



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2017 – 11:48 AM EDT

PDB ID : 5K1V
Title : Crystal structure of Endoplasmic Reticulum aminopeptidase 2 (ERAP2) in complex with a diaminobenzoic acid derivative ligand.
Authors : Saridakis, E.; Papakyriakou, A.; Giastas, P.; Mpakali, A.; Mavridis, I.M.; Stratikos, E.
Deposited on : 2016-05-18
Resolution : 2.90 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029077
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20029077

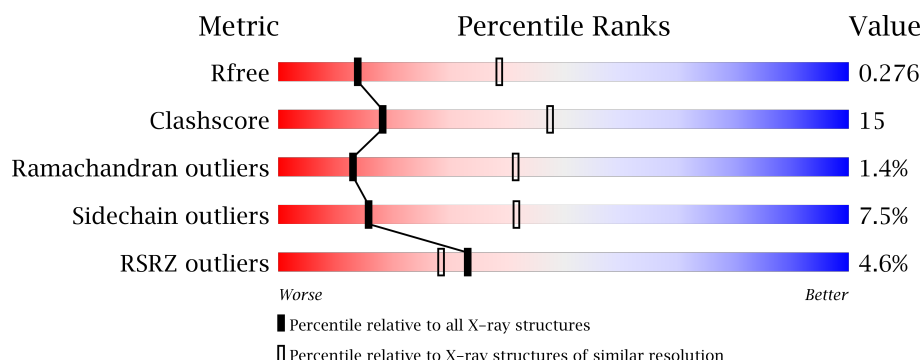
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	967	<div> <div>2%</div> <div>60%</div> <div>29%</div> <div>7%</div> </div>
1	B	967	<div> <div>6%</div> <div>54%</div> <div>30%</div> <div>12%</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
3	6PX	A	1002	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14637 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 Endoplasmic reticulum aminopeptidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	900	Total	C	N	O	S	0	4	1
			7345	4732	1225	1356	32			
1	B	849	Total	C	N	O	S	0	2	0
			6937	4482	1147	1281	27			

There are 14 discrepancies between the modelled and reference sequences:

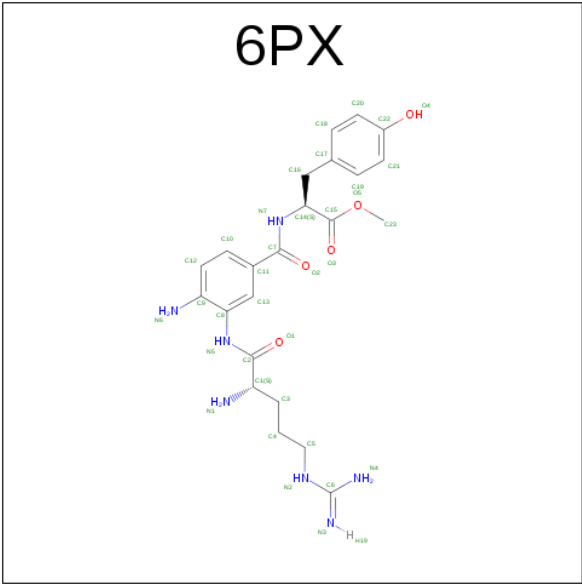
Chain	Residue	Modelled	Actual	Comment	Reference
A	961	ARG	-	expression tag	UNP Q6P179
A	962	HIS	-	expression tag	UNP Q6P179
A	963	HIS	-	expression tag	UNP Q6P179
A	964	HIS	-	expression tag	UNP Q6P179
A	965	HIS	-	expression tag	UNP Q6P179
A	966	HIS	-	expression tag	UNP Q6P179
A	967	HIS	-	expression tag	UNP Q6P179
B	961	ARG	-	expression tag	UNP Q6P179
B	962	HIS	-	expression tag	UNP Q6P179
B	963	HIS	-	expression tag	UNP Q6P179
B	964	HIS	-	expression tag	UNP Q6P179
B	965	HIS	-	expression tag	UNP Q6P179
B	966	HIS	-	expression tag	UNP Q6P179
B	967	HIS	-	expression tag	UNP Q6P179

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

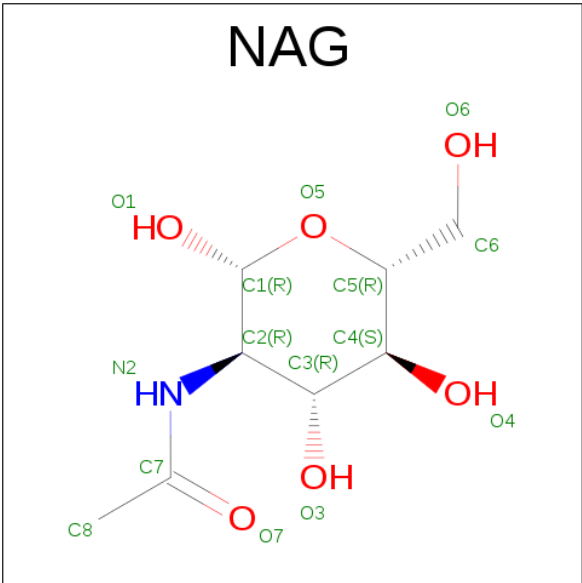
- Molecule 3 is methyl N-[4-amino-3-(L-arginylamino)benzene-1-carbonyl]-L-tyrosinate

(three-letter code: 6PX) (formula: C₂₃H₃₁N₇O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			35	23	7	5		

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		

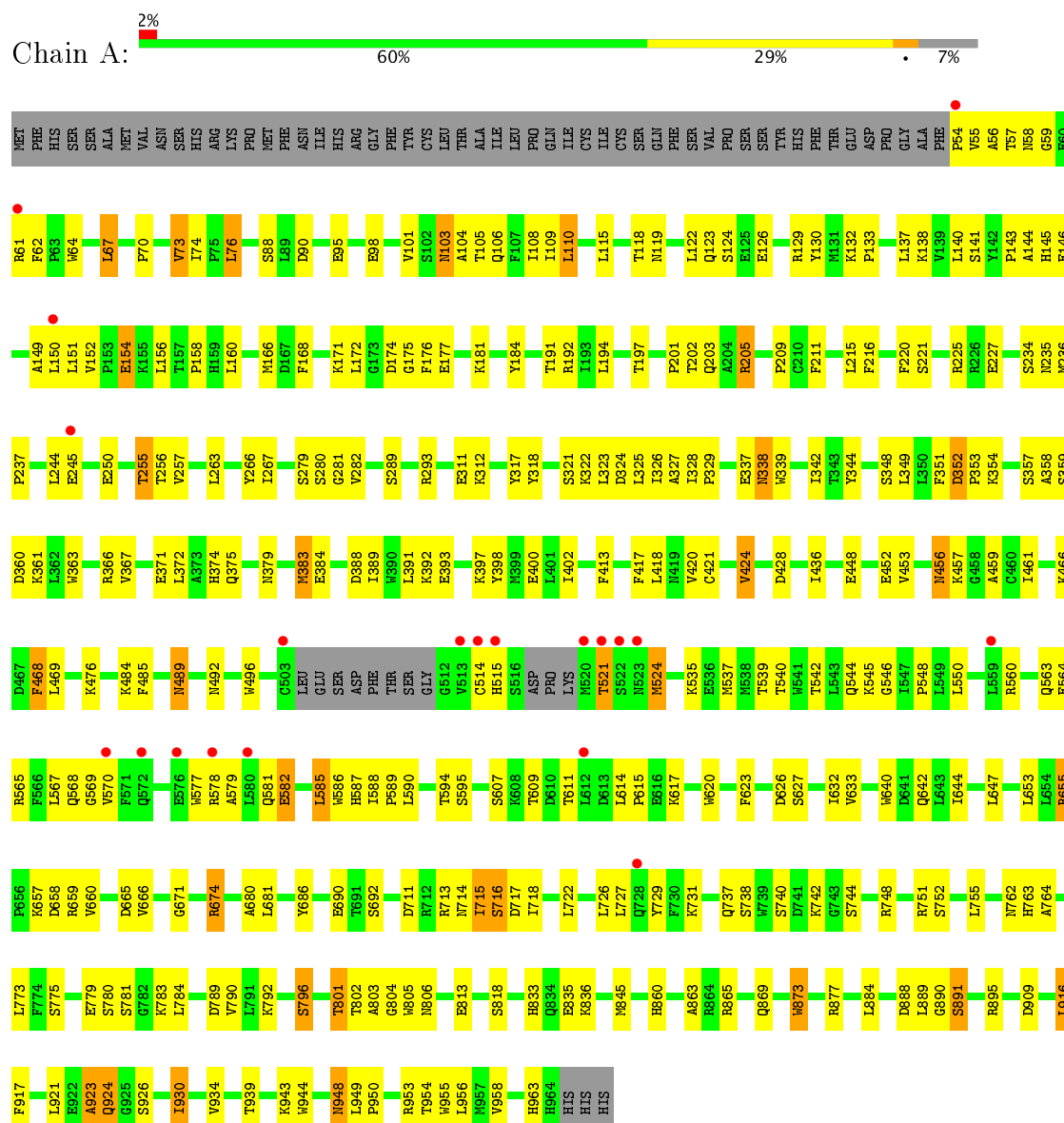
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	30	Total	O	0	0
			30	30		
6	B	14	Total	O	0	0
			14	14		

