Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:37 PM GMT

PDB ID	:	1PWP
Title	:	Crystal Structure of the Anthrax Lethal Factor complexed with Small Molecule Inhibitor NSC 12155
Authors	:	Wong, T.Y.; Schwarzenbacher, R.; Liddington, R.C.
Deposited on	:	2003-07-02
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

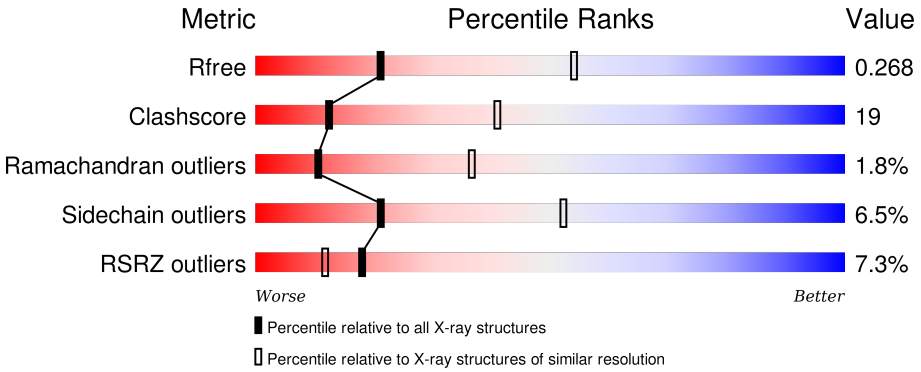
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (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 <=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	776	7%, 55%, 35%, 6%
1	B	776	7%, 60%, 32%

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	NSC	A	9002	X	-	-	X
3	NSC	B	9003	X	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12177 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.

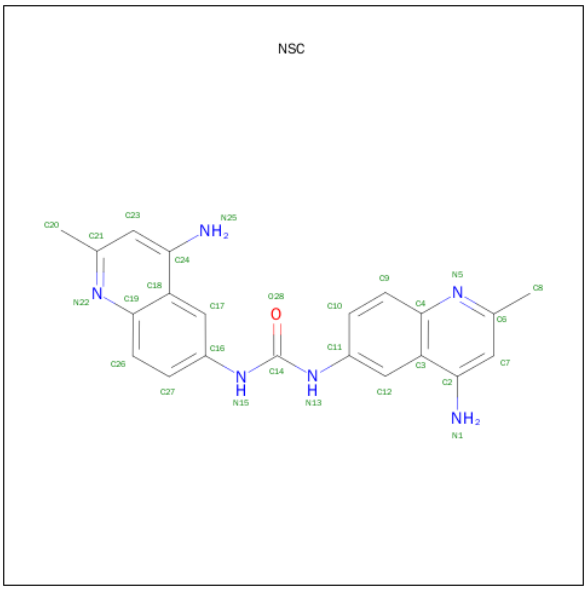
- Molecule 1 is a protein called Lethal factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	732	Total	C	N	O	S	0	0	0
			6014	3825	1011	1171	7			
1	B	743	Total	C	N	O	S	0	0	0
			6105	3877	1026	1195	7			

- 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 N,N'-BIS(4-AMINO-2-METHYLQUINOLIN-6-YL)UREA (three-letter code: NSC) (formula: $C_{21}H_{20}N_6O$).



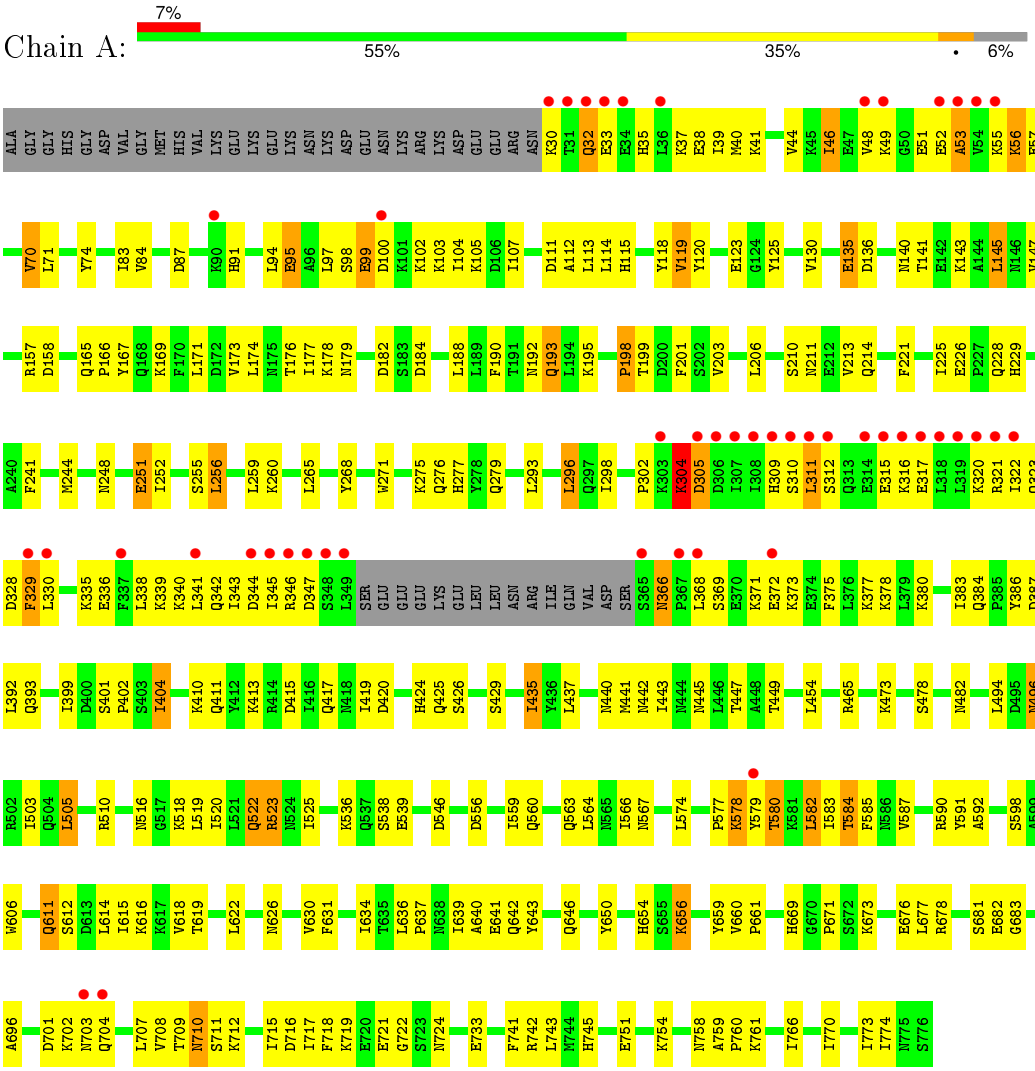
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			28	21	6	1		
3	B	1	Total	C	N	O	0	0
			28	21	6	1		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

