



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:03 AM GMT

PDB ID : 2ZAG
Title : Crystal structure of the SeMet-substituted soluble domain of STT3 from *P. furiosus*
Authors : Maita, N.
Deposited on : 2007-10-05
Resolution : 3.00 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

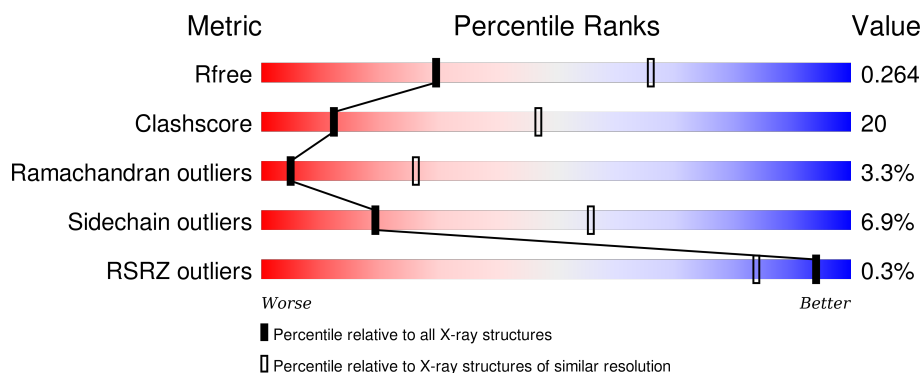
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	497	<div> <div>54%</div> <div>37%</div> <div>...</div> </div>
1	B	497	<div> <div>57%</div> <div>35%</div> <div>..</div> </div>
1	C	497	<div> <div>52%</div> <div>39%</div> <div>5% .</div> </div>
1	D	497	<div> <div>56%</div> <div>35%</div> <div>6% .</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CA	A	1	-	-	-	X
2	CA	B	2	-	-	-	X
2	CA	D	4	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 15179 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 Oligosaccharyl transferase stt3 subunit related protein.

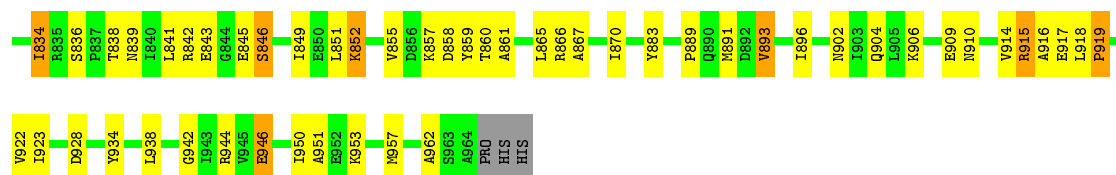
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	478	Total	C	N	O	S	Se	0	0	0
			3790	2444	615	725	2	4			
1	B	477	Total	C	N	O	S	Se	0	0	0
			3786	2441	617	722	2	4			
1	C	478	Total	C	N	O	S	Se	0	0	0
			3792	2445	618	723	2	4			
1	D	480	Total	C	N	O	S	Se	0	0	0
			3803	2452	621	724	2	4			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		

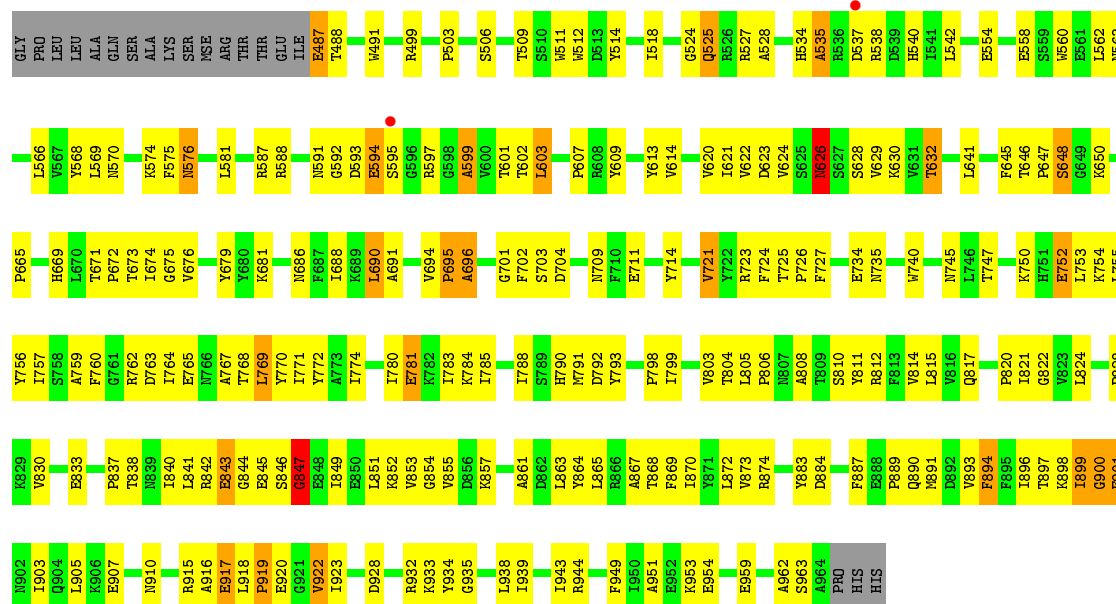
- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		



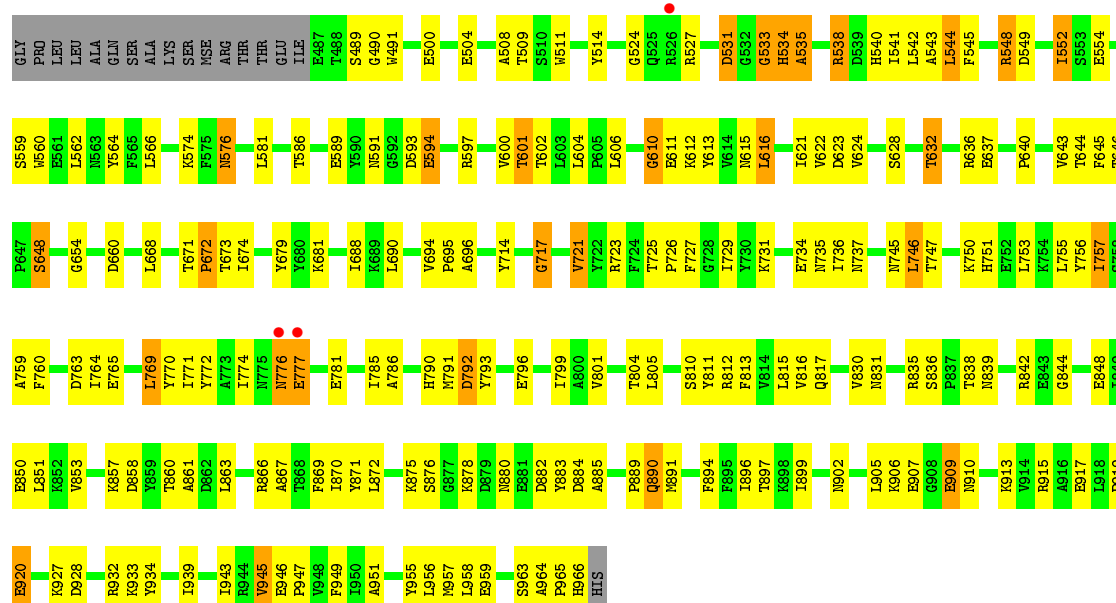
• Molecule 1: Oligosaccharyl transferase stt3 subunit related protein

Chain C: 52% 39% 5%



• Molecule 1: Oligosaccharyl transferase stt3 subunit related protein

Chain D: 56% 35% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	137.40 Å 266.40 Å 73.98 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 29.97 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-3.00) 100.0 (29.97-3.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.15 (at 3.00 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.220 , 0.272 0.216 , 0.264	Depositor DCC
R_{free} test set	3916 reflections (7.10%)	DCC
Wilson B-factor (Å ²)	55.1	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 49.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 55283 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15179	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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: CA, CL

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	0.48	0/3876	0.73	1/5261 (0.0%)
1	B	0.44	0/3872	0.70	1/5255 (0.0%)
1	C	0.41	1/3878 (0.0%)	0.66	1/5263 (0.0%)
1	D	0.47	0/3891	0.71	1/5283 (0.0%)
All	All	0.45	1/15517 (0.0%)	0.70	4/21062 (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	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	487	GLU	CB-CG	-5.25	1.42	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	847	GLY	N-CA-C	5.55	126.97	113.10
1	D	860	THR	N-CA-C	-5.52	96.09	111.00
1	A	566	LEU	CA-CB-CG	5.29	127.48	115.30
1	B	860	THR	N-CA-C	-5.05	97.36	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	955	TYR	Sidechain

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	3790	0	3721	146	0
1	B	3786	0	3724	131	0
1	C	3792	0	3728	177	0
1	D	3803	0	3726	154	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	1	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	1	0
All	All	15179	0	14899	593	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 20.