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 the various outlier classes 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: Endoplasmic reticulum aminopeptidase 2



• Molecule 1: Endoplasmic reticulum aminopeptidase 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.40 Å 135.17 Å 127.49 Å 90.00° 90.15° 90.00°	Depositor
Resolution (Å)	48.34 – 2.90 48.35 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.3 (48.34-2.90) 99.7 (48.35-2.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.91 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.205 , 0.273 0.208 , 0.276	Depositor DCC
R_{free} test set	2792 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	76.4	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 55.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14637	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 6PX, ZN, NAG, MAN

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	0.56	0/7537	0.69	1/10210 (0.0%)
1	B	0.43	0/7114	0.60	0/9636
All	All	0.50	0/14651	0.65	1/19846 (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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	205	ARG	NE-CZ-NH1	-5.02	117.79	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	54	PRO	Peptide

5.2 Too-close contacts [i](#)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7345	0	7282	193	0
1	B	6937	0	6887	242	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	35	0	0	3	0
4	A	140	0	128	1	0
4	B	112	0	102	3	0
5	B	22	0	19	1	0
6	A	30	0	0	3	0
6	B	14	0	0	0	0
All	All	14637	0	14418	434	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 15.

All (434) 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:B:592:TYR:HE1	1:B:601:HIS:HB2	1.13	1.07
1:B:599:VAL:HA	1:B:600:ILE:HG13	1.38	1.01
1:B:599:VAL:HG13	1:B:600:ILE:HB	1.42	0.98
1:B:599:VAL:HA	1:B:600:ILE:CG1	1.92	0.98
1:B:205:ARG:HH21	1:B:212:ASP:HB3	1.29	0.93
1:B:592:TYR:CE1	1:B:601:HIS:HB2	2.03	0.92
1:A:221:SER:OG	1:A:255:THR:OG1	1.92	0.87
1:B:442:THR:HG22	1:B:444:THR:H	1.40	0.84
1:B:258:LYS:HD3	4:B:1007:NAG:H61	1.58	0.83
1:A:108:ILE:HG23	1:A:150:LEU:HB2	1.59	0.83
1:B:540:THR:HG21	1:B:586:TRP:HA	1.60	0.82
1:A:55:VAL:HG22	1:A:62:PHE:H	1.45	0.81
1:B:599:VAL:HA	1:B:600:ILE:CB	2.09	0.81
1:A:560:ARG:HG2	1:A:611:THR:HG22	1.63	0.80
1:B:874:ASP:OD1	1:B:877:ARG:NH2	2.16	0.77
1:A:944:TRP:O	1:A:948:ASN:ND2	2.17	0.77
1:A:569:GLY:O	1:A:943:LYS:NZ	2.13	0.75
1:B:565:ARG:NH1	1:B:584:TYR:OH	2.20	0.75
1:B:599:VAL:CG1	1:B:600:ILE:HB	2.15	0.75
1:B:698:GLU:O	1:B:701:SER:OG	2.05	0.74
1:B:722:LEU:HG	1:B:956:LEU:HD21	1.69	0.74
1:B:316:ILE:HB	1:B:376:TRP:HE1	1.51	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:GLU:OE2	3:A:1002:6PX:N6	2.22	0.73
1:B:56:ALA:HB1	1:B:57:THR:HA	1.70	0.72
1:A:175:GLY:O	1:A:177:GLU:N	2.22	0.72
1:B:792:LYS:O	1:B:796:SER:OG	2.08	0.72
1:A:383:MET:HE3	1:A:383:MET:H	1.54	0.71
1:B:403:ALA:O	1:B:407:THR:OG1	2.08	0.71
1:B:622:LYS:NZ	1:B:623:PHE:O	2.23	0.71
1:B:599:VAL:CA	1:B:600:ILE:HG13	2.19	0.70
1:A:564:GLU:OE1	1:A:674:ARG:NH2	2.24	0.70
1:B:361:LYS:O	1:B:365:THR:OG1	2.10	0.70
1:A:137:LEU:O	6:A:1101:HOH:O	2.10	0.69
1:A:374:HIS:CE1	1:A:392:LYS:HG2	2.27	0.69
1:B:215:LEU:O	1:B:217:LYS:N	2.26	0.69
1:A:717:ASP:OD2	1:A:953:ARG:NH1	2.25	0.69
1:A:73:VAL:HG11	1:A:108:ILE:HG13	1.73	0.69
1:A:311:GLU:HG2	1:A:317:TYR:HA	1.77	0.67
1:B:218:ALA:O	1:B:258:LYS:HA	1.95	0.67
1:B:742:LYS:O	1:B:751:ARG:NH2	2.27	0.66
1:A:140:LEU:HB2	1:A:149:ALA:HB3	1.77	0.66
1:B:100:LEU:HD12	1:B:161:LYS:HG2	1.78	0.65
1:A:792:LYS:O	1:A:796:SER:OG	2.15	0.65
1:A:714:ASN:O	1:A:716:SER:N	2.31	0.64
1:B:55:VAL:HG13	1:B:62:PHE:HB2	1.80	0.64
1:B:856:ALA:HB1	1:B:896:MET:HG2	1.80	0.64
1:B:826:TYR:O	1:B:829:SER:OG	2.15	0.64
1:A:225:ARG:NH2	1:A:250:GLU:OE1	2.32	0.63
1:B:95:GLU:HG2	1:B:168:PHE:HE1	1.64	0.62
1:B:412:GLN:HE21	1:B:745:VAL:HB	1.65	0.62
1:A:468:PHE:CD1	1:A:469:LEU:HD23	2.34	0.62
1:B:599:VAL:HA	1:B:600:ILE:HB	1.80	0.62
1:A:95:GLU:HG2	1:A:168:PHE:HE2	1.64	0.62
1:B:352:ASP:O	1:B:356:SER:N	2.31	0.62
1:A:337:GLU:HG3	1:A:374:HIS:HB3	1.80	0.62
1:A:383:MET:HE2	1:A:392:LYS:HB2	1.82	0.62
1:A:55:VAL:HG21	1:A:61:ARG:HA	1.82	0.62
1:B:586:TRP:HB3	1:B:588:ILE:HG12	1.82	0.61
1:B:55:VAL:HG21	1:B:61:ARG:HA	1.81	0.61
1:B:599:VAL:HG12	1:B:601:HIS:CD2	2.35	0.61
1:A:805:TRP:CD2	1:A:836:LYS:HD2	2.35	0.61
1:A:877:ARG:HG2	1:A:917:PHE:CD1	2.36	0.61
1:B:332:ALA:O	1:B:345:ARG:NH2	2.33	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:738:SER:OG	1:A:751:ARG:NH1	2.34	0.60
1:A:888:ASP:O	1:A:891:SER:OG	2.19	0.60
1:B:797:VAL:O	1:B:799:ALA:N	2.35	0.60
1:B:299:ALA:O	1:B:303:SER:HB2	2.01	0.59
1:A:421:CYS:O	1:A:424:VAL:HG23	2.02	0.59
1:B:599:VAL:CG1	1:B:601:HIS:CD2	2.85	0.59
1:B:651:HIS:NE2	1:B:689:HIS:O	2.31	0.59
1:B:659:ARG:NH1	1:B:690:GLU:OE2	2.35	0.59
1:B:808:LEU:O	1:B:812:TYR:N	2.35	0.59
1:B:801:THR:HG22	1:B:803:ALA:H	1.68	0.59
1:A:548:PRO:HB3	1:A:586:TRP:CE3	2.38	0.59
1:A:398:TYR:OH	1:A:466:LYS:HD3	2.03	0.58
1:B:70:PRO:HD2	1:B:109:ILE:HG21	1.83	0.58
1:B:718:ILE:HD12	1:B:718:ILE:H	1.69	0.58
1:A:56:ALA:O	1:A:57:THR:HG22	2.04	0.58
1:A:448:GLU:HA	1:A:895:ARG:HH22	1.69	0.58
1:A:424:VAL:HG13	1:A:452:GLU:HB3	1.86	0.58
1:B:173:GLY:H	1:B:180:TYR:HA	1.69	0.58