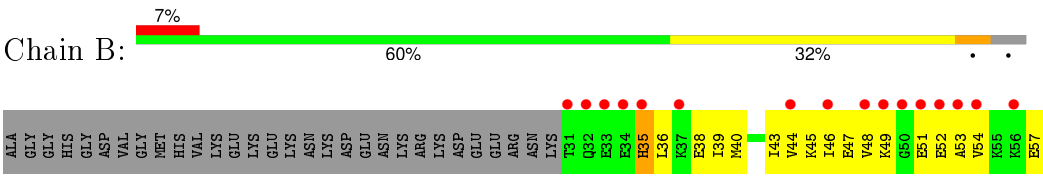
- Molecule 1: Lethal factor

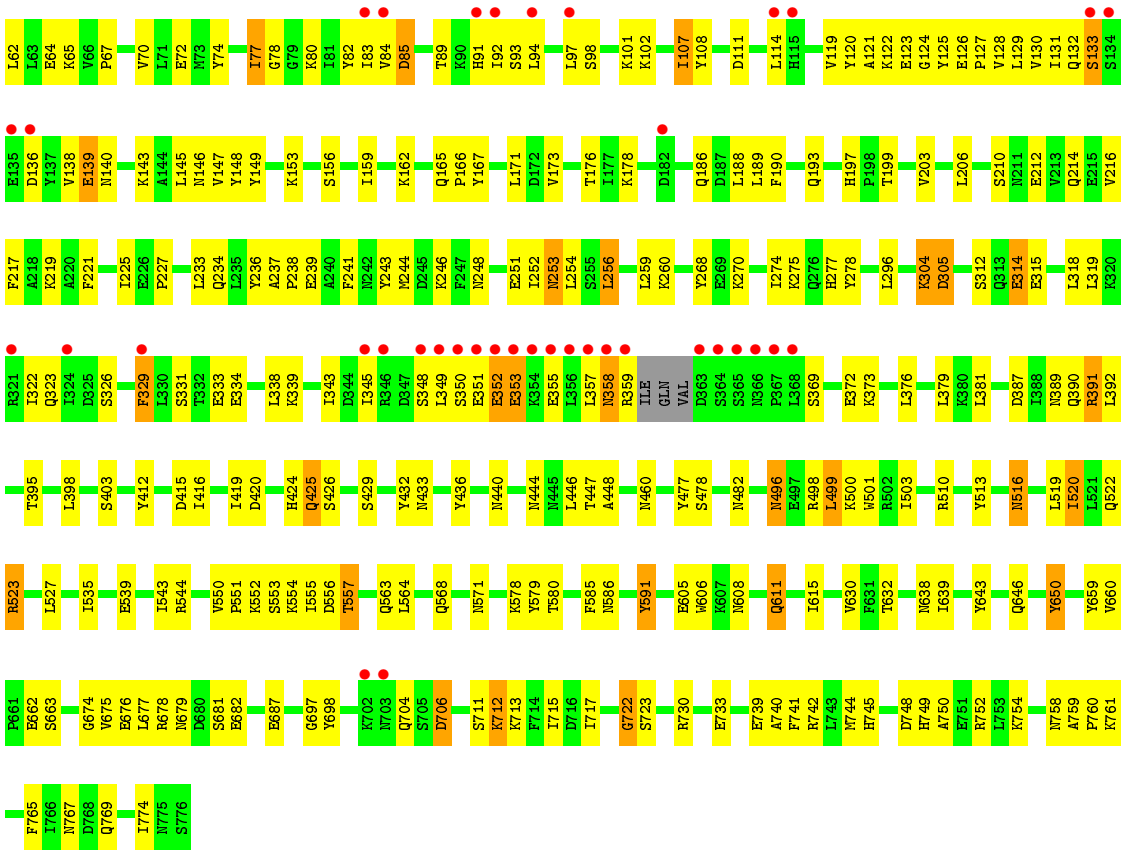
Chain A:



- Molecule 1: Lethal factor

Chain B:




L62 L63 E64 K65 V66 P67 V70 L71 E72 M73 Y74 I77 G78 G79 K80 I81 Y82 I83 V84 D85 T89 K90 H91 I92 S93 L94 L97 S98 K101 K102 I107 Y108 D111 L114 H115 V119 Y120 A121 K122 E123 G124 Y125 E126 P127 V128 L129 V130 I131 Q132 S133 S134
E135 D136 Y137 V138 E139 N140 K143 A144 L145 N146 V147 Y148 Y149 K153 S156 I159 K162 Q165 P166 Y167 L171 D172 V173 T176 I177 K178 D182 Q186 D187 L188 L189 F190 Q193 H197 P198 T199 V203 L206 S210 N211 E212 V213 Q214 E215 V216
F217 A218 K219 A220 F221 I225 E226 P227 L233 Q234 L235 Y236 A237 P238 E239 A240 F241 N242 Y243 M244 D245 K246 F247 N248 E251 I252 N253 L254 S255 L256 L259 K260 Y268 E269 K270 I274 K275 Q276 H277 Y278 L296 K304 D305 S312 Q313 E314 E315 I318 L319 K320
R321 I322 Q323 I324 D325 S326 F329 L330 S331 T332 E333 E334 I338 K339 I343 D344 I345 R346 D347 S348 L349 S350 E351 E352 E353 K354 E355 L356 I357 N358 R359 ILE GLN VAL D363 S364 S365 N366 P367 L368 S369 E372 K373 L376 L379 K380 L381 D387 I388 N389 Q390 R391 L392
T395 L398 S403 Y412 D415 I416 I419 D420 H424 Q425 S426 S429 Y432 N433 Y436 N440 N444 N445 L446 T447 A448 N460 Y477 S478 N482 N496 E497 R498 L499 K500 W501 R502 I503 R510 Y513 N516 L519 I520 L521 Q522
R523 L527 I535 E539 I543 R544 V550 P551 K552 S553 K554 I555 D556 T557 Q563 L564 Q568 N571 K578 Y579 T580 F585 N586 Y591 E605 W606 K607 N608 Q611 I615 V630 F631 T632 N638 I639 Y643 Q646 Y650 Y659 V660
P661 E662 S663 G674 V675 E676 L677 R678 N679 D680 S681 E682 E687 G697 Y698 K702 N703 Q704 S705 D706 S711 K712 K713 F714 I715 D716 I717 G722 S723 R730 E733 E739 A740 F741 R742 L743 M744 H745 D748 H749 A750 E751 R752 L753 K764 N758 A759 P760 K761
F765 I766 N767 D768 Q769 I774 N775 S776

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	96.70Å 137.40Å 98.30Å 90.00° 98.00° 90.00°	Depositor
Resolution (Å)	23.83 – 2.90 46.05 – 2.90	Depositor EDS
% Data completeness (in resolution range)	94.1 (23.83-2.90) 94.1 (46.05-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.50	Depositor
$< I/\sigma(I) >$ [1]	3.08 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.223 , 0.274 0.220 , 0.268	Depositor DCC
R_{free} test set	2595 reflections (4.89%)	DCC
Wilson B-factor (Å^2)	40.4	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 55.6	EDS
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 56344 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	12177	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.38	0/6122	0.62	0/8246
1	B	0.39	0/6213	0.62	0/8368
All	All	0.39	0/12335	0.62	0/16614

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	6014	0	6003	253	0
1	B	6105	0	6082	218	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	28	0	20	8	0
3	B	28	0	20	7	0
All	All	12177	0	12125	473	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 19.