All (593) 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:C:560:TRP:HE1	1:C:891:MSE:HE1	1.25	0.98
1:B:537:ASP:HB3	1:B:870:ILE:HD12	1.46	0.97
1:B:834:ILE:HD13	1:B:834:ILE:H	1.32	0.95
1:B:560:TRP:HE1	1:B:891:MSE:HE1	1.36	0.89
1:A:846:SER:HB3	1:A:917:GLU:HG3	1.57	0.87
1:A:863:LEU:HB3	1:A:900:GLY:HA3	1.54	0.87
1:C:487:GLU:CG	1:C:488:THR:H	1.87	0.86
1:D:757:ILE:HD13	1:D:757:ILE:H	1.40	0.85
1:C:841:LEU:HD11	1:C:916:ALA:HB1	1.59	0.85
1:D:535:ALA:HB3	1:D:538:ARG:HB2	1.60	0.84
1:D:755:LEU:HB2	1:D:799:ILE:HG22	1.61	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:906:LYS:H	1:D:910:ASN:HD21	1.30	0.78
1:A:541:ILE:HG23	1:A:555:VAL:HG21	1.64	0.78
1:A:606:LEU:HD23	1:A:615:ASN:HB2	1.66	0.77
1:B:569:LEU:HD12	1:B:718:ASN:HA	1.66	0.77
1:B:861:ALA:HB2	1:B:951:ALA:HB2	1.64	0.77
1:B:867:ALA:HB2	1:B:896:ILE:HD11	1.66	0.76
1:C:861:ALA:HB2	1:C:951:ALA:HB2	1.69	0.75
1:A:813:PHE:HB3	1:A:957:MSE:HE3	1.67	0.75
1:B:490:GLY:HA3	1:B:717:GLY:H	1.51	0.75
1:A:745:ASN:HB2	1:A:961:SER:O	1.87	0.74
1:C:771:ILE:HG13	1:C:785:ILE:HD13	1.69	0.73
1:A:569:LEU:HB2	1:A:718:ASN:HB3	1.70	0.73
1:D:747:THR:HG21	1:D:965:PRO:HB3	1.72	0.72
1:D:491:TRP:HZ3	1:D:566:LEU:HD23	1.54	0.72
1:D:791:MSE:O	1:D:792:ASP:HB3	1.89	0.72
1:D:747:THR:HG22	1:D:963:SER:HB2	1.72	0.72
1:D:600:VAL:HG12	1:D:601:THR:N	2.04	0.71
1:B:560:TRP:NE1	1:B:891:MSE:HE1	2.05	0.71
1:B:709:ASN:ND2	1:B:760:PHE:HB2	2.06	0.70
1:D:560:TRP:HE1	1:D:891:MSE:HE1	1.56	0.70
1:D:863:LEU:HD23	1:D:899:ILE:HG13	1.73	0.70
1:A:625:SER:O	1:A:626:ASN:HB3	1.92	0.70
1:B:569:LEU:HD23	1:B:691:ALA:HB1	1.73	0.69
1:B:852:LYS:HZ2	1:B:852:LYS:H	1.39	0.69
1:B:834:ILE:CD1	1:B:834:ILE:H	2.03	0.69
1:C:621:ILE:HB	1:C:632:THR:HG23	1.73	0.69
1:C:767:ALA:HB2	1:C:817:GLN:HE21	1.57	0.68
1:C:624:VAL:HG22	1:C:629:VAL:HG12	1.75	0.68
1:C:623:ASP:HB3	1:C:630:LYS:HB3	1.74	0.68
1:C:671:THR:HG22	1:C:673:THR:H	1.59	0.68
1:A:600:VAL:HG11	1:A:679:TYR:CD1	2.28	0.67
1:D:839:ASN:HA	1:D:945:VAL:HG23	1.75	0.67
1:B:593:ASP:HB2	1:B:594:GLU:OE2	1.93	0.67
1:A:934:TYR:CE2	1:D:897:THR:HG22	2.29	0.67
1:D:896:ILE:HG22	1:D:897:THR:HG23	1.76	0.67
1:C:767:ALA:HB2	1:C:817:GLN:HB3	1.75	0.66
1:B:834:ILE:HD13	1:B:834:ILE:N	2.07	0.66
1:C:560:TRP:NE1	1:C:891:MSE:HE1	2.07	0.66
1:C:867:ALA:HA	1:C:944:ARG:O	1.95	0.66
1:D:540:HIS:ND1	1:D:872:LEU:HD21	2.11	0.66
1:D:765:GLU:H	1:D:817:GLN:NE2	1.94	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:781:GLU:HG3	1:C:783:ILE:HG23	1.78	0.65
1:B:688:ILE:HG22	1:B:694:VAL:HB	1.79	0.65
1:C:863:LEU:HG	1:C:899:ILE:HD12	1.76	0.65
1:B:785:ILE:HB	1:B:801:VAL:HG21	1.79	0.65
1:C:735:ASN:HB3	1:C:752:GLU:HB3	1.79	0.65
1:A:767:ALA:HB2	1:A:817:GLN:HE21	1.61	0.65
1:A:765:GLU:H	1:A:817:GLN:HE22	1.43	0.65
1:C:641:LEU:HD11	1:C:665:PRO:HA	1.79	0.65
1:A:652:ILE:HD12	1:A:653:LYS:N	2.12	0.64
1:A:544:LEU:HD13	1:A:889:PRO:HG2	1.79	0.64
1:A:560:TRP:HE1	1:A:891:MSE:HE1	1.61	0.64
1:A:755:LEU:HB2	1:A:799:ILE:HG22	1.78	0.64
1:A:541:ILE:HG23	1:A:555:VAL:CG2	2.28	0.64
1:B:846:SER:OG	1:B:917:GLU:HG3	1.98	0.64
1:B:505:TYR:HE2	1:B:825:LEU:HD21	1.64	0.63
1:B:838:THR:HA	1:B:946:GLU:HG2	1.80	0.63
1:C:922:VAL:HG23	1:C:923:ILE:H	1.63	0.63
1:A:684:THR:HG21	1:A:698:THR:HG22	1.81	0.62
1:B:865:LEU:HD13	1:B:918:LEU:HD13	1.81	0.62
1:D:850:GLU:HG3	1:D:913:LYS:HG2	1.81	0.62
1:C:487:GLU:CG	1:C:488:THR:N	2.56	0.62
1:A:774:ILE:O	1:A:808:ALA:HB1	1.99	0.62
1:D:763:ASP:OD2	1:D:792:ASP:HA	2.00	0.61
1:D:870:ILE:HD11	1:D:891:MSE:HE3	1.81	0.61
1:B:767:ALA:HB2	1:B:817:GLN:HB3	1.82	0.61
1:C:671:THR:HB	1:C:674:ILE:O	2.00	0.61
1:B:637:GLU:H	1:B:659:SER:HB2	1.64	0.61
1:B:714:TYR:HB3	1:B:721:VAL:CG1	2.31	0.61
1:D:679:TYR:HE2	1:D:681:LYS:HD2	1.65	0.61
1:A:600:VAL:HG12	1:A:601:THR:N	2.14	0.61
1:D:774:ILE:HB	1:D:810:SER:OG	2.01	0.61
1:A:846:SER:HB3	1:A:917:GLU:CG	2.30	0.61
1:D:600:VAL:CG1	1:D:601:THR:N	2.64	0.61
1:A:586:THR:OG1	1:A:589:GLU:HG3	2.01	0.61
1:C:851:LEU:HD12	1:C:851:LEU:O	2.01	0.61
1:C:830:VAL:O	1:C:833:GLU:HG2	2.00	0.60
1:C:518:ILE:HD11	1:D:616:LEU:HD11	1.83	0.60
1:C:613:TYR:HB2	1:C:622:VAL:HB	1.82	0.60
1:D:714:TYR:HB3	1:D:721:VAL:CG1	2.31	0.60
1:A:934:TYR:HE2	1:D:897:THR:HG22	1.66	0.59
1:A:919:PRO:HB2	1:A:922:VAL:HG13	1.82	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:593:ASP:HA	1:C:883:TYR:CE2	2.37	0.59
1:A:698:THR:HG21	1:D:932:ARG:HE	1.68	0.59
1:A:746:LEU:O	1:A:962:ALA:HA	2.01	0.59
1:A:745:ASN:C	1:A:745:ASN:HD22	2.05	0.59
1:C:540:HIS:HD2	1:C:872:LEU:HD21	1.65	0.59
1:B:508:ALA:O	1:B:532:GLY:HA2	2.02	0.59
1:A:771:ILE:HG13	1:A:785:ILE:HD13	1.84	0.59
1:C:592:GLY:N	1:C:599:ALA:HB2	2.18	0.59
1:C:646:THR:O	1:C:672:PRO:HD3	2.02	0.59
1:D:842:ARG:HB2	1:D:842:ARG:HH11	1.67	0.59
1:C:491:TRP:HZ3	1:C:566:LEU:HD23	1.67	0.59
1:C:844:GLY:HA2	1:C:918:LEU:O	2.03	0.59
1:D:765:GLU:H	1:D:817:GLN:HE22	1.51	0.58
1:D:764:ILE:HA	1:D:817:GLN:HE22	1.68	0.58
1:D:759:ALA:HB3	1:D:793:TYR:HA	1.85	0.58
1:A:765:GLU:H	1:A:817:GLN:NE2	2.01	0.58
1:D:870:ILE:HD11	1:D:891:MSE:CE	2.33	0.58
1:D:671:THR:HG22	1:D:673:THR:H	1.69	0.58
1:B:569:LEU:HB2	1:B:718:ASN:HB3	1.85	0.58
1:C:750:LYS:HD2	1:C:804:THR:HG23	1.84	0.58
1:B:757:ILE:HD12	1:B:957:MSE:HE1	1.85	0.58
1:C:846:SER:O	1:C:916:ALA:HB3	2.04	0.58
1:C:918:LEU:HD12	1:C:919:PRO:HD2	1.86	0.58
1:B:612:LYS:HE2	1:B:623:ASP:OD2	2.04	0.58
1:D:600:VAL:HG11	1:D:679:TYR:CD1	2.39	0.58