1:B:318:TYR:CE2	1:B:323:LEU:HB2	2.39	0.58
1:B:737:GLN:NE2	1:B:750:LEU:HD23	2.19	0.58
1:B:475:GLN:O	1:B:479:ILE:HG13	2.05	0.57
1:A:577:TRP:O	1:A:581:GLN:HG2	2.05	0.57
1:A:801:THR:HG22	1:A:803:ALA:H	1.68	0.57
1:B:646:GLN:HE22	1:B:653:LEU:HD12	1.70	0.57
1:A:632:ILE:HG23	1:A:665:ASP:CG	2.25	0.57
1:B:424:VAL:O	1:B:428:ASP:N	2.31	0.57
1:B:549:LEU:HB2	1:B:566:PHE:HB2	1.87	0.56
1:A:711:ASP:OD2	6:A:1102:HOH:O	2.18	0.56
1:B:214:PRO:HA	1:B:260:SER:HB3	1.87	0.56
1:B:902:THR:OG1	1:B:934:VAL:HG11	2.06	0.56
1:B:635:TYR:HB3	1:B:639:GLY:HA3	1.86	0.56
1:B:389:ILE:HD11	1:B:449:MET:HE3	1.88	0.56
1:B:592:TYR:HD1	1:B:592:TYR:H	1.53	0.56
1:A:177:GLU:HB2	1:A:203:GLN:HG2	1.88	0.56
1:A:64:TRP:CD2	1:A:70:PRO:HG3	2.41	0.56
1:A:805:TRP:CE2	1:A:836:LYS:HD2	2.41	0.56
4:B:1002:NAG:O3	4:B:1002:NAG:O7	2.22	0.56
1:B:139:VAL:HA	1:B:150:LEU:HA	1.88	0.56
1:B:316:ILE:HD11	1:B:483:LYS:HE2	1.88	0.56
1:B:620:TRP:NE1	1:B:646:GLN:OE1	2.32	0.56
1:B:227:GLU:OE1	1:B:229:ARG:HD3	2.07	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:713:ARG:HB3	1:B:713:ARG:HH11	1.71	0.55
1:B:599:VAL:HG11	1:B:601:HIS:NE2	2.21	0.55
1:B:634:HIS:NE2	1:B:674:ARG:HB3	2.22	0.55
1:B:139:VAL:HG23	1:B:140:LEU:N	2.22	0.55
1:B:877:ARG:HA	1:B:917:PHE:CE1	2.42	0.55
1:A:537:MET:HG3	1:A:587:HIS:HB2	1.89	0.55
1:B:232:ALA:O	1:B:253:PHE:HZ	1.89	0.55
1:B:73:VAL:HG13	1:B:99:VAL:HG21	1.89	0.54
1:A:234:SER:OG	1:A:235:ASN:N	2.40	0.54
1:A:954:THR:O	1:A:958:VAL:HG23	2.07	0.54
1:A:374:HIS:HE1	1:A:392:LYS:HG2	1.72	0.54
1:B:718:ILE:HG13	1:B:953:ARG:HG3	1.88	0.54
1:B:442:THR:O	1:B:446:ILE:HG13	2.08	0.54
1:B:479:ILE:O	1:B:483:LYS:HG3	2.07	0.54
1:B:877:ARG:HG3	1:B:917:PHE:CD1	2.41	0.54
1:A:398:TYR:CZ	1:A:402:ILE:HD11	2.42	0.54
1:A:640:TRP:O	1:A:644:ILE:HG13	2.06	0.54
1:B:845:MET:HG3	1:B:875:PHE:HZ	1.73	0.54
1:B:140:LEU:HD12	1:B:141:SER:H	1.73	0.54
1:B:70:PRO:HG2	1:B:109:ILE:HG21	1.90	0.54
1:B:236:MET:SD	1:B:256:THR:HA	2.47	0.54
1:B:565:ARG:HD3	1:B:584:TYR:CE1	2.41	0.54
1:B:338:ASN:HB2	1:B:341:LEU:O	2.08	0.54
1:B:599:VAL:CA	1:B:600:ILE:CB	2.85	0.54
1:B:156:LEU:HD22	1:B:162:TYR:CE2	2.42	0.54
1:B:640:TRP:CZ3	1:B:666:VAL:HG22	2.43	0.53
1:B:763:HIS:CG	1:B:765:PRO:HD2	2.43	0.53
1:A:713:ARG:HB2	1:A:715:ILE:HG13	1.91	0.53
1:B:273:SER:HB3	1:B:287:TYR:CE1	2.43	0.53
1:B:386:TRP:CD1	1:B:446:ILE:HD13	2.43	0.53
1:B:479:ILE:HG22	1:B:483:LYS:HE3	1.89	0.53
1:B:464:MET:HG3	1:B:629:GLY:HA2	1.91	0.53
1:B:130:TYR:HE1	1:B:153:PRO:HG2	1.74	0.53
1:B:123:GLN:O	1:B:163:TYR:N	2.40	0.53
1:B:448:GLU:HA	1:B:895:ARG:NH1	2.24	0.53
1:B:640:TRP:CD1	1:B:675:LEU:HD11	2.44	0.53
1:B:922:GLU:HA	1:B:926:SER:HB3	1.90	0.52
1:A:397:LYS:O	1:A:400:GLU:HB2	2.09	0.52
1:A:141:SER:O	1:A:143:PRO:HD3	2.08	0.52
1:A:119:ASN:O	1:A:166:MET:HA	2.09	0.52
1:A:659:ARG:NH1	1:A:690:GLU:OE1	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:721:ASN:HB2	1:B:956:LEU:HD23	1.91	0.52
1:B:242:ILE:O	1:B:242:ILE:HG13	2.09	0.52
1:B:351:PHE:CZ	1:B:361:LYS:HD2	2.43	0.52
1:B:468:PHE:HD1	1:B:469:LEU:HG	1.75	0.52
1:B:599:VAL:CA	1:B:600:ILE:HB	2.40	0.52
1:B:388:ASP:OD1	1:B:437:SER:OG	2.21	0.51
1:B:469:LEU:O	1:B:473:LYS:HB2	2.09	0.51
1:B:929:ASP:N	1:B:929:ASP:OD1	2.44	0.51
1:B:311:GLU:HG2	1:B:317:TYR:HA	1.91	0.51
1:B:257:VAL:HG11	1:B:487:TYR:CE2	2.46	0.51
1:A:489:ASN:N	1:A:489:ASN:OD1	2.43	0.51
1:B:599:VAL:CG1	1:B:601:HIS:NE2	2.73	0.51
1:A:129:ARG:HD2	1:A:154:GLU:OE1	2.11	0.51
1:A:521:THR:O	1:A:524:MET:HB3	2.11	0.51
1:B:314:PHE:O	1:B:479:ILE:HG23	2.11	0.51
1:B:670:VAL:HG21	1:B:680:ALA:HB2	1.93	0.51
1:A:813:GLU:OE1	1:B:848:LYS:NZ	2.25	0.51
1:A:722:LEU:HG	1:A:956:LEU:HD11	1.93	0.51
1:A:383:MET:CE	1:A:392:LYS:HD3	2.42	0.50
1:A:236:MET:HB3	1:A:237:PRO:HD2	1.93	0.50
1:A:383:MET:HE1	1:A:392:LYS:HD3	1.94	0.50
1:A:939:THR:HG22	1:A:943:LYS:HE2	1.94	0.50
1:B:64:TRP:CZ3	1:B:70:PRO:HG3	2.47	0.50
1:B:731:LYS:H	1:B:732:PRO:HD2	1.76	0.50
1:A:138:LYS:HB3	1:A:151:LEU:HB2	1.93	0.50
1:A:311:GLU:CG	1:A:317:TYR:HA	2.41	0.50
1:A:570:VAL:HG12	1:A:577:TRP:HD1	1.76	0.50
1:B:122:LEU:HD12	1:B:163:TYR:O	2.11	0.50
1:B:446:ILE:O	1:B:449:MET:HB2	2.12	0.50
1:A:383:MET:CE	1:A:383:MET:H	2.21	0.50
1:B:662:LEU:O	1:B:666:VAL:HG23	2.12	0.50
1:A:388:ASP:OD2	1:A:492:ASN:HB2	2.12	0.50
1:A:727:LEU:O	1:A:731:LYS:HB2	2.10	0.50
1:A:833:HIS:HB2	1:A:836:LYS:HG2	1.92	0.50
1:B:818:SER:HA	1:B:821:GLN:HB2	1.93	0.50
1:A:104:ALA:HB2	1:A:158:PRO:HD3	1.93	0.50
1:B:226:ARG:NH1	1:B:230:HIS:O	2.44	0.50
1:A:614:LEU:HD12	1:A:615:PRO:HD2	1.94	0.49
1:A:398:TYR:OH	1:A:402:ILE:HD11	2.12	0.49
1:A:681:LEU:HB3	1:A:955:TRP:CE2	2.47	0.49
1:B:351:PHE:CE2	1:B:356:SER:HB3	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:SER:HB3	1:A:367:VAL:HG11	1.94	0.49
1:A:484:LYS:HG2	1:A:485:PHE:CE1	2.48	0.49
1:B:477:GLY:HA3	1:B:499:LEU:HD23	1.94	0.49
1:B:808:LEU:HA	1:B:811:GLN:HB3	1.94	0.49
1:A:594:THR:HG21	1:A:614:LEU:HD11	1.93	0.49
1:B:139:VAL:HG23	1:B:140:LEU:H	1.77	0.49
1:B:488:ARG:O	1:B:489:ASN:ND2	2.46	0.49
1:B:366:ARG:NH1	1:B:416:TYR:HE2	2.11	0.49
1:A:110:LEU:HB3	1:A:211:PHE:CE1	2.47	0.49
1:B:63:PRO:HB3	1:B:107:PHE:CE2	2.48	0.49
1:A:323:LEU:HD21	1:A:372:LEU:HD22	1.95	0.48
1:A:64:TRP:CE3	1:A:70:PRO:HG3	2.48	0.48
1:B:63:PRO:HB3	1:B:107:PHE:CD2	2.48	0.48