All (473) 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:304:LYS:HD3	1:B:304:LYS:H	1.17	1.06
1:B:510:ARG:H	1:B:522:GLN:HE21	1.10	0.97
1:A:563:GLN:HE21	1:A:585:PHE:H	1.17	0.90
1:B:675:VAL:HG22	1:B:676:GLU:HG2	1.53	0.89
1:B:319:LEU:HD23	1:B:345:ILE:HG13	1.53	0.88
1:B:611:GLN:HE21	1:B:774:ILE:HD13	1.39	0.87
1:A:501:TRP:HB3	1:A:503:ILE:HD11	1.57	0.87
1:B:659:TYR:HB3	3:B:9003:NSC:H26	1.58	0.86
1:A:563:GLN:NE2	1:A:585:PHE:H	1.73	0.84
1:A:46:ILE:H	1:A:46:ILE:HD12	1.43	0.84
1:B:712:LYS:HD2	1:B:712:LYS:H	1.44	0.83
1:B:304:LYS:HD3	1:B:304:LYS:N	1.92	0.82
1:B:123:GLU:HG2	1:B:124:GLY:H	1.45	0.82
1:B:107:ILE:HG21	1:B:145:LEU:HD11	1.62	0.80
1:A:435:ILE:H	1:A:435:ILE:HD12	1.46	0.80
1:A:766:ILE:O	1:A:770:ILE:HG12	1.84	0.78
1:A:32:GLN:HG3	1:A:33:GLU:H	1.49	0.77
1:B:176:THR:HG21	1:B:239:GLU:HG3	1.66	0.77
1:A:87:ASP:OD2	1:A:115:HIS:HA	1.85	0.77
1:B:632:THR:HG21	1:B:639:ILE:HD11	1.68	0.76
1:B:563:GLN:NE2	1:B:585:PHE:H	1.85	0.75
1:A:435:ILE:HD12	1:A:435:ILE:N	2.00	0.75
1:A:107:ILE:HG21	1:A:145:LEU:HD13	1.67	0.75
1:A:659:TYR:HB3	3:A:9002:NSC:H26	1.69	0.74
1:B:97:LEU:HD23	1:B:101:LYS:HE3	1.69	0.74
1:A:277:HIS:CE1	1:A:425:GLN:HE21	2.05	0.74
1:A:30:LYS:HA	1:A:32:GLN:HG2	1.70	0.74
1:A:193:GLN:HE21	1:A:193:GLN:HA	1.52	0.74
1:B:126:GLU:N	1:B:127:PRO:HD3	2.03	0.74
1:B:349:LEU:HG	1:B:350:SER:H	1.52	0.73
1:B:712:LYS:HD2	1:B:712:LYS:N	2.03	0.73
1:A:304:LYS:HD3	1:A:304:LYS:H	1.53	0.72
1:A:567:ASN:HD21	1:A:583:ILE:H	1.36	0.72
1:B:679:ASN:HD21	1:B:681:SER:HB2	1.53	0.72
1:B:39:ILE:O	1:B:43:ILE:HG12	1.90	0.71
1:B:424:HIS:HA	1:B:510:ARG:HD2	1.70	0.71
1:B:296:LEU:HD22	1:B:419:ILE:HD13	1.70	0.71
1:B:712:LYS:CD	1:B:712:LYS:H	1.97	0.71
1:A:99:GLU:OE1	1:A:102:LYS:HG3	1.91	0.71
1:B:339:LYS:O	1:B:343:ILE:HG12	1.93	0.69
1:A:46:ILE:HG12	1:A:56:LYS:HG2	1.75	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:770:ILE:O	1:A:774:ILE:HG12	1.92	0.69
1:A:389:ASN:OD1	1:A:482:ASN:HB2	1.93	0.69
1:B:611:GLN:NE2	1:B:774:ILE:HD13	2.08	0.68
1:A:277:HIS:CD2	1:A:429:SER:HB2	2.29	0.68
1:A:615:ILE:O	1:A:619:THR:HG23	1.92	0.68
1:A:634:ILE:HD11	1:A:639:ILE:HD12	1.75	0.68
1:B:233:LEU:HD22	1:B:237:ALA:HB3	1.75	0.67
1:B:535:ILE:HD13	1:B:544:ARG:HB2	1.75	0.67
1:B:136:ASP:O	1:B:140:ASN:HB3	1.95	0.67
1:B:759:ALA:N	1:B:760:PRO:HD3	2.10	0.66
1:B:516:ASN:HD22	1:B:516:ASN:N	1.93	0.66
1:A:733:GLU:H	1:A:733:GLU:CD	1.98	0.66
1:B:387:ASP:HB3	1:B:390:GLN:HB3	1.78	0.65
1:A:30:LYS:C	1:A:32:GLN:H	1.98	0.65
1:A:193:GLN:HE21	1:A:193:GLN:CA	2.10	0.65
1:A:577:PRO:O	1:A:580:THR:HG23	1.97	0.65
1:A:721:GLU:HA	1:A:724:ASN:HD21	1.61	0.64
1:B:206:LEU:O	1:B:206:LEU:HD23	1.97	0.64
1:B:440:ASN:HD21	1:B:500:LYS:NZ	1.94	0.64
1:A:721:GLU:HA	1:A:724:ASN:ND2	2.12	0.64
1:B:605:GLU:HG3	1:B:681:SER:OG	1.98	0.64
1:B:77:ILE:HD13	1:B:259:LEU:HD21	1.80	0.64
1:A:312:SER:O	1:A:316:LYS:HG3	1.98	0.63
1:B:391:ARG:HG3	1:B:412:TYR:CD1	2.33	0.63
1:A:707:LEU:HB3	1:A:709:THR:HG22	1.79	0.63
1:B:97:LEU:CD2	1:B:101:LYS:HE3	2.28	0.63
1:B:49:LYS:HG2	1:B:85:ASP:OD1	1.98	0.63
1:B:314:GLU:O	1:B:318:LEU:HD13	1.99	0.63
1:B:45:LYS:HD2	1:B:82:TYR:HE2	1.64	0.62
1:B:131:ILE:HG22	1:B:132:GLN:H	1.63	0.62
1:A:30:LYS:C	1:A:32:GLN:N	2.46	0.62
1:A:30:LYS:HE2	1:A:33:GLU:OE2	2.00	0.62
1:A:48:VAL:HG23	1:A:52:GLU:HG2	1.82	0.62
1:A:33:GLU:O	1:A:37:LYS:HG3	2.00	0.62
1:B:478:SER:HB3	1:B:527:LEU:HB2	1.80	0.62
1:B:36:LEU:O	1:B:40:MET:HG3	2.00	0.62
1:B:352:GLU:O	1:B:355:GLU:HB3	2.00	0.61
1:A:103:LYS:NZ	1:A:103:LYS:HB3	2.16	0.61
1:A:701:ASP:C	1:A:703:ASN:H	2.03	0.61
1:B:711:SER:O	1:B:715:ILE:HG13	2.00	0.61
1:A:107:ILE:HD12	1:A:149:TYR:HB2	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:SER:O	1:A:214:GLN:HG3	2.00	0.61
1:A:741:PHE:O	1:A:745:HIS:HD2	1.84	0.61
1:A:304:LYS:HD3	1:A:304:LYS:N	2.16	0.60
1:A:578:LYS:HB2	1:A:578:LYS:NZ	2.15	0.60
1:A:188:LEU:HG	1:A:188:LEU:O	2.01	0.60
1:A:516:ASN:ND2	1:A:518:LYS:HD2	2.16	0.60
1:B:553:SER:O	1:B:557:THR:HG23	2.01	0.60
1:A:329:PHE:HA	3:A:9002:NSC:H83	1.83	0.60
1:B:277:HIS:CD2	1:B:429:SER:HB2	2.36	0.60
1:B:107:ILE:HG21	1:B:145:LEU:CD1	2.31	0.60
1:A:316:LYS:O	1:A:320:LYS:HG3	2.01	0.60
1:B:52:GLU:O	1:B:52:GLU:HG3	2.00	0.60
1:B:171:LEU:HD21	1:B:206:LEU:HD12	1.84	0.60