1:B:792:ASP:HB3	1:B:795:ASN:HB2	1.86	0.58
1:A:746:LEU:HD12	1:A:960:VAL:HG21	1.86	0.57
1:B:526:ARG:O	1:B:527:ARG:HG2	2.03	0.57
1:D:964:ALA:HB1	1:D:966:HIS:ND1	2.19	0.57
1:C:852:LYS:NZ	1:C:852:LYS:HB2	2.19	0.57
1:B:857:LYS:HG2	1:B:858:ASP:H	1.69	0.57
1:B:852:LYS:NZ	1:B:852:LYS:H	2.02	0.57
1:C:626:ASN:ND2	1:C:628:SER:H	2.02	0.57
1:C:838:THR:HG23	1:C:944:ARG:HG2	1.86	0.57
1:D:964:ALA:HB1	1:D:966:HIS:CE1	2.39	0.57
1:D:560:TRP:NE1	1:D:891:MSE:HE1	2.20	0.57
1:D:769:LEU:N	1:D:769:LEU:HD23	2.20	0.57
1:B:788:ILE:HD11	1:B:799:ILE:HD13	1.86	0.57
1:B:746:LEU:O	1:B:962:ALA:HA	2.04	0.57
1:B:560:TRP:HE1	1:B:891:MSE:CE	2.13	0.57
1:A:679:TYR:HE2	1:A:681:LYS:HD2	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:511:TRP:HH2	1:D:581:LEU:HD12	1.68	0.57
1:C:774:ILE:O	1:C:808:ALA:HB1	2.05	0.57
1:A:735:ASN:C	1:A:735:ASN:HD22	2.08	0.56
1:C:540:HIS:CD2	1:C:872:LEU:HD21	2.40	0.56
1:A:499:ARG:HG3	1:A:500:GLU:HG3	1.86	0.56
1:B:544:LEU:HD12	1:B:548:ARG:HG3	1.85	0.56
1:A:528:ALA:HB3	1:A:530:ALA:O	2.06	0.56
1:C:840:ILE:HG23	1:C:841:LEU:HG	1.87	0.56
1:A:705:LYS:HB3	1:A:758:SER:OG	2.05	0.56
1:B:643:VAL:HG13	1:B:668:LEU:HD23	1.87	0.56
1:A:731:LYS:HG3	1:A:742:GLN:NE2	2.21	0.56
1:A:840:ILE:O	1:A:841:LEU:HD12	2.06	0.56
1:D:597:ARG:NH1	1:D:597:ARG:HB3	2.21	0.56
1:D:772:TYR:HB2	1:D:812:ARG:HB2	1.88	0.56
1:C:701:GLY:O	1:C:703:SER:N	2.39	0.55
1:C:772:TYR:HB2	1:C:812:ARG:HB2	1.88	0.55
1:B:671:THR:HG22	1:B:673:THR:HG22	1.86	0.55
1:A:614:VAL:HG23	1:A:620:VAL:O	2.06	0.55
1:D:640:PRO:O	1:D:654:GLY:HA3	2.06	0.55
1:D:858:ASP:OD2	1:D:906:LYS:HA	2.06	0.55
1:C:726:PRO:HB2	1:C:727:PHE:CE1	2.42	0.55
1:C:714:TYR:HB3	1:C:721:VAL:HG13	1.87	0.55
1:D:490:GLY:HA3	1:D:717:GLY:H	1.71	0.55
1:D:906:LYS:N	1:D:910:ASN:HD21	2.02	0.55
1:A:791:MSE:HG3	1:A:797:TYR:CE2	2.40	0.55
1:D:586:THR:OG1	1:D:589:GLU:HG3	2.06	0.55
1:D:750:LYS:HB3	1:D:804:THR:HA	1.89	0.55
1:B:606:LEU:HD23	1:B:615:ASN:HB2	1.89	0.54
1:C:535:ALA:HB3	1:C:538:ARG:HB2	1.89	0.54
1:C:740:TRP:CZ3	1:C:754:LYS:HG3	2.42	0.54
1:A:765:GLU:N	1:A:817:GLN:HE22	2.05	0.54
1:A:680:TYR:CE1	1:D:933:LYS:HB2	2.42	0.54
1:D:805:LEU:HB3	1:D:811:TYR:CE2	2.42	0.54
1:C:601:THR:HG22	1:C:601:THR:O	2.07	0.54
1:B:775:ASN:O	1:B:777:GLU:N	2.40	0.54
1:A:880:ASN:ND2	1:A:939:ILE:HD11	2.23	0.54
1:C:727:PHE:CD2	1:C:764:ILE:HG12	2.43	0.54
1:D:905:LEU:HA	1:D:910:ASN:ND2	2.23	0.54
1:B:821:ILE:HG23	1:B:953:LYS:HD2	1.90	0.54
1:D:757:ILE:HD13	1:D:757:ILE:N	2.16	0.53
1:A:604:LEU:HG	1:A:615:ASN:HD22	1.72	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:558:GLU:HA	1:C:558:GLU:OE2	2.07	0.53
1:B:505:TYR:CE2	1:B:825:LEU:HD21	2.42	0.53
1:B:714:TYR:O	1:B:721:VAL:HG12	2.08	0.53
1:D:811:TYR:O	1:D:959:GLU:HA	2.08	0.53
1:C:780:ILE:O	1:C:781:GLU:HG2	2.08	0.53
1:C:874:ARG:HD3	1:C:887:PHE:HE1	1.72	0.53
1:C:537:ASP:HB2	1:C:870:ILE:HG21	1.90	0.53
1:D:548:ARG:HH21	1:D:875:LYS:NZ	2.06	0.53
1:B:568:TYR:HB3	1:B:571:ASP:OD2	2.08	0.53
1:D:769:LEU:HD22	1:D:815:LEU:CD2	2.38	0.53
1:C:814:VAL:HG11	1:C:954:GLU:HG2	1.89	0.53
1:A:488:THR:HG21	1:A:492:GLU:HG2	1.90	0.53
1:B:534:HIS:O	1:B:538:ARG:HG3	2.08	0.53
1:C:861:ALA:HB2	1:C:951:ALA:CB	2.37	0.53
1:C:609:TYR:HB2	1:C:614:VAL:HG12	1.91	0.53
1:C:511:TRP:HH2	1:C:581:LEU:HD12	1.74	0.53
1:B:825:LEU:HD13	1:B:909:GLU:HG2	1.90	0.53
1:D:576:ASN:ND2	1:D:602:THR:H	2.07	0.53
1:C:603:LEU:HD21	1:C:688:ILE:HD11	1.91	0.53
1:A:768:THR:HG23	1:A:784:LYS:HE2	1.91	0.53
1:C:554:GLU:HG2	1:C:760:PHE:CE1	2.44	0.53
1:D:928:ASP:HB3	1:D:932:ARG:NH2	2.24	0.53
1:C:688:ILE:HG22	1:C:694:VAL:HB	1.90	0.53
1:D:844:GLY:HA2	1:D:920:GLU:HG3	1.90	0.53
1:B:734:GLU:HG3	1:B:753:LEU:HD23	1.90	0.53
1:D:776:ASN:O	1:D:777:GLU:HB2	2.09	0.53
1:D:688:ILE:HG22	1:D:694:VAL:HB	1.91	0.53
1:B:861:ALA:HB1	1:B:950:ILE:O	2.08	0.53
1:A:819:GLY:HA3	1:A:953:LYS:HD3	1.90	0.53
1:A:616:LEU:HD11	1:B:518:ILE:HD11	1.92	0.52
1:C:745:ASN:ND2	1:C:963:SER:HB2	2.24	0.52
1:C:781:GLU:OE1	1:C:806:PRO:HG3	2.10	0.52
1:C:626:ASN:N	1:C:626:ASN:HD22	2.06	0.52
1:D:791:MSE:O	1:D:792:ASP:CB	2.57	0.52
1:A:861:ALA:HB2	1:A:951:ALA:HB2	1.90	0.52
1:C:763:ASP:OD2	1:C:792:ASP:HA	2.09	0.52
1:A:560:TRP:NE1	1:A:891:MSE:HE1	2.24	0.52
1:D:853:VAL:HG21	1:D:949:PHE:CE1	2.45	0.52
1:A:860:THR:HG23	1:A:904:GLN:NE2	2.24	0.52
1:A:576:ASN:HD21	1:A:602:THR:H	1.58	0.52
1:A:694:VAL:C	1:A:696:ALA:H	2.13	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:874:ARG:HH11	1:C:874:ARG:HG2	1.75	0.52
1:B:604:LEU:HD21	1:B:618:ALA:CB	2.39	0.52
1:B:725:THR:O	1:B:725:THR:HG23	2.09	0.52
1:C:785:ILE:HG22	1:C:803:VAL:HG11	1.91	0.52
1:D:489:SER:O	1:D:717:GLY:HA3	2.09	0.52
1:D:876:SER:O	1:D:885:ALA:HA	2.10	0.52
1:D:613:TYR:HB2	1:D:622:VAL:HB	1.91	0.52
1:C:558:GLU:HB3	1:C:762:ARG:NE	2.25	0.52
1:A:640:PRO:O	1:A:654:GLY:HA3	2.10	0.52
1:A:715:GLU:OE1	1:A:715:GLU:N	2.43	0.51
1:D:746:LEU:HD21	1:D:753:LEU:HD21	1.92	0.51
1:C:499:ARG:HG2	1:C:527:ARG:NH1	2.25	0.51
1:A:857:LYS:HE2	1:A:859:TYR:CZ	2.46	0.51
1:D:757:ILE:HD11	1:D:791:MSE:HE1	1.92	0.51
1:B:684:THR:HG22	1:B:696:ALA:O	2.11	0.51
1:D:871:TYR:CD2	1:D:871:TYR:N	2.77	0.51
1:B:859:TYR:O	1:B:904:GLN:HA	2.10	0.51
1:A:650:LYS:HD3	1:A:651:THR:H	1.75	0.51
1:A:680:TYR:CD1	1:D:933:LYS:HB2	2.46	0.51
1:B:788:ILE:HD12	1:B:788:ILE:N	2.25	0.51
1:C:769:LEU:HD11	1:C:815:LEU:HD12	1.91	0.51
1:D:714:TYR:HB3	1:D:721:VAL:HG13	1.93	0.51
