	A	711	ASN
1	A	720	GLN
1	A	767	HIS
1	A	774	ASN
1	A	779	ASN
1	A	796	GLN
1	B	524	HIS
1	B	565	ASN
1	B	576	ASN
1	B	582	GLN
1	B	794	GLN
1	B	796	GLN
1	C	501	GLN
1	C	538	ASN
1	C	566	HIS
1	C	576	ASN
1	C	692	HIS
1	C	720	GLN
1	C	793	GLN
1	C	796	GLN
1	D	576	ASN
1	D	792	GLN
1	D	793	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 oligosaccharides in this entry.

5.6 Ligand geometry

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	C	3	-	4,4,4	0.27	0	6,6,6	0.33	0
2	SO4	D	2	-	4,4,4	0.40	0	6,6,6	0.46	0
2	SO4	A	6	-	4,4,4	0.30	0	6,6,6	0.15	0
2	SO4	B	1	-	4,4,4	0.38	0	6,6,6	0.24	0
2	SO4	B	7	-	4,4,4	0.38	0	6,6,6	0.44	0
2	SO4	D	4	-	4,4,4	0.24	0	6,6,6	0.33	0
2	SO4	A	5	-	4,4,4	0.25	0	6,6,6	0.24	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	B	1	SO4	1	0
2	B	7	SO4	1	0
2	A	5	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%)	0.08	5 (1%) 72 65	53, 74, 86, 89	0
1	B	194/391 (49%)	-0.01	1 (0%) 87 85	52, 65, 82, 85	0
1	C	337/391 (86%)	0.14	7 (2%) 63 55	52, 76, 92, 100	0
1	D	199/391 (50%)	-0.10	2 (1%) 79 75	47, 62, 85, 91	0
All	All	1064/1564 (68%)	0.05	15 (1%) 73 67	47, 71, 89, 100	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	433	VAL	3.0
1	C	689	ILE	2.9
1	A	688	ILE	2.8
1	C	451	LEU	2.6
1	B	431	ASP	2.5
1	C	677	ARG	2.5
1	A	689	ILE	2.5
1	D	802	GLU	2.4
1	A	573	ILE	2.3
1	D	630	PHE	2.2
1	A	802	GLU	2.2
1	C	571	ARG	2.2
1	C	489	ASP	2.1
1	C	691	LEU	2.0
1	A	718	TYR	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 oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	6	5/5	0.90	0.07	109,110,111,111	0
2	SO4	A	5	5/5	0.91	0.06	97,97,98,98	0
2	SO4	C	3	5/5	0.95	0.11	67,67,69,70	0
2	SO4	B	7	5/5	0.96	0.14	70,70,71,71	0
2	SO4	D	2	5/5	0.96	0.08	55,57,60,61	0
2	SO4	B	1	5/5	0.97	0.05	64,65,66,67	0
2	SO4	D	4	5/5	0.98	0.06	72,73,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.