1:A:198:PRO:HG2	1:A:199:THR:H	1.67	0.60
1:B:46:ILE:HD13	1:B:83:ILE:HB	1.82	0.60
1:A:501:TRP:HB3	1:A:503:ILE:CD1	2.30	0.60
1:A:38:GLU:O	1:A:41:LYS:HG2	2.01	0.60
1:B:256:LEU:HD22	1:B:260:LYS:HE2	1.84	0.60
1:A:70:VAL:HG12	1:A:252:ILE:HD11	1.84	0.59
1:A:612:SER:O	1:A:616:LYS:HG3	2.02	0.59
1:A:759:ALA:N	1:A:760:PRO:HD3	2.17	0.59
1:A:522:GLN:HE21	1:A:525:ILE:HG13	1.67	0.59
1:A:256:LEU:HD22	1:A:260:LYS:HE3	1.84	0.59
1:A:304:LYS:HG2	1:A:305:ASP:H	1.66	0.59
1:A:393:GLN:HE22	1:A:445:ASN:HD21	1.50	0.59
1:B:253:ASN:N	1:B:253:ASN:HD22	1.99	0.59
1:A:496:ASN:C	1:A:496:ASN:HD22	2.04	0.59
1:A:614:LEU:HD22	1:A:770:ILE:HD12	1.83	0.59
1:B:403:SER:OG	1:B:638:ASN:ND2	2.34	0.59
1:A:56:LYS:HD3	1:A:56:LYS:O	2.01	0.59
1:A:125:TYR:HA	1:B:268:TYR:HE2	1.67	0.59
1:B:733:GLU:CD	1:B:733:GLU:H	2.06	0.58
1:B:91:HIS:CD2	1:B:93:SER:H	2.21	0.58
1:A:46:ILE:N	1:A:46:ILE:HD12	2.15	0.58
1:A:577:PRO:HD2	1:A:580:THR:HG21	1.84	0.58
3:A:9002:NSC:H12	3:A:9002:NSC:O28	2.03	0.58
1:A:369:SER:HB3	1:A:372:GLU:HB2	1.86	0.58
1:B:754:LYS:O	1:B:758:ASN:HB2	2.04	0.57
1:A:338:LEU:HD23	1:A:341:LEU:HD12	1.86	0.57
3:B:9003:NSC:H12	3:B:9003:NSC:O28	2.04	0.57
1:A:701:ASP:C	1:A:703:ASN:N	2.56	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:LEU:O	1:A:341:LEU:HB2	2.04	0.57
1:A:296:LEU:O	1:A:296:LEU:HD22	2.03	0.57
1:B:563:GLN:HE21	1:B:585:PHE:HB2	1.70	0.57
1:A:516:ASN:HD21	1:A:518:LYS:HD2	1.69	0.57
1:B:606:TRP:CE2	1:B:615:ILE:HD12	2.39	0.57
1:A:104:ILE:HG22	1:A:105:LYS:H	1.69	0.57
1:B:682:GLU:HG2	1:B:742:ARG:HD3	1.87	0.57
1:A:324:ILE:HG22	1:A:335:LYS:HG2	1.87	0.57
1:B:123:GLU:HG2	1:B:124:GLY:N	2.18	0.57
1:B:460:ASN:O	1:B:498:ARG:NH2	2.37	0.57
1:A:48:VAL:CG2	1:A:52:GLU:HG2	2.35	0.57
1:B:496:ASN:N	1:B:496:ASN:HD22	2.03	0.56
1:A:226:GLU:OE1	1:A:229:HIS:ND1	2.30	0.56
1:A:312:SER:HB3	1:A:315:GLU:HB2	1.87	0.56
1:B:513:TYR:HA	1:B:519:LEU:HD23	1.87	0.56
1:A:437:LEU:HD11	1:A:519:LEU:HD12	1.87	0.56
1:B:107:ILE:HG13	1:B:145:LEU:HD13	1.87	0.56
3:B:9003:NSC:O28	3:B:9003:NSC:H17	2.06	0.56
1:B:606:TRP:CH2	1:B:615:ILE:HG23	2.41	0.56
1:A:30:LYS:CA	1:A:32:GLN:HG2	2.35	0.55
1:B:212:GLU:O	1:B:216:VAL:HG23	2.05	0.55
1:A:711:SER:O	1:A:715:ILE:HG13	2.06	0.55
1:B:45:LYS:HB2	1:B:82:TYR:CD2	2.41	0.55
1:B:606:TRP:CZ2	1:B:615:ILE:HD12	2.41	0.55
1:A:696:ALA:HB3	1:A:708:VAL:HG11	1.88	0.55
1:B:237:ALA:N	1:B:238:PRO:HD3	2.22	0.55
1:A:70:VAL:HG12	1:A:252:ILE:CD1	2.36	0.55
1:A:611:GLN:OE1	1:A:770:ILE:HG21	2.07	0.55
1:A:48:VAL:HG21	1:A:55:LYS:HD2	1.89	0.55
1:A:701:ASP:O	1:A:703:ASN:N	2.39	0.55
1:B:643:TYR:HA	1:B:646:GLN:HG3	1.89	0.55
1:B:477:TYR:HB2	1:B:555:ILE:HD13	1.88	0.55
1:A:754:LYS:O	1:A:758:ASN:HB2	2.06	0.55
1:B:516:ASN:ND2	1:B:516:ASN:H	2.06	0.54
1:B:338:LEU:HD22	1:B:379:LEU:HD13	1.87	0.54
1:A:606:TRP:CH2	1:A:615:ILE:HG23	2.41	0.54
1:A:309:HIS:C	1:A:311:LEU:H	2.10	0.54
1:A:38:GLU:OE2	1:A:41:LYS:HE2	2.07	0.54
1:B:659:TYR:H	3:B:9003:NSC:C27	2.21	0.54
1:B:713:LYS:O	1:B:717:ILE:HG12	2.07	0.54
1:B:420:ASP:OD2	1:B:523:ARG:NH1	2.38	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:LEU:HD13	1:A:115:HIS:HE1	1.73	0.54
3:A:9002:NSC:H17	3:A:9002:NSC:O28	2.06	0.54
1:A:53:ALA:O	1:A:57:GLU:HB2	2.08	0.54
1:B:444:ASN:ND2	1:B:448:ALA:HA	2.23	0.53
1:A:244:MET:HE3	1:A:244:MET:HA	1.90	0.53
1:A:302:PRO:HG2	1:A:383:ILE:O	2.08	0.53
1:A:426:SER:HA	1:A:510:ARG:HA	1.89	0.53
1:A:275:LYS:NZ	1:A:279:GLN:HE22	2.06	0.53
1:B:305:ASP:N	1:B:305:ASP:OD2	2.42	0.53
1:B:94:LEU:HD22	1:B:97:LEU:HD11	1.91	0.53
1:A:317:GLU:O	1:A:320:LYS:HB2	2.08	0.53
1:B:126:GLU:N	1:B:127:PRO:CD	2.72	0.53
1:A:256:LEU:HD22	1:A:260:LYS:HG3	1.91	0.53
1:B:552:LYS:HE2	1:B:556:ASP:OD1	2.09	0.53
1:B:769:GLN:HA	1:B:769:GLN:NE2	2.24	0.53
1:A:424:HIS:O	1:A:510:ARG:HD2	2.09	0.52
1:A:387:ASP:HB3	1:A:390:GLN:HB3	1.91	0.52
1:B:722:GLY:HA3	1:B:730:ARG:HH11	1.74	0.52
1:B:436:TYR:HA	1:B:503:ILE:O	2.10	0.52
1:A:686:HIS:HB2	1:A:742:ARG:HD3	1.92	0.52
1:A:339:LYS:O	1:A:343:ILE:HG12	2.10	0.52
1:B:107:ILE:HG12	1:B:149:TYR:CG	2.45	0.52
1:A:701:ASP:OD2	1:A:704:GLN:HB3	2.10	0.52
1:B:51:GLU:OE1	1:B:53:ALA:HB2	2.10	0.52
1:B:369:SER:O	1:B:373:LYS:HG3	2.10	0.51
1:B:426:SER:HA	1:B:510:ARG:HA	1.93	0.51