1:D:671:THR:HB	1:D:674:ILE:O	2.11	0.51
1:D:731:LYS:HD2	1:D:756:TYR:CE1	2.45	0.51
1:C:841:LEU:HD21	1:C:849:ILE:HD11	1.92	0.51
1:A:863:LEU:HD13	1:A:949:PHE:CE2	2.46	0.51
1:C:671:THR:HG23	1:C:672:PRO:HD2	1.93	0.51
1:B:730:TYR:CZ	1:B:756:TYR:HB3	2.46	0.51
1:D:857:LYS:HA	1:D:907:GLU:HG2	1.93	0.50
1:A:852:LYS:HD3	1:A:909:GLU:OE1	2.11	0.50
1:A:705:LYS:HG2	1:A:730:TYR:CE2	2.46	0.50
1:B:604:LEU:HD21	1:B:618:ALA:HB3	1.93	0.50
1:A:913:LYS:O	1:A:914:VAL:HG23	2.11	0.50
1:C:811:TYR:O	1:C:959:GLU:HA	2.11	0.50
1:B:588:ARG:HB2	1:B:883:TYR:HB3	1.93	0.50
1:D:905:LEU:HD23	1:D:910:ASN:HD22	1.76	0.50
1:D:745:ASN:O	1:D:746:LEU:HB2	2.11	0.50
1:D:866:ARG:NH1	3:D:8:CL:CL	2.78	0.50
1:A:668:LEU:HD21	1:A:670:LEU:HD21	1.93	0.50
1:D:576:ASN:ND2	1:D:602:THR:OG1	2.42	0.50
1:D:813:PHE:HB3	1:D:957:MSE:HE3	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:PHE:HB3	1:B:562:LEU:HD12	1.92	0.50
1:D:560:TRP:HE1	1:D:891:MSE:CE	2.24	0.50
1:A:764:ILE:O	1:A:790:HIS:HA	2.10	0.50
1:D:830:VAL:HB	1:D:835:ARG:HG3	1.92	0.50
1:D:541:ILE:HG13	1:D:891:MSE:HE3	1.93	0.50
1:B:519:GLU:HG2	1:B:525:GLN:NE2	2.26	0.50
1:C:846:SER:O	1:C:847:GLY:O	2.29	0.50
1:C:849:ILE:HG12	1:C:916:ALA:HB2	1.94	0.50
1:A:499:ARG:HB3	1:A:499:ARG:NH1	2.27	0.50
1:B:531:ASP:OD1	1:B:531:ASP:N	2.41	0.50
1:B:775:ASN:O	1:B:776:ASN:HB3	2.11	0.50
1:B:624:VAL:HG13	1:B:629:VAL:HG12	1.93	0.49
1:B:914:VAL:HG12	1:B:915:ARG:O	2.12	0.49
1:A:600:VAL:HG12	1:A:601:THR:H	1.77	0.49
1:A:680:TYR:O	1:D:932:ARG:HD2	2.12	0.49
1:A:568:TYR:HB3	1:A:571:ASP:OD2	2.11	0.49
1:C:828:PRO:HD3	1:C:837:PRO:HG3	1.94	0.49
1:C:568:TYR:CZ	1:C:570:ASN:HB2	2.47	0.49
1:C:853:VAL:HG21	1:C:949:PHE:CE2	2.47	0.49
1:B:537:ASP:CB	1:B:870:ILE:HD12	2.32	0.49
1:C:842:ARG:O	1:C:918:LEU:HD23	2.12	0.49
1:B:613:TYR:CE1	1:B:670:LEU:HD22	2.47	0.49
1:D:880:ASN:ND2	1:D:939:ILE:HD11	2.27	0.49
1:A:909:GLU:C	1:A:910:ASN:HD22	2.14	0.49
1:C:799:ILE:O	1:C:799:ILE:HG23	2.12	0.49
1:B:769:LEU:HD12	1:B:785:ILE:CG1	2.42	0.49
1:A:631:VAL:HB	1:A:638:CYS:O	2.12	0.49
1:D:838:THR:HA	1:D:946:GLU:HG2	1.93	0.49
1:C:745:ASN:HD21	1:C:963:SER:HB2	1.77	0.49
1:A:780:ILE:O	1:A:781:GLU:HB2	2.12	0.49
1:A:853:VAL:HG21	1:A:949:PHE:CE1	2.47	0.49
1:C:709:ASN:OD1	1:C:760:PHE:HB2	2.12	0.49
1:A:534:HIS:O	1:A:538:ARG:HB2	2.13	0.49
1:A:724:PHE:CG	1:A:725:THR:N	2.80	0.49
1:D:871:TYR:CE2	1:D:890:GLN:HB3	2.47	0.49
1:C:811:TYR:HE1	1:C:962:ALA:HB2	1.78	0.49
1:C:568:TYR:CE2	1:C:570:ASN:HB2	2.48	0.49
1:D:508:ALA:HA	1:D:564:TYR:O	2.13	0.49
1:B:849:ILE:HG22	1:B:851:LEU:HD23	1.94	0.49
1:A:600:VAL:HG13	1:A:666:TYR:OH	2.13	0.49
1:C:509:THR:OG1	1:C:562:LEU:HD13	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:866:ARG:NH1	3:A:5:CL:CL	2.81	0.49
1:B:496:LYS:HA	1:B:499:ARG:CZ	2.43	0.49
1:D:491:TRP:CZ3	1:D:566:LEU:HD23	2.41	0.48
1:D:548:ARG:NH2	1:D:875:LYS:NZ	2.61	0.48
1:C:626:ASN:ND2	1:C:626:ASN:N	2.59	0.48
1:C:853:VAL:HG12	1:C:854:GLY:N	2.28	0.48
1:B:537:ASP:OD1	1:B:942:GLY:HA3	2.12	0.48
1:C:764:ILE:O	1:C:790:HIS:HA	2.13	0.48
1:C:747:THR:HB	1:C:963:SER:O	2.13	0.48
1:B:922:VAL:O	1:B:923:ILE:HB	2.14	0.48
1:D:867:ALA:HB3	1:D:894:PHE:CE2	2.48	0.48
1:A:557:PHE:HB3	1:A:562:LEU:HD23	1.96	0.48
1:C:669:HIS:HB2	1:C:676:VAL:HG13	1.94	0.48
1:D:610:GLY:C	1:D:612:LYS:H	2.16	0.48
1:C:647:PRO:O	1:C:648:SER:HB3	2.14	0.48
1:B:830:VAL:HG22	1:B:849:ILE:HG12	1.95	0.48
1:C:898:LYS:HG2	1:C:901:GLU:OE2	2.13	0.48
1:D:734:GLU:HG2	1:D:735:ASN:N	2.29	0.48
1:A:594:GLU:O	1:B:587:ARG:NH2	2.47	0.48
1:D:726:PRO:HG2	1:D:727:PHE:CD1	2.49	0.48
1:A:813:PHE:HB3	1:A:957:MSE:CE	2.42	0.48
1:C:790:HIS:HE1	1:C:792:ASP:HB2	1.77	0.48
1:D:548:ARG:HH21	1:D:875:LYS:HZ1	1.61	0.48
1:B:836:SER:C	1:B:838:THR:H	2.16	0.48
1:D:836:SER:C	1:D:838:THR:H	2.17	0.48
1:C:558:GLU:HB2	1:C:726:PRO:HG3	1.96	0.48
1:C:765:GLU:H	1:C:817:GLN:NE2	2.12	0.48
1:C:770:TYR:HB2	1:C:772:TYR:HE1	1.79	0.48
1:C:855:VAL:HG23	1:C:907:GLU:HA	1.96	0.48
1:B:554:GLU:HA	1:B:760:PHE:CZ	2.49	0.48
1:A:666:TYR:HB3	1:A:677:LEU:HD11	1.95	0.48
1:D:729:ILE:HG12	1:D:757:ILE:HG22	1.96	0.47
1:D:544:LEU:HD12	1:D:548:ARG:HG3	1.95	0.47
1:D:514:TYR:OH	1:D:574:LYS:HE2	2.13	0.47
1:C:754:LYS:HB3	1:C:754:LYS:NZ	2.29	0.47
1:B:736:ILE:HD12	1:B:741:LYS:HD3	1.95	0.47
1:D:848:GLU:OE1	1:D:913:LYS:HD3	2.14	0.47
1:A:805:LEU:HB3	1:A:811:TYR:CE2	2.49	0.47
1:A:689:LYS:HE3	1:A:696:ALA:O	2.13	0.47
1:A:714:TYR:HB3	1:A:721:VAL:CG1	2.44	0.47
1:A:736:ILE:O	1:A:737:ASN:HB2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:593:ASP:HB2	1:D:594:GLU:OE1	2.14	0.47
1:C:853:VAL:HG21	1:C:949:PHE:HE2	1.79	0.47
1:A:566:LEU:HD12	1:A:721:VAL:HB	1.95	0.47
1:C:869:PHE:CE1	1:C:943:ILE:HG23	2.50	0.47
1:B:857:LYS:HG2	1:B:858:ASP:N	2.28	0.47
1:A:694:VAL:O	1:A:696:ALA:N	2.40	0.47
1:D:723:ARG:NH2	1:D:956:LEU:O	2.48	0.47
1:C:759:ALA:HB3	1:C:793:TYR:HA	1.96	0.47
1:C:674:ILE:HG13	1:C:675:GLY:N	2.29	0.47
1:C:774:ILE:HB	1:C:810:SER:OG	2.15	0.47
1:A:826:ASP:OD1	1:A:852:LYS:HD2	2.14	0.47
1:B:641:LEU:HD11	1:B:665:PRO:HA	1.96	0.47
1:B:609:TYR:HB2	1:B:614:VAL:HG12	1.96	0.47
1:A:867:ALA:HB2	1:A:896:ILE:HD11	1.97	0.47
1:C:903:ILE:N	1:C:903:ILE:HD12	2.30	0.47
1:D:734:GLU:HA	1:D:753:LEU:HD23	1.97	0.47
1:A:548:ARG:NH1	1:A:552:ILE:HG21	2.30	0.47
1:B:511:TRP:CE2	1:B:578:ILE:HG12	2.50	0.47
1:C:771:ILE:HG13	1:C:785:ILE:HG21	1.96	0.47
1:A:759:ALA:HB3	1:A:793:TYR:HA	1.96	0.47