1:A:383:MET:HE3	1:A:383:MET:HB3	1.59	0.48
1:A:55:VAL:CG2	1:A:62:PHE:H	2.22	0.48
1:B:122:LEU:HD11	1:B:162:TYR:HB3	1.94	0.48
1:A:263:LEU:O	1:A:338:ASN:HB3	2.13	0.48
1:A:152:VAL:HG21	1:A:156:LEU:HD21	1.95	0.48
1:A:351:PHE:CZ	1:A:361:LYS:HE3	2.48	0.48
1:A:666:VAL:HG11	1:A:680:ALA:HA	1.95	0.48
3:A:1002:6PX:N7	3:A:1002:6PX:C18	2.75	0.48
1:A:514:CYS:HA	1:A:515:HIS:HA	1.65	0.48
1:A:588:ILE:O	1:A:590:LEU:N	2.47	0.48
1:B:731:LYS:N	1:B:732:PRO:HD2	2.27	0.48
1:A:585:LEU:HD21	1:A:607:SER:HA	1.95	0.48
1:B:60:GLU:HG2	1:B:61:ARG:H	1.78	0.48
1:B:797:VAL:C	1:B:799:ALA:H	2.16	0.48
1:A:780:SER:HB2	1:A:783:LYS:HB2	1.96	0.48
1:A:921:LEU:O	1:A:926:SER:HB2	2.14	0.48
1:A:122:LEU:HB2	1:A:137:LEU:HD21	1.96	0.48
1:A:324:ASP:C	1:A:325:LEU:HD12	2.34	0.48
1:A:115:LEU:HD13	1:A:209:PRO:HD3	1.95	0.47
1:A:801:THR:HB	1:A:804:GLY:H	1.78	0.47
1:B:156:LEU:O	1:B:158:PRO:HD3	2.14	0.47
1:B:409:PRO:HD2	1:B:410:GLU:OE1	2.14	0.47
1:A:752:SER:OG	1:A:789:ASP:O	2.30	0.47
1:A:863:ALA:HA	1:A:869:GLN:HA	1.96	0.47
1:B:200:GLU:OE2	1:B:392:LYS:NZ	2.45	0.47
1:B:907:SER:O	1:B:942:ILE:HD11	2.13	0.47
1:A:352:ASP:HA	1:A:353:PRO:HD3	1.71	0.47
1:A:215:LEU:HD13	1:A:384:GLU:HG3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:ASP:OD1	1:B:453:VAL:HB	2.14	0.47
1:B:62:PHE:HA	1:B:63:PRO:HD3	1.70	0.47
1:B:223:LYS:O	1:B:224:ILE:HD13	2.14	0.47
1:A:923:ALA:N	1:A:924:GLN:O	2.48	0.47
1:B:55:VAL:HG21	1:B:62:PHE:H	1.79	0.47
1:B:790:VAL:HG12	1:B:794:VAL:HG23	1.97	0.47
1:A:143:PRO:O	1:A:146:GLU:N	2.42	0.47
1:A:397:LYS:HB3	1:A:459:ALA:HB2	1.95	0.47
1:A:436:ILE:HA	1:A:453:VAL:HG12	1.97	0.47
1:B:77:HIS:ND1	1:B:219:ASN:HB2	2.30	0.47
1:B:500:SER:HB3	1:B:534:VAL:HG21	1.96	0.47
1:A:201:PRO:HG2	1:A:202:THR:HG23	1.97	0.47
1:A:595:SER:HB3	1:A:620:TRP:CE2	2.49	0.47
1:B:122:LEU:HD12	1:B:123:GLN:H	1.80	0.47
1:B:600:ILE:HG22	1:B:600:ILE:O	2.14	0.47
1:B:847:GLY:HA2	1:B:850:ILE:O	2.14	0.47
1:A:428:ASP:O	1:A:546:GLY:HA2	2.14	0.46
1:A:775:SER:O	1:A:779:GLU:HG2	2.14	0.46
1:B:911:LEU:HD13	1:B:938:ILE:HB	1.96	0.46
1:A:363:TRP:O	1:A:367:VAL:HG23	2.15	0.46
1:A:550:LEU:HD22	1:A:590:LEU:HD22	1.98	0.46
1:A:393:GLU:OE2	3:A:1002:6PX:N1	2.49	0.46
1:B:591:THR:O	1:B:624:ASN:N	2.43	0.46
1:A:568:GLN:HE21	1:A:671:GLY:HA3	1.80	0.46
1:A:626:ASP:OD1	1:A:657:LYS:HB2	2.16	0.46
1:A:873:TRP:CZ2	1:A:877:ARG:HD3	2.51	0.46
1:B:142:TYR:HD1	1:B:143:PRO:HD2	1.80	0.46
1:B:302:ALA:O	1:B:306:LEU:HB2	2.15	0.46
1:B:383:MET:HG3	1:B:383:MET:H	1.41	0.46
1:B:718:ILE:HG22	1:B:722:LEU:HD12	1.98	0.46
1:A:197:THR:HG23	1:A:266:TYR:O	2.14	0.46
1:A:535:LYS:O	1:A:539:THR:HG23	2.16	0.46
1:B:80:LEU:HB3	1:B:222:ILE:HD13	1.96	0.46
1:A:388:ASP:OD2	1:A:492:ASN:N	2.44	0.46
1:A:780:SER:HB3	1:A:784:LEU:HD12	1.98	0.46
1:B:298:TYR:CD1	1:B:361:LYS:HE2	2.51	0.46
1:B:687:LEU:HD11	1:B:699:GLY:HA3	1.97	0.46
1:A:389:ILE:HD11	1:A:392:LYS:HE3	1.97	0.46
1:B:239:VAL:HG12	1:B:240:LYS:HG2	1.97	0.46
1:A:418:LEU:HD21	1:A:627:SER:HB2	1.98	0.46
1:B:411:LEU:HA	1:B:745:VAL:HG21	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:GLU:HB3	1:A:160:LEU:HD22	1.98	0.45
1:A:930:ILE:O	1:A:934:VAL:HG23	2.16	0.45
1:B:591:THR:HG22	1:B:602:ARG:HD3	1.97	0.45
1:A:545:LYS:HD2	1:A:565:ARG:NH2	2.31	0.45
1:B:316:ILE:HD11	1:B:483:LYS:HG2	1.99	0.45
1:B:867:LYS:HA	1:B:867:LYS:HD2	1.78	0.45
1:B:226:ARG:NH1	1:B:249:LEU:HD12	2.32	0.45
1:B:99:VAL:HG23	1:B:100:LEU:O	2.17	0.45
1:A:174:ASP:N	1:A:174:ASP:OD1	2.50	0.45
1:A:192:ARG:HA	1:B:190:GLU:HG2	1.99	0.45
1:B:918:PHE:O	1:B:922:GLU:HG2	2.16	0.45
1:A:762:ASN:O	1:A:764:ALA:N	2.50	0.45
1:B:592:TYR:HA	1:B:623:PHE:HA	1.97	0.45
1:B:820:GLU:O	1:B:824:ILE:HG13	2.17	0.45
1:B:464:MET:SD	1:B:630:TYR:N	2.70	0.45
1:B:64:TRP:CE3	1:B:70:PRO:HG3	2.52	0.45
1:B:776:GLN:HB3	1:B:784:LEU:HD12	1.99	0.45
1:B:73:VAL:HG13	1:B:99:VAL:CG2	2.47	0.45
1:B:201:PRO:HD2	1:B:203:GLN:OE1	2.17	0.44
1:B:205:ARG:NE	1:B:212:ASP:OD2	2.51	0.44
1:B:386:TRP:O	1:B:389:ILE:HG13	2.17	0.44
1:B:592:TYR:CD1	1:B:592:TYR:N	2.84	0.44
1:A:496:TRP:HZ2	1:A:542:THR:HG21	1.83	0.44
1:B:258:LYS:HE3	1:B:258:LYS:HB2	1.68	0.44
1:B:894:ILE:HD13	1:B:894:ILE:HA	1.71	0.44
1:B:906:SER:HB3	1:B:941:ASN:HB3	1.99	0.44
1:B:677:LEU:HD21	1:B:952:LEU:HD13	1.99	0.44
1:A:755:LEU:HD23	1:A:755:LEU:HA	1.65	0.44
1:A:191:THR:HB	1:B:191:THR:HG23	1.98	0.44
1:B:55:VAL:HG12	1:B:56:ALA:N	2.33	0.44
1:B:738:SER:O	1:B:751:ARG:HD3	2.17	0.44
1:A:383:MET:CE	1:A:392:LYS:HB2	2.48	0.44
1:A:718:ILE:HD12	1:A:949:LEU:HD11	2.00	0.44
1:B:656:PRO:O	1:B:659:ARG:HB2	2.17	0.44
1:B:385:TRP:CG	1:B:386:TRP:N	2.85	0.44
1:B:236:MET:HB3	1:B:236:MET:HE2	1.86	0.44
1:A:742:LYS:O	1:A:751:ARG:NH2	2.51	0.43
1:B:640:TRP:NE1	1:B:675:LEU:HD11	2.33	0.43
1:A:184:TYR:CE1	1:A:289:SER:HB2	2.53	0.43
1:B:306:LEU:HD22	1:B:310:TYR:CE2	2.53	0.43
1:B:444:THR:HG21	1:B:889:LEU:HD23	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:680:ALA:O	1:B:683:MET:HB3	2.18	0.43
1:B:70:PRO:HB3	1:B:72:VAL:HG23	2.01	0.43
1:A:877:ARG:HA	1:A:917:PHE:CE1	2.53	0.43
1:A:383:MET:N	1:A:383:MET:HE3	2.27	0.43
1:B:235:ASN:O	1:B:322:LYS:HE3	2.19	0.43
1:B:436:ILE:HD11	1:B:457:LYS:HG2	2.01	0.43
1:B:532:ALA:O	1:B:536:GLU:HG3	2.19	0.43
1:B:763:HIS:CD2	1:B:765:PRO:HD2	2.54	0.43
1:A:873:TRP:CZ3	1:A:877:ARG:HG3	2.54	0.43
1:B:134:GLY:HA2	1:B:135:LYS:HA	1.80	0.43