1:A:618:VAL:O	1:A:622:LEU:HG	2.10	0.51
1:A:743:LEU:HD22	1:A:751:GLU:HG2	1.92	0.51
1:A:234:GLN:NE2	1:A:241:PHE:CE1	2.79	0.51
1:A:100:ASP:C	1:A:102:LYS:H	2.14	0.51
1:B:501:TRP:HB3	1:B:503:ILE:HD11	1.93	0.51
1:A:659:TYR:HB3	3:A:9002:NSC:C26	2.39	0.51
1:B:516:ASN:ND2	1:B:516:ASN:N	2.56	0.51
1:B:107:ILE:HG22	1:B:108:TYR:CD1	2.46	0.51
1:B:586:ASN:HB3	1:B:632:THR:HB	1.93	0.51
1:A:123:GLU:HG3	1:A:157:ARG:CZ	2.41	0.51
1:B:510:ARG:H	1:B:522:GLN:NE2	1.94	0.51
1:A:373:LYS:O	1:A:377:LYS:HG3	2.10	0.51
1:B:392:LEU:HD21	1:B:416:ILE:HD13	1.93	0.51
1:A:315:GLU:HB3	1:A:375:PHE:CE1	2.46	0.51
1:B:236:TYR:C	1:B:238:PRO:HD3	2.32	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:640:ALA:O	1:A:642:GLN:N	2.44	0.50
1:A:342:GLN:O	1:A:345:ILE:HG22	2.11	0.50
1:A:40:MET:O	1:A:44:VAL:HB	2.11	0.50
1:B:312:SER:OG	1:B:315:GLU:HG3	2.11	0.50
1:A:443:ILE:CD1	1:A:454:LEU:HD22	2.41	0.50
1:B:167:TYR:OH	1:B:203:VAL:HG21	2.12	0.50
1:B:496:ASN:H	1:B:496:ASN:ND2	2.10	0.50
1:A:643:TYR:HA	1:A:646:GLN:HG3	1.93	0.50
1:B:65:LYS:HB2	1:B:148:TYR:OH	2.11	0.50
1:A:32:GLN:CG	1:A:33:GLU:H	2.20	0.50
1:B:304:LYS:CD	1:B:304:LYS:H	2.02	0.50
1:B:662:GLU:H	1:B:662:GLU:CD	2.13	0.50
1:B:107:ILE:HD13	1:B:219:LYS:HG2	1.94	0.49
1:A:583:ILE:HG23	1:A:631:PHE:HE1	1.77	0.49
1:B:578:LYS:O	1:B:579:TYR:HB2	2.12	0.49
1:A:602:ILE:HG23	1:A:681:SER:HA	1.93	0.49
1:A:614:LEU:HB2	1:A:774:ILE:HD11	1.94	0.49
1:B:94:LEU:HD21	1:B:120:TYR:HD2	1.77	0.49
1:A:566:ILE:HG13	1:A:600:TYR:CE2	2.47	0.49
1:B:121:ALA:HA	1:B:128:VAL:O	2.12	0.49
1:A:392:LEU:HD13	1:A:482:ASN:HA	1.93	0.49
1:B:47:GLU:O	1:B:84:VAL:HG23	2.12	0.49
1:B:496:ASN:H	1:B:496:ASN:HD22	1.59	0.49
1:B:564:LEU:O	1:B:568:GLN:HG3	2.12	0.49
1:A:410:LYS:HB3	1:A:410:LYS:NZ	2.27	0.49
1:B:233:LEU:HD13	1:B:241:PHE:HB2	1.95	0.49
1:A:317:GLU:HA	1:A:320:LYS:HD2	1.95	0.49
1:B:358:ASN:HD22	1:B:358:ASN:C	2.15	0.49
1:A:329:PHE:HA	3:A:9002:NSC:C8	2.42	0.49
1:A:330:LEU:O	1:A:335:LYS:HE3	2.12	0.49
1:B:630:VAL:HG11	1:B:639:ILE:HD13	1.95	0.48
1:A:293:LEU:HD22	1:A:520:ILE:HD12	1.95	0.48
1:B:440:ASN:HD21	1:B:500:LYS:HZ2	1.58	0.48
1:A:221:PHE:CE2	1:A:225:ILE:HG13	2.48	0.48
1:A:443:ILE:HD12	1:A:454:LEU:HD22	1.95	0.48
1:A:366:ASN:H	1:A:366:ASN:HD22	1.62	0.48
1:A:67:PRO:HG2	1:A:248:ASN:OD1	2.13	0.48
1:B:748:ASP:OD1	1:B:750:ALA:HB3	2.13	0.48
1:B:173:VAL:HG21	1:B:243:TYR:CD2	2.48	0.48
1:A:496:ASN:C	1:A:496:ASN:ND2	2.66	0.48
1:B:369:SER:HB2	1:B:372:GLU:HG3	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:741:PHE:O	1:B:745:HIS:HD2	1.96	0.48
1:A:74:TYR:CZ	1:A:154:ILE:HD13	2.49	0.48
1:B:234:GLN:HB2	1:B:241:PHE:CD2	2.49	0.48
1:A:496:ASN:HD22	1:A:497:GLU:N	2.11	0.48
1:B:89:THR:C	1:B:91:HIS:H	2.17	0.48
1:B:774:ILE:O	1:B:774:ILE:HG22	2.13	0.48
1:B:233:LEU:CD1	1:B:241:PHE:HA	2.44	0.48
1:B:149:TYR:CZ	1:B:153:LYS:HE3	2.49	0.48
1:A:437:LEU:CD1	1:A:519:LEU:HD12	2.43	0.48
1:B:165:GLN:HA	1:B:166:PRO:C	2.34	0.48
1:B:77:ILE:HG13	1:B:162:LYS:HE2	1.96	0.47
1:B:322:ILE:HD13	1:B:376:LEU:HD21	1.95	0.47
1:A:380:LYS:O	1:A:384:GLN:HG2	2.14	0.47
1:B:687:GLU:OE2	3:B:9003:NSC:H27	2.14	0.47
1:A:556:ASP:O	1:A:560:GLN:HG3	2.13	0.47
1:A:104:ILE:HG22	1:A:105:LYS:N	2.29	0.47
1:B:722:GLY:HA3	1:B:730:ARG:NH1	2.28	0.47
1:A:192:ASN:HA	1:A:195:LYS:HB2	1.97	0.47
1:B:178:LYS:HB2	1:B:190:PHE:HE1	1.79	0.47
1:A:203:VAL:HG21	1:A:465:ARG:NH2	2.30	0.47
1:B:97:LEU:HB2	1:B:102:LYS:HE3	1.95	0.47
1:B:674:GLY:HA3	1:B:677:LEU:HD12	1.97	0.47
1:A:94:LEU:HD11	1:A:130:VAL:HG21	1.97	0.47
1:B:62:LEU:HD21	1:B:147:VAL:HG11	1.96	0.47
1:B:84:VAL:O	1:B:132:GLN:HA	2.14	0.47
1:A:611:GLN:H	1:A:611:GLN:NE2	2.13	0.47
1:B:632:THR:CG2	1:B:639:ILE:HD11	2.42	0.47
1:A:437:LEU:HD12	1:A:505:LEU:HD21	1.95	0.47
1:B:74:TYR:HA	1:B:159:ILE:HD11	1.97	0.47
1:B:446:LEU:HG	1:B:591:TYR:HB2	1.97	0.47
1:B:520:ILE:O	1:B:520:ILE:HG23	2.15	0.47
1:B:156:SER:HB2	1:B:217:PHE:CD2	2.50	0.47
1:B:662:GLU:OE2	1:B:662:GLU:N	2.26	0.47
1:A:193:GLN:NE2	1:A:193:GLN:CA	2.78	0.47
1:B:107:ILE:HG13	1:B:145:LEU:CD1	2.45	0.47
1:B:759:ALA:N	1:B:760:PRO:CD	2.78	0.47
1:A:48:VAL:HG11	1:A:55:LYS:HD3	1.97	0.47
1:B:252:ILE:HG23	1:B:253:ASN:N	2.30	0.47
1:A:710:ASN:O	1:A:710:ASN:ND2	2.48	0.47
1:A:268:TYR:CE2	1:B:125:TYR:HB3	2.50	0.47