1:D:917:GLU:O	1:D:919:PRO:HD3	2.15	0.47
1:B:498:LEU:HD21	1:B:721:VAL:HG21	1.97	0.46
1:B:674:ILE:HG12	1:B:675:GLY:N	2.29	0.46
1:C:740:TRP:HZ3	1:C:753:LEU:HA	1.79	0.46
1:C:756:TYR:CD2	1:C:798:PRO:HB3	2.50	0.46
1:C:838:THR:CG2	1:C:944:ARG:HG2	2.45	0.46
1:D:540:HIS:CE1	1:D:872:LEU:HD11	2.50	0.46
1:A:657:THR:HG22	1:A:662:ASN:O	2.15	0.46
1:A:625:SER:O	1:A:626:ASN:CB	2.62	0.46
1:A:735:ASN:HD22	1:A:736:ILE:N	2.14	0.46
1:B:688:ILE:CG2	1:B:694:VAL:HB	2.44	0.46
1:C:734:GLU:HG3	1:C:735:ASN:N	2.30	0.46
1:B:842:ARG:O	1:B:918:LEU:HD23	2.16	0.46
1:C:701:GLY:O	1:C:704:ASP:N	2.48	0.46
1:D:731:LYS:HD2	1:D:756:TYR:CD1	2.50	0.46
1:A:836:SER:C	1:A:838:THR:H	2.19	0.46
1:C:894:PHE:O	1:C:894:PHE:HD2	1.98	0.46
1:C:853:VAL:HG12	1:C:854:GLY:H	1.81	0.46
1:A:514:TYR:O	1:A:518:ILE:HG12	2.15	0.46
1:A:604:LEU:HG	1:A:615:ASN:ND2	2.30	0.46
1:C:514:TYR:HE2	1:D:616:LEU:O	1.99	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:544:LEU:HD22	1:B:889:PRO:HG2	1.97	0.46
1:A:624:VAL:HG22	1:A:629:VAL:HG22	1.98	0.46
1:D:757:ILE:O	1:D:796:GLU:HG2	2.14	0.46
1:D:815:LEU:HD13	1:D:816:VAL:N	2.31	0.46
1:A:736:ILE:HD12	1:A:741:LYS:HD3	1.97	0.46
1:B:919:PRO:O	1:B:922:VAL:HG22	2.16	0.46
1:A:610:GLY:C	1:A:612:LYS:H	2.18	0.46
1:B:713:VAL:HG22	1:B:721:VAL:O	2.16	0.46
1:A:805:LEU:HB3	1:A:811:TYR:HE2	1.81	0.46
1:D:621:ILE:HB	1:D:632:THR:HG23	1.97	0.46
1:B:538:ARG:HH11	1:B:944:ARG:NH2	2.13	0.46
1:B:757:ILE:O	1:B:796:GLU:HG2	2.16	0.46
1:D:812:ARG:HG3	1:D:959:GLU:HG3	1.98	0.45
1:C:727:PHE:CE2	1:C:764:ILE:HG12	2.51	0.45
1:B:569:LEU:HD21	1:B:691:ALA:O	2.16	0.45
1:D:747:THR:HG22	1:D:963:SER:CB	2.44	0.45
1:D:612:LYS:HE2	1:D:623:ASP:OD2	2.17	0.45
1:D:543:ALA:O	1:D:545:PHE:N	2.50	0.45
1:C:933:LYS:HG2	1:C:934:TYR:CE2	2.51	0.45
1:C:587:ARG:NH2	1:D:594:GLU:O	2.49	0.45
1:C:768:THR:HG21	1:C:784:LYS:HE2	1.98	0.45
1:D:861:ALA:HB2	1:D:951:ALA:HB2	1.98	0.45
1:C:905:LEU:HA	1:C:910:ASN:ND2	2.30	0.45
1:D:958:LEU:HD12	1:D:959:GLU:H	1.81	0.45
1:D:576:ASN:HD21	1:D:602:THR:H	1.63	0.45
1:A:626:ASN:HD21	1:A:628:SER:CB	2.30	0.45
1:C:769:LEU:HD21	1:C:788:ILE:CD1	2.47	0.45
1:A:562:LEU:HD11	1:A:564:TYR:O	2.16	0.45
1:C:669:HIS:HB2	1:C:676:VAL:CG1	2.47	0.45
1:D:643:VAL:HG22	1:D:668:LEU:HB3	1.99	0.45
1:A:618:ALA:O	1:A:619:LYS:HB2	2.15	0.45
1:C:845:GLU:HG2	1:C:846:SER:H	1.82	0.45
1:C:791:MSE:O	1:C:792:ASP:HB3	2.16	0.45
1:A:953:LYS:HE2	1:A:955:TYR:CE2	2.52	0.45
1:C:868:THR:HA	1:C:893:VAL:HG12	1.98	0.45
1:B:709:ASN:HD22	1:B:760:PHE:HB2	1.78	0.45
1:D:540:HIS:HE1	1:D:872:LEU:HD11	1.82	0.45
1:D:872:LEU:HD23	1:D:889:PRO:HA	1.98	0.45
1:C:814:VAL:HG12	1:C:815:LEU:N	2.32	0.45
1:B:551:ASN:OD1	1:B:794:LEU:HD22	2.17	0.45
1:A:909:GLU:C	1:A:910:ASN:ND2	2.71	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:ARG:HB3	1:A:548:ARG:HH11	1.81	0.45
1:C:686:ASN:O	1:C:690:LEU:HB2	2.16	0.45
1:B:726:PRO:O	1:B:759:ALA:HA	2.16	0.45
1:A:601:THR:O	1:A:601:THR:HG22	2.17	0.44
1:C:781:GLU:CD	1:C:806:PRO:HG3	2.36	0.44
1:A:735:ASN:HD21	1:A:738:GLY:N	2.15	0.44
1:D:909:GLU:HG2	1:D:909:GLU:H	1.51	0.44
1:B:841:LEU:HD23	1:B:845:GLU:OE2	2.17	0.44
1:D:600:VAL:CG1	1:D:601:THR:H	2.30	0.44
1:C:595:SER:HB3	1:C:597:ARG:NH2	2.32	0.44
1:A:567:VAL:HG11	1:A:690:LEU:HB3	1.99	0.44
1:B:768:THR:HG23	1:B:784:LYS:HE2	1.98	0.44
1:C:576:ASN:ND2	1:C:602:THR:OG1	2.48	0.44
1:B:852:LYS:HA	1:B:910:ASN:O	2.17	0.44
1:D:830:VAL:O	1:D:831:ASN:HB2	2.18	0.44
1:D:606:LEU:HD23	1:D:615:ASN:HB2	1.98	0.44
1:C:499:ARG:CD	1:C:525:GLN:HE22	2.31	0.44
1:B:524:GLY:O	1:B:525:GLN:HB3	2.18	0.44
1:A:613:TYR:HB2	1:A:622:VAL:HB	1.98	0.44
1:B:934:TYR:HB2	1:B:938:LEU:HB2	2.00	0.44
1:C:873:VAL:HG23	1:C:890:GLN:HG3	2.00	0.44
1:B:593:ASP:C	1:B:595:SER:H	2.21	0.44
1:D:842:ARG:HB2	1:D:842:ARG:NH1	2.31	0.44
1:B:727:PHE:HB3	1:B:957:MSE:HE3	2.00	0.44
1:C:928:ASP:O	1:C:932:ARG:HG2	2.18	0.44
1:A:863:LEU:HB3	1:A:900:GLY:CA	2.38	0.44
1:A:783:ILE:O	1:A:785:ILE:HG23	2.18	0.44
1:A:742:GLN:HG2	1:A:744:TYR:CZ	2.53	0.44
1:C:714:TYR:HB3	1:C:721:VAL:CG1	2.47	0.44
1:A:733:GLU:OE2	1:A:754:LYS:HD2	2.17	0.44
1:C:805:LEU:HB3	1:C:811:TYR:CE2	2.53	0.44
1:B:511:TRP:CZ2	1:B:578:ILE:HG12	2.53	0.44
1:C:765:GLU:H	1:C:817:GLN:HE22	1.64	0.43
1:C:852:LYS:HZ3	1:C:852:LYS:HB2	1.83	0.43
1:C:569:LEU:HD23	1:C:691:ALA:HB1	2.00	0.43
1:B:646:THR:O	1:B:672:PRO:HD3	2.18	0.43
1:C:594:GLU:HA	1:D:883:TYR:OH	2.18	0.43
1:C:506:SER:HA	1:C:563:ASN:OD1	2.18	0.43
1:C:842:ARG:HB2	1:C:845:GLU:HB2	2.00	0.43
1:A:569:LEU:HD12	1:A:691:ALA:HB1	1.99	0.43
1:B:600:VAL:CG1	1:B:601:THR:N	2.80	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:882:ASP:OD2	1:D:884:ASP:HB2	2.18	0.43
1:C:820:PRO:O	1:C:953:LYS:HD2	2.18	0.43
1:D:500:GLU:HG2	1:D:500:GLU:O	2.19	0.43
1:C:558:GLU:HB2	1:C:726:PRO:CG	2.49	0.43
1:A:568:TYR:CE2	1:A:570:ASN:HB2	2.54	0.43
1:B:586:THR:HG23	1:B:589:GLU:OE1	2.17	0.43
1:D:645:PHE:HB3	1:D:648:SER:HB3	2.00	0.43
1:A:593:ASP:HA	1:A:883:TYR:CE2	2.53	0.43
1:A:763:ASP:OD1	1:A:792:ASP:HA	2.18	0.43
1:B:669:HIS:CG	1:B:694:VAL:HG11	2.54	0.43
1:B:866:ARG:HD2	1:B:893:VAL:CG2	2.48	0.43
1:C:711:GLU:OE2	1:C:723:ARG:NH1	2.52	0.43
1:C:898:LYS:O	1:C:899:ILE:HG23	2.17	0.43
1:D:878:LYS:HG2	1:D:882:ASP:OD1	2.18	0.43
1:A:727:PHE:CE2	1:A:764:ILE:HG12	2.53	0.43
1:A:639:ASP:OD1	1:A:655:THR:HG23	2.19	0.43
1:B:640:PRO:O	1:B:654:GLY:HA3	2.18	0.43