1:B:145:HIS:O	1:B:147:GLN:HG3	2.19	0.43
1:B:430:LEU:HD22	1:B:936:GLU:OE1	2.17	0.43
1:A:108:ILE:CG2	1:A:150:LEU:HB2	2.40	0.43
1:A:57:THR:O	1:A:57:THR:HG23	2.19	0.43
1:B:205:ARG:NH2	1:B:212:ASP:HB3	2.12	0.43
1:B:55:VAL:CG2	1:B:62:PHE:H	2.32	0.43
1:A:244:LEU:HA	1:A:244:LEU:HD23	1.87	0.43
1:A:220:PHE:O	1:A:256:THR:HG23	2.19	0.43
1:A:647:LEU:HD21	1:A:659:ARG:HG2	2.01	0.43
1:B:836:LYS:HA	1:B:836:LYS:HD3	1.82	0.43
1:A:101:VAL:HG12	1:A:103:ASN:O	2.18	0.43
1:B:780:SER:O	1:B:783:LYS:HG2	2.19	0.43
1:A:227:GLU:OE2	4:A:1003:NAG:H3	2.19	0.43
1:A:366:ARG:HD2	1:A:413:PHE:CE1	2.54	0.43
1:B:96:LYS:HG3	1:B:165:ALA:HB2	2.00	0.43
1:B:833:HIS:HB3	1:B:835:GLU:HG3	2.01	0.43
1:B:106:GLN:HG3	1:B:107:PHE:CD2	2.54	0.42
1:B:646:GLN:NE2	1:B:650:ASN:O	2.52	0.42
1:A:267:ILE:HD13	1:A:326:ILE:HD13	1.99	0.42
1:B:261:THR:O	1:B:263:LEU:N	2.52	0.42
1:B:105:THR:HG22	1:B:107:PHE:H	1.84	0.42
1:B:118:THR:OG1	1:B:119:ASN:N	2.51	0.42
1:B:746:TRP:HA	1:B:749:MET:HB2	2.02	0.42
1:A:342:ILE:HG22	1:A:344:TYR:CE1	2.54	0.42
1:A:436:ILE:HD11	1:A:457:LYS:HG2	2.00	0.42
1:A:773:LEU:HD23	1:A:773:LEU:HA	1.78	0.42
1:B:639:GLY:O	1:B:643:LEU:HD12	2.18	0.42
1:A:375:GLN:HA	1:A:379:ASN:HB2	2.00	0.42
1:A:744:SER:O	1:A:748:ARG:HG3	2.19	0.42
1:B:306:LEU:HD22	1:B:310:TYR:HE2	1.83	0.42
1:B:351:PHE:O	1:B:353:PRO:HD3	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:LEU:HD21	1:B:372:LEU:HD22	2.02	0.42
1:A:245[A]:GLU:CD	1:A:245[A]:GLU:H	2.23	0.42
1:A:889:LEU:N	1:A:890:GLY:HA3	2.34	0.42
1:B:397:LYS:O	1:B:400:GLU:HB2	2.19	0.42
1:B:877:ARG:HG3	1:B:917:PHE:CE1	2.55	0.42
1:B:222:ILE:O	1:B:253:PHE:HD2	2.03	0.42
1:B:274:LEU:O	1:B:285:SER:HA	2.20	0.42
1:B:665:ASP:O	1:B:669:LEU:HG	2.19	0.42
1:A:109:ILE:HD13	1:A:149:ALA:HA	2.01	0.42
1:A:620:TRP:HB3	1:A:642:GLN:HB3	2.01	0.42
1:B:352:ASP:O	1:B:356:SER:HB2	2.19	0.42
1:B:876:VAL:HG21	1:B:901:THR:HG21	2.02	0.42
1:A:537:MET:HE2	1:A:587:HIS:O	2.20	0.42
1:A:722:LEU:HD23	1:A:722:LEU:HA	1.81	0.42
1:B:390:TRP:HH2	1:B:496:TRP:CZ2	2.38	0.42
1:B:496:TRP:CE3	1:B:538:MET:HG3	2.55	0.42
1:B:627:SER:OG	1:B:661:GLY:HA3	2.20	0.42
1:B:737:GLN:HE21	1:B:750:LEU:HD23	1.84	0.42
1:A:67:LEU:HA	1:A:67:LEU:HD23	1.70	0.41
1:A:737:GLN:HA	6:A:1113:HOH:O	2.19	0.41
1:A:949:LEU:HB3	1:A:950:PRO:HD3	2.01	0.41
1:B:257:VAL:HG11	1:B:487:TYR:HE2	1.84	0.41
1:A:655:ARG:HB2	1:A:658:ASP:OD2	2.19	0.41
1:A:726:LEU:HA	1:A:726:LEU:HD23	1.75	0.41
4:B:1003:NAG:H61	4:B:1004:NAG:C1	2.50	0.41
1:B:126:GLU:OE1	1:B:160:LEU:HA	2.20	0.41
1:A:279:SER:C	1:A:281:GLY:H	2.23	0.41
1:A:391:LEU:HD23	1:A:391:LEU:HA	1.90	0.41
1:A:563:GLN:OE1	1:A:586:TRP:N	2.49	0.41
1:A:884:LEU:HD23	1:A:884:LEU:HA	1.83	0.41
1:A:328:ILE:HA	1:A:329:PRO:HD3	1.91	0.41
1:A:327:ALA:HB2	1:A:349:LEU:HD23	2.02	0.41
1:B:325:LEU:HD23	1:B:349:LEU:HD11	2.02	0.41
1:B:258:LYS:NZ	1:B:487:TYR:O	2.33	0.41
1:B:880:TRP:CE2	1:B:921:LEU:HD22	2.55	0.41
1:B:926:SER:HA	1:B:927:HIS:HA	1.80	0.41
1:A:468:PHE:HD1	1:A:469:LEU:HD23	1.81	0.41
1:B:127:ASP:HB2	1:B:160:LEU:HD12	2.01	0.41
1:B:777:TRP:HD1	1:B:784:LEU:O	2.02	0.41
1:A:456:ASN:N	1:A:456:ASN:OD1	2.53	0.41
1:A:88:SER:OG	1:A:90:ASP:OD1	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:537:MET:HG3	1:B:587:HIS:HB3	2.01	0.41
1:A:140:LEU:HD23	1:A:140:LEU:HA	1.82	0.41
1:A:448:GLU:HA	1:A:895:ARG:NH2	2.34	0.41
1:B:420:VAL:HG13	1:B:456:ASN:CG	2.40	0.41
1:B:738:SER:OG	1:B:751:ARG:NH1	2.54	0.41
1:B:79:ASP:O	1:B:95:GLU:HA	2.21	0.41
1:A:124:SER:N	1:A:130:TYR:O	2.43	0.41
1:A:579:ALA:O	1:A:582:GLU:HG3	2.21	0.41
1:A:623:PHE:HB3	1:A:633:VAL:HG11	2.01	0.41
1:A:76:LEU:HD12	1:A:98:GLU:HG2	2.03	0.41
1:A:146:GLU:OE1	1:A:205:ARG:NH1	2.49	0.41
1:A:151:LEU:HA	1:A:151:LEU:HD23	1.84	0.41
1:A:916:LEU:HD12	1:A:916:LEU:HA	1.90	0.41
1:B:339:TRP:CE2	1:B:379:ASN:HB3	2.56	0.41
1:A:184:TYR:HB3	1:A:329:PRO:HG2	2.02	0.41
1:A:540:THR:O	1:A:544:GLN:HB2	2.21	0.41
1:A:564:GLU:HG2	1:A:581:GLN:OE1	2.21	0.41
1:A:845:MET:HB3	1:A:845:MET:HE3	1.75	0.41
1:B:235:ASN:HB3	1:B:339:TRP:O	2.21	0.41
1:B:323:LEU:HD21	1:B:372:LEU:CD2	2.51	0.41
1:A:282:VAL:HG11	1:A:318:TYR:CD2	2.56	0.41
1:A:55:VAL:CG2	1:A:61:ARG:HA	2.48	0.41
1:B:434:ARG:NH2	1:B:451:ASP:OD1	2.50	0.41
1:A:417:PHE:O	1:A:420:VAL:HB	2.21	0.40
1:B:282:VAL:HG12	1:B:284:VAL:HG23	2.02	0.40
1:B:859:LEU:HD12	1:B:859:LEU:HA	1.78	0.40
1:A:375:GLN:O	1:A:379:ASN:HB2	2.21	0.40
1:A:358:ALA:HB2	1:A:748:ARG:NH1	2.36	0.40
1:B:435:PRO:HB2	1:B:437:SER:O	2.21	0.40
1:B:476:LYS:HA	1:B:476:LYS:HD3	1.64	0.40
1:B:55:VAL:HG12	1:B:56:ALA:O	2.21	0.40
1:B:634:HIS:ND1	1:B:669:LEU:HD13	2.36	0.40
1:B:930:ILE:O	1:B:934:VAL:HG23	2.21	0.40
1:A:565:ARG:O	1:A:567:LEU:HG	2.21	0.40
1:A:132:LYS:HA	1:A:133:PRO:HA	1.71	0.40
1:A:256:THR:OG1	1:A:257:VAL:O	2.33	0.40
1:A:293:ARG:NH1	5:B:1005:MAN:O2	2.54	0.40
1:A:357:SER:N	1:A:360:ASP:OD2	2.51	0.40
1:A:647:LEU:HA	1:A:647:LEU:HD23	1.78	0.40
1:A:191:THR:HB	1:B:191:THR:H	1.86	0.40
1:B:600:ILE:CG2	1:B:600:ILE:O	2.69	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:917:PHE:CE2	1:B:921:LEU:HD11	2.56	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	898/967 (93%)	788 (88%)	96 (11%)	14 (2%)	11	37
1	B	841/967 (87%)	725 (86%)	105 (12%)	11 (1%)	14	43
All	All	1739/1934 (90%)	1513 (87%)	201 (12%)	25 (1%)	13	41