1:A:559:ILE:HD13	1:A:587:VAL:HB	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:550:VAL:HB	1:B:551:PRO:HD2	1.96	0.46
1:A:717:ILE:HG23	1:A:761:LYS:HB3	1.97	0.46
1:B:678:ARG:HG2	1:B:682:GLU:OE1	2.15	0.46
1:A:182:ASP:OD1	1:A:184:ASP:HB2	2.16	0.46
1:A:118:TYR:N	1:A:118:TYR:CD1	2.84	0.46
1:B:659:TYR:H	3:B:9003:NSC:H27	1.79	0.46
1:A:567:ASN:ND2	1:A:582:LEU:H	2.13	0.46
1:A:125:TYR:HA	1:B:268:TYR:CE2	2.50	0.46
1:A:141:THR:HG21	1:A:228:GLN:HG3	1.97	0.46
1:A:673:LYS:NZ	1:A:678:ARG:HA	2.30	0.46
1:A:656:LYS:O	1:A:656:LYS:HD3	2.15	0.46
1:B:331:SER:OG	1:B:334:GLU:HG3	2.15	0.46
1:A:598:SER:O	1:A:602:ILE:HG13	2.16	0.46
1:A:119:VAL:HG11	1:A:147:VAL:HG13	1.98	0.46
1:B:114:LEU:HD23	1:B:114:LEU:O	2.15	0.46
1:A:103:LYS:HG3	1:A:112:ALA:O	2.15	0.46
1:B:765:PHE:O	1:B:769:GLN:HG2	2.16	0.46
1:A:717:ILE:CD1	1:A:761:LYS:HD2	2.45	0.46
1:A:577:PRO:O	1:A:580:THR:CG2	2.63	0.46
1:B:91:HIS:CG	1:B:92:ILE:N	2.84	0.46
1:A:107:ILE:HG21	1:A:145:LEU:CD1	2.44	0.46
1:A:343:ILE:HG22	1:A:343:ILE:O	2.16	0.46
1:A:366:ASN:N	1:A:366:ASN:HD22	2.13	0.46
1:A:611:GLN:H	1:A:611:GLN:HE21	1.63	0.46
1:A:32:GLN:HG3	1:A:33:GLU:N	2.25	0.46
1:B:387:ASP:HB3	1:B:390:GLN:CB	2.46	0.46
1:B:40:MET:HA	1:B:44:VAL:HG23	1.98	0.46
1:B:122:LYS:HE2	1:B:128:VAL:HG22	1.97	0.45
1:A:378:LYS:HE2	1:A:650:TYR:CE2	2.51	0.45
1:A:135:GLU:N	1:A:135:GLU:CD	2.70	0.45
1:A:440:ASN:HD21	1:A:500:LYS:NZ	2.13	0.45
1:A:371:LYS:N	1:A:371:LYS:HD2	2.31	0.45
1:A:46:ILE:HG12	1:A:56:LYS:CG	2.45	0.45
1:A:157:ARG:HG3	1:A:214:GLN:HE22	1.81	0.45
1:A:345:ILE:HG13	1:A:345:ILE:O	2.17	0.45
1:A:35:HIS:O	1:A:39:ILE:HG12	2.16	0.45
1:A:176:THR:HG21	1:A:239:GLU:HG3	1.98	0.45
1:A:677:LEU:HD13	1:A:683:GLY:HA2	1.99	0.45
1:A:309:HIS:O	1:A:311:LEU:N	2.49	0.45
1:A:640:ALA:HA	1:A:643:TYR:CE2	2.52	0.45
1:A:277:HIS:CE1	1:A:425:GLN:NE2	2.80	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:GLU:OE1	1:A:228:GLN:HB2	2.16	0.45
1:A:584:THR:HG23	1:A:630:VAL:HG22	1.99	0.45
1:A:83:ILE:HD12	1:A:83:ILE:N	2.32	0.45
1:B:395:THR:HB	1:B:398:LEU:O	2.17	0.45
1:A:114:LEU:HD21	1:A:120:TYR:CD1	2.52	0.45
1:A:640:ALA:C	1:A:642:GLN:N	2.71	0.44
1:A:567:ASN:ND2	1:A:583:ILE:H	2.10	0.44
1:B:679:ASN:ND2	1:B:681:SER:HB2	2.26	0.44
1:B:444:ASN:HD22	1:B:448:ALA:HA	1.80	0.44
1:B:551:PRO:HG2	1:B:554:LYS:HG3	1.98	0.44
1:B:119:VAL:HA	1:B:130:VAL:O	2.17	0.44
1:B:244:MET:HA	1:B:244:MET:HE3	1.98	0.44
1:B:739:GLU:OE1	1:B:739:GLU:HA	2.17	0.44
1:B:571:ASN:ND2	1:B:580:THR:HB	2.32	0.44
1:B:210:SER:O	1:B:214:GLN:HG3	2.17	0.44
1:B:353:GLU:OE1	1:B:357:LEU:HG	2.18	0.44
1:B:717:ILE:HG23	1:B:761:LYS:HB2	1.98	0.44
1:A:538:SER:O	1:A:539:GLU:HB2	2.17	0.44
1:A:171:LEU:HG	1:A:206:LEU:HD13	2.00	0.44
1:A:336:GLU:HG3	1:A:340:LYS:HE3	1.98	0.44
1:B:304:LYS:HG2	1:B:305:ASP:H	1.81	0.44
1:B:516:ASN:HD22	1:B:516:ASN:H	1.60	0.44
1:A:311:LEU:HD23	1:A:316:LYS:HG2	2.00	0.44
1:A:391:ARG:NH1	1:A:404:ILE:HD12	2.33	0.44
1:B:188:LEU:HG	1:B:189:LEU:HG	1.98	0.44
1:B:197:HIS:HD2	1:B:199:THR:O	2.00	0.44
1:B:496:ASN:ND2	1:B:496:ASN:N	2.65	0.44
1:A:321:ARG:HA	1:A:321:ARG:HD2	1.75	0.44
1:A:614:LEU:O	1:A:618:VAL:HG23	2.18	0.43
1:B:54:VAL:HA	1:B:57:GLU:HB3	2.00	0.43
1:A:401:SER:HA	1:A:402:PRO:HD3	1.73	0.43
1:B:749:HIS:CE1	1:B:752:ARG:NH1	2.86	0.43
1:A:178:LYS:HD2	1:A:201:PHE:CE1	2.53	0.43
1:B:139:GLU:HG2	1:B:140:ASN:H	1.81	0.43
1:B:440:ASN:HD21	1:B:500:LYS:HZ3	1.63	0.43
1:B:740:ALA:O	1:B:744:MET:HG3	2.17	0.43
1:A:174:LEU:HD11	1:A:213:VAL:HG13	2.00	0.43
1:B:167:TYR:CZ	1:B:203:VAL:HG21	2.54	0.43
1:B:186:GLN:HG3	1:B:190:PHE:CD1	2.53	0.43
1:B:143:LYS:O	1:B:147:VAL:HG23	2.19	0.43
1:B:322:ILE:HD11	1:B:376:LEU:HD11	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:ILE:O	1:A:324:ILE:N	2.52	0.43
1:A:424:HIS:HA	1:A:510:ARG:HD2	2.00	0.43
1:A:420:ASP:OD1	1:A:523:ARG:HD3	2.19	0.43
1:B:318:LEU:O	1:B:322:ILE:HB	2.19	0.43
1:B:45:LYS:HE3	1:B:80:LYS:HD2	2.00	0.43
1:A:326:SER:O	1:A:368:LEU:HD21	2.19	0.43
1:A:118:TYR:CZ	1:A:143:LYS:HG2	2.53	0.43
1:A:708:VAL:O	1:A:708:VAL:HG22	2.18	0.43
1:B:176:THR:CG2	1:B:239:GLU:HG3	2.43	0.42
1:B:45:LYS:HB2	1:B:82:TYR:HD2	1.81	0.42
1:B:244:MET:CE	1:B:248:ASN:HD21	2.32	0.42
1:B:35:HIS:CE1	1:B:38:GLU:HG2	2.54	0.42