1:B:671:THR:HB	1:B:674:ILE:O	2.19	0.43
1:C:591:ASN:HD21	1:D:591:ASN:ND2	2.16	0.43
1:D:624:VAL:HA	1:D:628:SER:O	2.18	0.43
1:D:597:ARG:HH11	1:D:597:ARG:HB3	1.82	0.42
1:A:600:VAL:CG1	1:A:601:THR:N	2.81	0.42
1:C:512:TRP:HE3	1:C:514:TYR:CE1	2.36	0.42
1:A:867:ALA:HA	1:A:944:ARG:O	2.19	0.42
1:D:771:ILE:HG13	1:D:785:ILE:HD13	2.01	0.42
1:C:865:LEU:HA	1:C:865:LEU:HD23	1.93	0.42
1:C:872:LEU:HD23	1:C:889:PRO:HA	2.01	0.42
1:B:526:ARG:C	1:B:527:ARG:HG2	2.38	0.42
1:A:850:GLU:HG3	1:A:913:LYS:HG2	2.00	0.42
1:D:785:ILE:HB	1:D:801:VAL:CG2	2.49	0.42
1:B:769:LEU:CD1	1:B:785:ILE:HD11	2.49	0.42
1:C:537:ASP:HB2	1:C:870:ILE:HG13	2.02	0.42
1:A:848:GLU:OE1	1:A:913:LYS:HD3	2.19	0.42
1:C:811:TYR:CE1	1:C:962:ALA:HB2	2.54	0.42
1:B:915:ARG:HG3	1:B:916:ALA:N	2.32	0.42
1:C:607:PRO:HA	1:C:674:ILE:HD12	2.01	0.42
1:C:641:LEU:CD1	1:C:665:PRO:HA	2.49	0.42
1:A:684:THR:HG21	1:A:698:THR:N	2.35	0.42
1:A:705:LYS:HG2	1:A:730:TYR:CD2	2.54	0.42
1:D:533:GLY:O	1:D:534:HIS:C	2.57	0.42
1:A:558:GLU:HA	1:A:558:GLU:OE2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:896:ILE:HG22	1:C:897:THR:HG23	2.01	0.42
1:B:705:LYS:HG2	1:B:730:TYR:CE2	2.55	0.42
1:C:915:ARG:HH11	1:C:915:ARG:HG2	1.84	0.42
1:A:767:ALA:HB2	1:A:817:GLN:HB3	2.02	0.42
1:B:538:ARG:HD2	1:B:560:TRP:CZ2	2.54	0.42
1:B:489:SER:O	1:B:717:GLY:HA3	2.19	0.42
1:D:812:ARG:CG	1:D:959:GLU:HG3	2.50	0.42
1:C:828:PRO:CD	1:C:837:PRO:HG3	2.50	0.42
1:A:829:LYS:HA	1:A:833:GLU:O	2.20	0.42
1:A:878:LYS:HE2	1:D:765:GLU:OE1	2.20	0.42
1:A:871:TYR:CD2	1:A:871:TYR:N	2.86	0.42
1:B:728:GLY:HA2	1:B:957:MSE:HB3	2.02	0.42
1:D:769:LEU:HD22	1:D:815:LEU:HD23	2.01	0.42
1:C:614:VAL:HG23	1:C:620:VAL:O	2.19	0.42
1:A:857:LYS:HB3	1:A:859:TYR:CE1	2.55	0.42
1:A:769:LEU:HD21	1:A:815:LEU:HD12	2.02	0.42
1:A:874:ARG:HH11	1:A:874:ARG:HG2	1.85	0.42
1:C:588:ARG:HB2	1:C:883:TYR:HB3	2.02	0.41
1:C:769:LEU:HD22	1:C:769:LEU:N	2.35	0.41
1:A:576:ASN:ND2	1:A:602:THR:HG23	2.35	0.41
1:A:648:SER:OG	1:A:650:LYS:HB2	2.20	0.41
1:C:755:LEU:O	1:C:798:PRO:HA	2.19	0.41
1:D:554:GLU:HG2	1:D:760:PHE:CE1	2.55	0.41
1:D:764:ILE:O	1:D:790:HIS:HA	2.21	0.41
1:D:688:ILE:CG2	1:D:694:VAL:HB	2.50	0.41
1:D:869:PHE:CE1	1:D:943:ILE:HD13	2.55	0.41
1:A:706:LEU:C	1:A:706:LEU:HD23	2.41	0.41
1:C:645:PHE:HB2	1:C:650:LYS:HB3	2.01	0.41
1:A:666:TYR:HB3	1:A:677:LEU:CD1	2.50	0.41
1:D:562:LEU:HD11	1:D:564:TYR:O	2.20	0.41
1:C:868:THR:CB	1:C:893:VAL:HG12	2.50	0.41
1:D:636:ARG:HE	1:D:660:ASP:CG	2.23	0.41
1:D:646:THR:O	1:D:672:PRO:HD3	2.20	0.41
1:C:863:LEU:HD12	1:C:864:TYR:N	2.35	0.41
1:A:548:ARG:HH12	1:A:552:ILE:HG21	1.86	0.41
1:D:947:PRO:O	1:D:947:PRO:HG2	2.20	0.41
1:B:714:TYR:HB3	1:B:721:VAL:HG11	2.02	0.41
1:C:938:LEU:HD12	1:C:939:ILE:H	1.85	0.41
1:B:768:THR:CG2	1:B:784:LYS:HE2	2.51	0.41
1:C:679:TYR:HE2	1:C:681:LYS:HD2	1.86	0.41
1:B:773:ALA:HB3	1:B:780:ILE:HB	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:846:SER:HA	1:C:917:GLU:HA	2.03	0.41
1:D:933:LYS:HD3	1:D:934:TYR:CZ	2.56	0.41
1:C:822:GLY:HA2	1:C:854:GLY:O	2.21	0.41
1:A:552:ILE:O	1:A:552:ILE:HG12	2.19	0.41
1:C:849:ILE:CG1	1:C:916:ALA:HB2	2.50	0.41
1:A:534:HIS:HB3	1:A:535:ALA:H	1.72	0.41
1:C:695:PRO:HG2	1:C:696:ALA:H	1.85	0.41
1:C:764:ILE:HA	1:C:817:GLN:HE22	1.85	0.41
1:C:872:LEU:HB2	1:C:939:ILE:HB	2.02	0.41
1:B:671:THR:CG2	1:B:673:THR:HG22	2.51	0.41
1:B:587:ARG:O	1:B:590:TYR:HB3	2.21	0.41
1:C:759:ALA:O	1:C:793:TYR:HB2	2.20	0.41
1:C:602:THR:HA	1:C:679:TYR:HB2	2.03	0.41
1:C:724:PHE:CG	1:C:725:THR:N	2.89	0.41
1:C:725:THR:HA	1:C:726:PRO:HD3	1.92	0.41
1:D:544:LEU:HD22	1:D:889:PRO:HB2	2.03	0.41
1:C:863:LEU:HB3	1:C:900:GLY:HA3	2.03	0.41
1:C:514:TYR:HE1	1:C:574:LYS:HE3	1.85	0.41
1:A:496:LYS:HE2	1:A:500:GLU:OE1	2.21	0.41
1:B:626:ASN:C	1:B:628:SER:H	2.24	0.41
1:D:527:ARG:HB2	1:D:531:ASP:OD2	2.21	0.41
1:A:915:ARG:HG3	1:A:916:ALA:N	2.35	0.41
1:B:622:VAL:HG13	1:B:631:VAL:HG22	2.02	0.41
1:B:727:PHE:O	1:B:957:MSE:HG2	2.21	0.41
1:A:554:GLU:OE1	1:A:794:LEU:HD23	2.21	0.41
1:B:567:VAL:CG2	1:B:720:ILE:HB	2.50	0.41
1:D:542:LEU:HA	1:D:542:LEU:HD23	1.85	0.41
1:A:870:ILE:HD11	1:A:891:MSE:CE	2.51	0.40
1:C:815:LEU:C	1:C:815:LEU:HD23	2.41	0.40
1:D:544:LEU:HD11	1:D:552:ILE:HG12	2.04	0.40
1:A:562:LEU:HD12	1:A:563:ASN:H	1.86	0.40
1:B:545:PHE:O	1:B:686:ASN:HB2	2.21	0.40
1:B:679:TYR:HE2	1:B:681:LYS:HD2	1.86	0.40
1:B:491:TRP:HZ3	1:B:566:LEU:HD13	1.86	0.40
1:C:843:GLU:O	1:C:920:GLU:HA	2.20	0.40
1:A:680:TYR:CE1	1:D:933:LYS:HG3	2.56	0.40
1:B:705:LYS:HG2	1:B:730:TYR:CD2	2.57	0.40
1:C:821:ILE:HG22	1:C:953:LYS:HE3	2.02	0.40
1:D:736:ILE:HG22	1:D:736:ILE:O	2.20	0.40
1:B:765:GLU:O	1:B:766:ASN:C	2.58	0.40
1:C:896:ILE:HG21	1:C:918:LEU:CD1	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:851:LEU:HA	1:B:852:LYS:HZ1	1.86	0.40
1:C:757:ILE:HD13	1:C:791:MSE:HE1	2.04	0.40
1:D:769:LEU:HG	1:D:786:ALA:HB3	2.02	0.40
1:B:914:VAL:HG12	1:B:915:ARG:N	2.37	0.40
1:B:521:SER:O	1:B:523:LEU:N	2.53	0.40
1:B:822:GLY:HA2	1:B:855:VAL:HG12	2.02	0.40
1:D:746:LEU:HD13	1:D:805:LEU:HD11	2.03	0.40
1:D:610:GLY:O	1:D:611:GLU:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	476/497 (96%)	414 (87%)	49 (10%)	13 (3%)	6	32
1	B	475/497 (96%)	408 (86%)	54 (11%)	13 (3%)	6	32
1	C	476/497 (96%)	398 (84%)	59 (12%)	19 (4%)	4	21
1	D	478/497 (96%)	410 (86%)	50 (10%)	18 (4%)	4	22
All	All	1905/1988 (96%)	1630 (86%)	212 (11%)	63 (3%)	5	26