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	PHE
1	A	582	GLU
1	A	715	ILE
1	B	140	LEU
1	B	216	PHE
1	B	600	ILE
1	B	715	ILE
1	A	763	HIS
1	B	139	VAL
1	B	798	GLY
1	B	924	GLN
1	A	59	GLY
1	A	216	PHE
1	A	280	SER
1	A	617	LYS
1	A	923	ALA
1	A	74	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	144	ALA
1	A	468	PHE
1	A	589	PRO
1	B	72	VAL
1	B	689	HIS
1	A	58	ASN
1	B	257	VAL
1	B	666	VAL

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	812/870 (93%)	750 (92%)	62 (8%)	15	41
1	B	764/870 (88%)	708 (93%)	56 (7%)	16	43
All	All	1576/1740 (91%)	1458 (92%)	118 (8%)	16	42

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	LEU
1	A	73	VAL
1	A	76	LEU
1	A	103	ASN
1	A	105	THR
1	A	106	GLN
1	A	110	LEU
1	A	118	THR
1	A	123	GLN
1	A	145	HIS
1	A	154	GLU
1	A	171	LYS
1	A	172	LEU
1	A	181	LYS
1	A	194	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	255	THR
1	A	312	LYS
1	A	321	SER
1	A	322	LYS
1	A	338	ASN
1	A	339	TRP
1	A	352	ASP
1	A	354	LYS
1	A	359	SER
1	A	383	MET
1	A	424	VAL
1	A	456	ASN
1	A	461	ILE
1	A	476	LYS
1	A	489	ASN
1	A	521	THR
1	A	524	MET
1	A	578	ARG
1	A	585	LEU
1	A	609	THR
1	A	653	LEU
1	A	655	ARG
1	A	660	VAL
1	A	674	ARG
1	A	686	TYR
1	A	692	SER
1	A	716	SER
1	A	729	TYR
1	A	740	SER
1	A	781	SER
1	A	790	VAL
1	A	796	SER
1	A	801	THR
1	A	802	THR
1	A	806	ASN
1	A	818	SER
1	A	835	GLU
1	A	860	HIS
1	A	865	ARG
1	A	873	TRP
1	A	891	SER
1	A	909	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	916	LEU
1	A	924	GLN
1	A	930	ILE
1	A	948	ASN
1	A	963	HIS
1	B	57	THR
1	B	71	SER
1	B	86	LEU
1	B	96	LYS
1	B	99	VAL
1	B	106	GLN
1	B	112	SER
1	B	114	ASP
1	B	128	SER
1	B	138	LYS
1	B	191	THR
1	B	193	ILE
1	B	194	LEU
1	B	196	VAL
1	B	203	GLN
1	B	219	ASN
1	B	235	ASN
1	B	236	MET
1	B	257	VAL
1	B	259	MET
1	B	274	LEU
1	B	289	SER
1	B	321	SER
1	B	322	LYS
1	B	339	TRP
1	B	348	SER
1	B	356	SER
1	B	365	THR
1	B	383	MET
1	B	389	ILE
1	B	395	PHE
1	B	421	CYS
1	B	424	VAL
1	B	465	LEU
1	B	497	SER
1	B	563	GLN
1	B	588	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	592	TYR
1	B	609	THR
1	B	612	LEU
1	B	684	THR
1	B	705	SER
1	B	713	ARG
1	B	727	LEU
1	B	747	ASP
1	B	752	SER
1	B	818	SER
1	B	832	LYS
1	B	833	HIS
1	B	859	LEU
1	B	867	LYS
1	B	877	ARG
1	B	894	ILE
1	B	921	LEU
1	B	927	HIS
1	B	929	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	412	GLN
1	B	959	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 23 ligands modelled in this entry, 2 are monoatomic - leaving 21 for Mogul analysis.