1:B:83:ILE:CD1	1:B:131:ILE:HD12	2.49	0.42
1:B:65:LYS:HE2	1:B:227:PRO:HD3	2.02	0.42
1:B:97:LEU:HB2	1:B:102:LYS:CE	2.49	0.42
1:A:578:LYS:HD3	1:A:579:TYR:CZ	2.54	0.42
1:B:769:GLN:HA	1:B:769:GLN:HE21	1.84	0.42
1:B:723:SER:HB3	1:B:730:ARG:HD3	2.01	0.42
1:B:389:ASN:OD1	1:B:482:ASN:HB2	2.18	0.42
1:A:386:TYR:OH	1:A:411:GLN:HG3	2.19	0.42
1:A:98:SER:C	1:A:100:ASP:H	2.22	0.42
1:A:252:ILE:O	1:A:255:SER:HB2	2.19	0.42
1:A:154:ILE:O	1:A:158:ASP:HB2	2.19	0.42
1:A:167:TYR:CZ	1:A:536:LYS:HB2	2.55	0.42
1:A:606:TRP:CZ2	1:A:615:ILE:HG23	2.55	0.42
1:A:516:ASN:HB2	1:B:539:GLU:CD	2.40	0.42
1:A:393:GLN:NE2	1:A:445:ASN:HD21	2.15	0.42
1:A:51:GLU:N	1:A:51:GLU:CD	2.73	0.42
1:A:46:ILE:CD1	1:A:46:ILE:H	2.23	0.42
1:B:270:LYS:O	1:B:274:ILE:HG12	2.20	0.42
1:A:669:HIS:CE1	1:A:671:PRO:HB2	2.55	0.42
1:B:225:ILE:HD13	1:B:225:ILE:HA	1.89	0.42
1:A:640:ALA:HA	1:A:643:TYR:CD2	2.55	0.42
1:A:338:LEU:HA	1:A:341:LEU:HD12	2.02	0.42
1:A:437:LEU:HD12	1:A:505:LEU:HG	2.02	0.42
1:B:381:LEU:HD11	1:B:650:TYR:HA	2.02	0.42
1:B:139:GLU:HG2	1:B:140:ASN:N	2.35	0.41
1:A:578:LYS:HZ3	1:A:578:LYS:HB2	1.84	0.41
1:A:682:GLU:OE2	1:A:742:ARG:NH1	2.52	0.41
1:A:178:LYS:HG3	1:A:179:ASN:N	2.35	0.41
1:A:265:LEU:HD23	1:A:265:LEU:HA	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:GLU:HG2	1:A:64:GLU:O	2.18	0.41
1:A:165:GLN:HB3	1:A:166:PRO:HA	2.02	0.41
1:A:103:LYS:HZ3	1:A:103:LYS:HB3	1.84	0.41
1:A:244:MET:CE	1:A:248:ASN:HD21	2.33	0.41
1:B:221:PHE:HD1	1:B:244:MET:HE1	1.84	0.41
1:A:84:VAL:HG11	1:A:91:HIS:HD2	1.86	0.41
1:B:278:TYR:CE2	1:B:425:GLN:HB3	2.55	0.41
1:A:339:LYS:O	1:A:342:GLN:HG2	2.21	0.41
1:A:271:TRP:O	1:A:271:TRP:HD1	2.03	0.41
3:A:9002:NSC:C12	3:A:9002:NSC:O28	2.68	0.41
1:B:237:ALA:N	1:B:238:PRO:CD	2.83	0.41
1:A:759:ALA:N	1:A:760:PRO:CD	2.82	0.41
1:B:275:LYS:HG3	1:B:513:TYR:CZ	2.55	0.41
1:B:519:LEU:HD23	1:B:519:LEU:HA	1.94	0.41
1:B:717:ILE:HG23	1:B:761:LYS:CB	2.50	0.41
1:A:440:ASN:HD21	1:A:500:LYS:HZ2	1.67	0.41
1:B:675:VAL:O	1:B:676:GLU:HB2	2.21	0.41
1:B:132:GLN:O	1:B:133:SER:C	2.58	0.41
1:A:95:GLU:C	1:A:97:LEU:H	2.24	0.41
1:A:309:HIS:C	1:A:311:LEU:N	2.73	0.41
1:A:173:VAL:O	1:A:177:ILE:HG12	2.20	0.41
1:A:399:ILE:HD12	1:A:413:LYS:HG3	2.01	0.41
1:B:149:TYR:OH	1:B:153:LYS:HE3	2.20	0.41
1:A:328:ASP:O	3:A:9002:NSC:H82	2.20	0.41
1:A:715:ILE:O	1:A:719:LYS:HG2	2.21	0.41
1:A:660:VAL:HA	1:A:661:PRO:HD2	1.92	0.41
1:A:298:ILE:HG13	1:A:298:ILE:O	2.20	0.41
1:A:693:ASP:CG	1:A:709:THR:HB	2.41	0.41
1:A:157:ARG:HB2	1:A:214:GLN:NE2	2.36	0.41
1:A:30:LYS:O	1:A:30:LYS:HG2	2.20	0.41
1:B:45:LYS:HB2	1:B:82:TYR:CE2	2.55	0.41
1:A:437:LEU:HD12	1:A:505:LEU:CD2	2.51	0.41
1:A:696:ALA:HB2	1:A:773:ILE:HD11	2.03	0.41
1:A:640:ALA:C	1:A:642:GLN:H	2.24	0.41
1:B:398:LEU:H	1:B:398:LEU:HD22	1.86	0.41
1:B:697:GLY:HA3	1:B:706:ASP:O	2.21	0.41
1:B:499:LEU:HD12	1:B:543:ILE:HB	2.02	0.41
1:B:304:LYS:HG2	1:B:305:ASP:N	2.36	0.41
3:B:9003:NSC:C12	3:B:9003:NSC:O28	2.69	0.41
1:A:275:LYS:HZ2	1:A:279:GLN:HE22	1.68	0.41
1:A:169:LYS:NZ	1:A:251:GLU:OE2	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:ASP:O	1:B:419:ILE:HG13	2.21	0.40
1:A:399:ILE:CD1	1:A:413:LYS:HG3	2.51	0.40
1:A:718:PHE:O	1:A:722:GLY:HA3	2.21	0.40
1:B:67:PRO:HB2	1:B:70:VAL:HG23	2.03	0.40
1:B:254:LEU:HD23	1:B:254:LEU:HA	1.91	0.40
1:B:48:VAL:HB	1:B:85:ASP:OD2	2.21	0.40
1:A:366:ASN:N	1:A:366:ASN:ND2	2.69	0.40
1:A:119:VAL:HA	1:A:130:VAL:O	2.21	0.40
1:A:478:SER:OG	1:A:590:ARG:HA	2.22	0.40
1:A:190:PHE:CD2	1:A:190:PHE:N	2.89	0.40
1:A:136:ASP:O	1:A:140:ASN:N	2.49	0.40
1:A:415:ASP:O	1:A:419:ILE:HG13	2.21	0.40
1:B:440:ASN:ND2	1:B:500:LYS:HZ3	2.19	0.40
1:A:105:LYS:HE2	1:A:111:ASP:OD2	2.20	0.40
1:B:660:VAL:HB	1:B:663:SER:OG	2.21	0.40
1:B:40:MET:O	1:B:44:VAL:HB	2.22	0.40
1:B:553:SER:O	1:B:557:THR:CG2	2.68	0.40
1:A:716:ASP:O	1:A:719:LYS:HB2	2.21	0.40
1:A:637:PRO:HD3	1:A:654:HIS:HB2	2.03	0.40
1:B:59:ALA:C	1:B:61:LYS:H	2.25	0.40
1:A:441:MET:HG2	1:A:442:ASN:N	2.36	0.40
1:A:323:GLN:O	1:A:324:ILE:C	2.59	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	728/776 (94%)	643 (88%)	69 (10%)	16 (2%)	8	31
1	B	739/776 (95%)	652 (88%)	76 (10%)	11 (2%)	13	42
All	All	1467/1552 (94%)	1295 (88%)	145 (10%)	27 (2%)	11	37