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	535	ALA
1	A	626	ASN
1	A	696	ALA
1	B	529	SER
1	B	777	GLU
1	B	843	GLU
1	C	626	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	648	SER
1	C	696	ALA
1	C	702	PHE
1	C	847	GLY
1	D	695	PRO
1	A	524	GLY
1	A	796	GLU
1	B	520	SER
1	B	522	LEU
1	B	594	GLU
1	B	716	SER
1	C	901	GLU
1	C	922	VAL
1	D	534	HIS
1	D	535	ALA
1	D	610	GLY
1	D	776	ASN
1	A	625	SER
1	A	695	PRO
1	A	806	PRO
1	A	907	GLU
1	B	525	GLN
1	B	737	ASN
1	C	524	GLY
1	C	528	ALA
1	C	535	ALA
1	C	781	GLU
1	C	900	GLY
1	D	544	LEU
1	D	717	GLY
1	D	737	ASN
1	D	746	LEU
1	A	919	PRO
1	B	717	GLY
1	C	917	GLU
1	C	935	GLY
1	D	524	GLY
1	D	696	ALA
1	D	902	ASN
1	A	629	VAL
1	D	781	GLU
1	D	792	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	524	GLY
1	C	503	PRO
1	C	599	ALA
1	D	648	SER
1	A	939	ILE
1	C	899	ILE
1	C	919	PRO
1	D	533	GLY
1	A	837	PRO
1	C	695	PRO
1	D	552	ILE
1	D	672	PRO
1	B	780	ILE
1	B	919	PRO