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
3	6PX	A	1002	2	36,36,36	2.33	6 (16%)	44,48,48	1.67	12 (27%)
4	NAG	A	1003	1,4	14,14,15	0.48	0	15,19,21	0.45	0
4	NAG	A	1004	4	14,14,15	0.29	0	15,19,21	0.73	1 (6%)
4	NAG	A	1005	1,4	14,14,15	0.38	0	15,19,21	1.66	3 (20%)
4	NAG	A	1006	4	14,14,15	1.09	1 (7%)	15,19,21	1.19	1 (6%)
4	NAG	A	1007	1	14,14,15	0.53	0	15,19,21	0.51	0
4	NAG	A	1008	1	14,14,15	0.63	1 (7%)	15,19,21	0.50	0
4	NAG	A	1009	1	14,14,15	0.44	0	15,19,21	0.65	0
4	NAG	A	1010	1	14,14,15	0.96	2 (14%)	15,19,21	0.61	0
4	NAG	A	1011	1	14,14,15	0.22	0	15,19,21	0.48	0
4	NAG	A	1012	1	14,14,15	0.83	1 (7%)	15,19,21	0.59	0
4	NAG	B	1002	1	14,14,15	0.57	0	15,19,21	0.63	0
4	NAG	B	1003	1,4	14,14,15	1.18	1 (7%)	15,19,21	0.91	1 (6%)
4	NAG	B	1004	5,4	14,14,15	0.91	1 (7%)	15,19,21	1.11	1 (6%)
5	MAN	B	1005	5,4	11,11,12	1.30	1 (9%)	13,15,17	1.47	2 (15%)
5	MAN	B	1006	5	11,11,12	1.33	1 (9%)	13,15,17	1.01	2 (15%)
4	NAG	B	1007	1	14,14,15	0.58	0	15,19,21	0.38	0
4	NAG	B	1008	1	14,14,15	0.78	1 (7%)	15,19,21	0.49	0
4	NAG	B	1009	1	14,14,15	0.40	0	15,19,21	0.90	1 (6%)
4	NAG	B	1010	1	14,14,15	0.32	0	15,19,21	0.44	0
4	NAG	B	1011	1	14,14,15	1.58	2 (14%)	15,19,21	1.48	1 (6%)

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
3	6PX	A	1002	2	-	2/33/33/33	0/2/2/2
4	NAG	A	1003	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1004	4	-	0/6/23/26	0/1/1/1
4	NAG	A	1005	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1006	4	-	0/6/23/26	0/1/1/1
4	NAG	A	1007	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1008	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1009	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1010	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1011	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1012	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1002	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1003	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1004	5,4	-	0/6/23/26	0/1/1/1
5	MAN	B	1005	5,4	-	0/2/19/22	0/1/1/1
5	MAN	B	1006	5	-	0/2/19/22	0/1/1/1
4	NAG	B	1007	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1008	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1009	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1010	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1011	1	-	0/6/23/26	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1003	NAG	O5-C1	-3.84	1.37	1.43
5	B	1006	MAN	O5-C1	-3.60	1.37	1.43
4	A	1010	NAG	O5-C1	-2.04	1.40	1.43
4	A	1008	NAG	C1-C2	2.08	1.55	1.52
4	B	1011	NAG	C1-C2	2.27	1.55	1.52
3	A	1002	6PX	O2-C7	2.36	1.28	1.23
4	B	1008	NAG	C1-C2	2.48	1.55	1.52
4	A	1012	NAG	C1-C2	2.53	1.55	1.52
4	A	1010	NAG	C1-C2	2.54	1.56	1.52
3	A	1002	6PX	C11-C7	2.55	1.55	1.50
5	B	1005	MAN	C4-C5	2.76	1.58	1.53
4	B	1004	NAG	O5-C1	3.27	1.49	1.43
4	A	1006	NAG	C1-C2	3.87	1.57	1.52
3	A	1002	6PX	O5-C15	3.91	1.43	1.33
4	B	1011	NAG	O5-C1	5.39	1.52	1.43
3	A	1002	6PX	C7-N7	5.70	1.47	1.34
3	A	1002	6PX	C2-N5	6.73	1.47	1.35
3	A	1002	6PX	C6-N2	7.86	1.48	1.33

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	6PX	C12-C10-C11	-4.42	115.85	120.79
3	A	1002	6PX	C11-C7-N7	-3.79	109.97	116.97
3	A	1002	6PX	C18-C20-C22	-3.11	116.35	119.88
5	B	1005	MAN	O2-C2-C3	-2.59	105.09	110.17
3	A	1002	6PX	C17-C16-C14	-2.44	106.59	113.41
5	B	1006	MAN	O2-C2-C3	-2.42	105.42	110.17
4	A	1005	NAG	C4-C3-C2	-2.41	107.49	111.02
4	B	1003	NAG	C4-C3-C2	-2.30	107.65	111.02
3	A	1002	6PX	C21-C19-C17	-2.23	117.94	121.02
3	A	1002	6PX	C16-C14-C15	-2.15	105.07	110.43
4	A	1004	NAG	C1-O5-C5	2.05	114.99	112.17
5	B	1006	MAN	C1-O5-C5	2.12	115.09	112.17
3	A	1002	6PX	C10-C11-C13	2.15	121.76	119.23
3	A	1002	6PX	O2-C7-C11	2.40	125.19	120.94
3	A	1002	6PX	C20-C22-C21	2.47	124.19	119.74
3	A	1002	6PX	C14-N7-C7	2.57	128.21	121.56
3	A	1002	6PX	C15-C14-N7	2.58	116.77	110.70
3	A	1002	6PX	C3-C1-N1	2.63	117.23	110.50
4	B	1009	NAG	C1-O5-C5	2.91	116.18	112.17
4	B	1004	NAG	C1-O5-C5	3.23	116.62	112.17
5	B	1005	MAN	C1-O5-C5	3.46	116.94	112.17
4	A	1005	NAG	O4-C4-C5	3.64	118.47	109.28
4	A	1006	NAG	C1-O5-C5	3.89	117.53	112.17
4	A	1005	NAG	C1-O5-C5	4.04	117.74	112.17
4	B	1011	NAG	C1-O5-C5	5.54	119.81	112.17

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	6PX	C3-C1-C2-N5
3	A	1002	6PX	O1-C2-C1-C3

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	6PX	3	0
4	A	1003	NAG	1	0
4	B	1002	NAG	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1003	NAG	1	0
4	B	1004	NAG	1	0
5	B	1005	MAN	1	0
4	B	1007	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	900/967 (93%)	-0.04	20 (2%) 62 59	24, 55, 100, 147	0
1	B	849/967 (87%)	0.50	60 (7%) 17 12	26, 97, 133, 156	0
All	All	1749/1934 (90%)	0.22	80 (4%) 33 28	24, 70, 127, 156	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	640	TRP	7.3
1	A	520	MET	6.4
1	B	623	PHE	5.9
1	B	615	PRO	5.9
1	A	503	CYS	5.7
1	B	612	LEU	5.2
1	B	614	LEU	5.2
1	A	522	SER	5.0
1	B	150	LEU	5.0
1	A	559	LEU	5.0
1	B	107	PHE	5.0
1	B	105	THR	4.4
1	B	647	LEU	4.4
1	B	609	THR	4.3
1	A	523	ASN	4.3
1	A	514	CYS	4.3
1	B	592	TYR	4.2
1	A	513	VAL	4.1
1	A	515	HIS	4.1
1	B	648	ASN	4.0
1	B	106	GLN	4.0
1	B	108	ILE	4.0
1	A	521	THR	3.9
1	B	152	VAL	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	153	PRO	3.6
1	B	154	GLU	3.5
1	B	102	SER	3.4
1	B	635	TYR	3.2
1	B	643	LEU	3.2
1	B	687	LEU	3.2
1	B	64	TRP	3.1
1	B	925	GLY	3.1
1	B	602	ARG	3.1
1	A	61	ARG	3.1
1	A	612	LEU	3.0
1	B	72	VAL	3.0
1	B	621	VAL	2.9
1	A	576	GLU	2.9
1	B	136	GLU	2.9
1	B	122	LEU	2.9
1	B	952	LEU	2.9
1	A	580	LEU	2.9
1	B	610	ASP	2.9
1	A	572	GLN	2.8
1	B	779	GLU	2.8
1	B	649	GLN	2.8
1	B	681	LEU	2.7
1	B	121	THR	2.7
1	B	601	HIS	2.6
1	B	956	LEU	2.6
1	B	73	VAL	2.6
1	B	419	ASN	2.6
1	B	162	TYR	2.6
1	B	421	CYS	2.5
1	B	620	TRP	2.5
1	B	638	HIS	2.5
1	A	578	ARG	2.5
1	B	912	GLN	2.5
1	B	603	HIS	2.4
1	A	570	VAL	2.4
1	B	120	ALA	2.4
1	B	803	ALA	2.4
1	B	151	LEU	2.3
1	B	667	PHE	2.3
1	B	689	HIS	2.3
1	B	721	ASN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	599	VAL	2.2
1	A	728	GLN	2.2
1	B	613	ASP	2.2
1	B	637	GLY	2.2
1	B	801	THR	2.2
1	A	54	PRO	2.1
1	B	837	LEU	2.1
1	A	150	LEU	2.1
1	B	99	VAL	2.1
1	A	245[A]	GLU	2.1
1	B	723	LYS	2.1
1	B	607	SER	2.0
1	B	703	LEU	2.0
1	B	118	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [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
3	6PX	A	1002	35/35	0.86	0.35	3.56	38,65,89,92	0
4	NAG	A	1004	14/15	0.92	0.25	0.04	86,93,99,101	0
4	NAG	B	1007	14/15	0.86	0.17	-0.07	94,114,129,131	0
2	ZN	B	1001	1/1	0.99	0.25	-0.15	54,54,54,54	0
2	ZN	A	1001	1/1	1.00	0.24	-0.44	32,32,32,32	0
4	NAG	A	1003	14/15	0.96	0.16	-0.60	48,66,86,86	0
4	NAG	B	1004	14/15	0.88	0.14	-0.74	57,88,107,124	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	B	1003	14/15	0.93	0.14	-0.82	50,63,74,80	0
4	NAG	A	1011	14/15	0.89	0.13	-0.94	99,107,116,119	0
4	NAG	A	1007	14/15	0.93	0.13	-1.06	84,92,96,98	0
4	NAG	A	1005	14/15	0.96	0.13	-1.07	42,55,66,71	0
4	NAG	A	1009	14/15	0.75	0.20	-	96,107,123,125	0
4	NAG	A	1012	14/15	0.77	0.18	-	90,117,127,130	0
5	MAN	B	1005	11/12	0.81	0.13	-	112,137,143,143	0
4	NAG	A	1008	14/15	0.87	0.14	-	105,114,120,130	0
4	NAG	A	1006	14/15	0.82	0.22	-	77,86,98,99	0
4	NAG	A	1010	14/15	0.78	0.14	-	107,119,131,136	0
4	NAG	B	1010	14/15	0.79	0.26	-	108,118,127,127	0
5	MAN	B	1006	11/12	0.77	0.20	-	140,150,157,158	0
4	NAG	B	1011	14/15	0.69	0.34	-	103,119,134,137	0
4	NAG	B	1009	14/15	0.80	0.29	-	100,119,123,124	0
4	NAG	B	1002	14/15	0.81	0.26	-	114,127,135,135	0
4	NAG	B	1008	14/15	0.57	0.27	-	124,136,145,146	0

6.5 Other polymers

There are no such residues in this entry.