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	404/419 (96%)	368 (91%)	36 (9%)	12	42
1	B	404/419 (96%)	376 (93%)	28 (7%)	19	56
1	C	404/419 (96%)	386 (96%)	18 (4%)	34	74
1	D	404/419 (96%)	374 (93%)	30 (7%)	17	52
All	All	1616/1676 (96%)	1504 (93%)	112 (7%)	19	56

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	503	PRO
1	A	507	THR
1	A	509	THR
1	A	525	GLN
1	A	527	ARG
1	A	531	ASP
1	A	548	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	549	ASP
1	A	555	VAL
1	A	561	GLU
1	A	566	LEU
1	A	576	ASN
1	A	594	GLU
1	A	623	ASP
1	A	625	SER
1	A	637	GLU
1	A	646	THR
1	A	652	ILE
1	A	657	THR
1	A	672	PRO
1	A	690	LEU
1	A	698	THR
1	A	703	SER
1	A	715	GLU
1	A	721	VAL
1	A	723	ARG
1	A	725	THR
1	A	735	ASN
1	A	745	ASN
1	A	777	GLU
1	A	795	ASN
1	A	836	SER
1	A	915	ARG
1	A	919	PRO
1	A	946	GLU
1	A	948	VAL
1	B	509	THR
1	B	531	ASP
1	B	534	HIS
1	B	538	ARG
1	B	548	ARG
1	B	562	LEU
1	B	576	ASN
1	B	594	GLU
1	B	608	ARG
1	B	623	ASP
1	B	646	THR
1	B	684	THR
1	B	690	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	716	SER
1	B	770	TYR
1	B	783	ILE
1	B	789	SER
1	B	807	ASN
1	B	834	ILE
1	B	839	ASN
1	B	846	SER
1	B	852	LYS
1	B	893	VAL
1	B	902	ASN
1	B	906	LYS
1	B	915	ARG
1	B	928	ASP
1	B	946	GLU
1	C	525	GLN
1	C	534	HIS
1	C	542	LEU
1	C	575	PHE
1	C	576	ASN
1	C	594	GLU
1	C	603	LEU
1	C	626	ASN
1	C	632	THR
1	C	690	LEU
1	C	721	VAL
1	C	752	GLU
1	C	769	LEU
1	C	824	LEU
1	C	843	GLU
1	C	857	LYS
1	C	884	ASP
1	C	894	PHE
1	D	504	GLU
1	D	509	THR
1	D	531	ASP
1	D	538	ARG
1	D	548	ARG
1	D	549	ASP
1	D	559	SER
1	D	576	ASN
1	D	594	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	601	THR
1	D	604	LEU
1	D	616	LEU
1	D	632	THR
1	D	637	GLU
1	D	644	THR
1	D	690	LEU
1	D	721	VAL
1	D	725	THR
1	D	751	HIS
1	D	757	ILE
1	D	769	LEU
1	D	770	TYR
1	D	777	GLU
1	D	851	LEU
1	D	890	GLN
1	D	909	GLU
1	D	915	ARG
1	D	920	GLU
1	D	927	LYS
1	D	945	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	576	ASN
1	A	591	ASN
1	A	615	ASN
1	A	626	ASN
1	A	662	ASN
1	A	709	ASN
1	A	718	ASN
1	A	735	ASN
1	A	742	GLN
1	A	745	ASN
1	A	776	ASN
1	A	807	ASN
1	A	817	GLN
1	A	839	ASN
1	A	890	GLN
1	A	902	ASN
1	A	904	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	525	GLN
1	B	737	ASN
1	B	807	ASN
1	B	839	ASN
1	B	890	GLN
1	B	904	GLN
1	B	931	GLN
1	C	525	GLN
1	C	540	HIS
1	C	570	ASN
1	C	576	ASN
1	C	591	ASN
1	C	626	ASN
1	C	662	ASN
1	C	718	ASN
1	C	737	ASN
1	C	742	GLN
1	C	745	ASN
1	C	790	HIS
1	C	817	GLN
1	C	904	GLN
1	D	570	ASN
1	D	576	ASN
1	D	591	ASN
1	D	709	ASN
1	D	742	GLN
1	D	802	ASN
1	D	817	GLN
1	D	910	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [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	474/497 (95%)	-0.43	0 100 100	12, 41, 67, 82	0
1	B	473/497 (95%)	-0.36	1 (0%) 95 87	14, 49, 71, 85	0
1	C	474/497 (95%)	-0.26	2 (0%) 93 80	25, 61, 86, 97	0
1	D	476/497 (95%)	-0.43	3 (0%) 90 73	13, 41, 81, 99	0
All	All	1897/1988 (95%)	-0.37	6 (0%) 94 84	12, 47, 79, 99	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	595	SER	3.2
1	B	776	ASN	3.2
1	D	777	GLU	2.3
1	D	776	ASN	2.3
1	D	526	ARG	2.1
1	C	537	ASP	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	CA	B	2	1/1	0.96	0.24	4.29	34,34,34,34	0
2	CA	D	4	1/1	0.95	0.20	2.73	30,30,30,30	0
2	CA	A	1	1/1	0.96	0.23	2.48	32,32,32,32	0
2	CA	C	3	1/1	0.94	0.19	0.73	57,57,57,57	0
3	CL	D	8	1/1	0.96	0.17	0.46	48,48,48,48	0
3	CL	B	6	1/1	0.93	0.18	-0.03	69,69,69,69	0
3	CL	C	7	1/1	0.95	0.18	-0.60	79,79,79,79	0
3	CL	A	5	1/1	0.93	0.14	-0.67	48,48,48,48	0

6.5 Other polymers ⓘ

There are no such residues in this entry.