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	251	GLU
1	B	138	VAL
1	A	53	ALA
1	A	198	PRO
1	A	310	SER
1	A	311	LEU
1	A	329	PHE
1	A	473	LYS
1	A	592	ALA
1	B	98	SER
1	B	133	SER
1	B	326	SER
1	A	641	GLU
1	A	702	LYS
1	B	64	GLU
1	B	251	GLU
1	B	329	PHE
1	A	324	ILE
1	A	347	ASP
1	B	650	TYR
1	B	722	GLY
1	A	32	GLN
1	A	49	LYS
1	A	304	LYS
1	B	433	ASN
1	A	305	ASP
1	B	78	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	671/710 (94%)	626 (93%)	45 (7%)	20 50
1	B	682/710 (96%)	639 (94%)	43 (6%)	22 54
All	All	1353/1420 (95%)	1265 (94%)	88 (6%)	21 52

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ILE
1	A	56	LYS
1	A	70	VAL
1	A	71	LEU
1	A	95	GLU
1	A	99	GLU
1	A	119	VAL
1	A	135	GLU
1	A	145	LEU
1	A	193	GLN
1	A	211	ASN
1	A	233	LEU
1	A	256	LEU
1	A	259	LEU
1	A	276	GLN
1	A	296	LEU
1	A	304	LYS
1	A	344	ASP
1	A	346	ARG
1	A	366	ASN
1	A	404	ILE
1	A	417	GLN
1	A	435	ILE
1	A	447	THR
1	A	449	THR
1	A	494	LEU
1	A	496	ASN
1	A	505	LEU
1	A	522	GLN
1	A	523	ARG
1	A	546	ASP
1	A	564	LEU
1	A	574	LEU
1	A	578	LYS
1	A	580	THR
1	A	582	LEU
1	A	584	THR
1	A	591	TYR
1	A	611	GLN
1	A	626	ASN
1	A	636	LEU
1	A	656	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	676	GLU
1	A	710	ASN
1	A	712	LYS
1	B	35	HIS
1	B	72	GLU
1	B	77	ILE
1	B	85	ASP
1	B	107	ILE
1	B	111	ASP
1	B	129	LEU
1	B	139	GLU
1	B	146	ASN
1	B	193	GLN
1	B	246	LYS
1	B	253	ASN
1	B	256	LEU
1	B	304	LYS
1	B	305	ASP
1	B	314	GLU
1	B	323	GLN
1	B	329	PHE
1	B	333	GLU
1	B	348	SER
1	B	351	GLU
1	B	352	GLU
1	B	353	GLU
1	B	358	ASN
1	B	359	ARG
1	B	391	ARG
1	B	425	GLN
1	B	432	TYR
1	B	447	THR
1	B	496	ASN
1	B	499	LEU
1	B	516	ASN
1	B	520	ILE
1	B	523	ARG
1	B	557	THR
1	B	591	TYR
1	B	608	ASN
1	B	611	GLN
1	B	698	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	704	GLN
1	B	706	ASP
1	B	712	LYS
1	B	767	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	HIS
1	A	140	ASN
1	A	164	ASN
1	A	193	GLN
1	A	197	HIS
1	A	209	ASN
1	A	214	GLN
1	A	234	GLN
1	A	242	ASN
1	A	262	GLN
1	A	277	HIS
1	A	279	GLN
1	A	366	ASN
1	A	393	GLN
1	A	440	ASN
1	A	496	ASN
1	A	504	GLN
1	A	522	GLN
1	A	524	ASN
1	A	563	GLN
1	A	567	ASN
1	A	571	ASN
1	A	608	ASN
1	A	611	GLN
1	A	652	GLN
1	A	710	ASN
1	A	724	ASN
1	A	745	HIS
1	A	767	ASN
1	A	769	GLN
1	B	42	HIS
1	B	91	HIS
1	B	164	ASN
1	B	197	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	209	ASN
1	B	214	GLN
1	B	228	GLN
1	B	234	GLN
1	B	242	ASN
1	B	248	ASN
1	B	250	GLN
1	B	253	ASN
1	B	262	GLN
1	B	297	GLN
1	B	313	GLN
1	B	323	GLN
1	B	358	ASN
1	B	440	ASN
1	B	444	ASN
1	B	445	ASN
1	B	496	ASN
1	B	504	GLN
1	B	516	ASN
1	B	522	GLN
1	B	524	ASN
1	B	533	GLN
1	B	563	GLN
1	B	571	ASN
1	B	608	ASN
1	B	609	ASN
1	B	611	GLN
1	B	638	ASN
1	B	645	HIS
1	B	679	ASN
1	B	704	GLN
1	B	745	HIS
1	B	756	GLN
1	B	769	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	NSC	A	9002	-	31,31,31	1.46	6 (19%)	39,45,45	1.28	4 (10%)
3	NSC	B	9003	-	31,31,31	1.46	6 (19%)	39,45,45	1.28	4 (10%)

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	NSC	A	9002	-	6/6/1/3	0/8/8/8	0/4/4/4
3	NSC	B	9003	-	6/6/1/3	0/8/8/8	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	9003	NSC	C16-N15	-3.08	1.35	1.41
3	A	9002	NSC	C11-N13	-3.07	1.35	1.41
3	A	9002	NSC	C16-N15	-3.05	1.35	1.41
3	B	9003	NSC	C11-N13	-2.93	1.36	1.41
3	A	9002	NSC	C26-C27	2.15	1.41	1.36
3	A	9002	NSC	C9-C10	2.29	1.41	1.36
3	B	9003	NSC	C26-C27	2.30	1.41	1.36
3	A	9002	NSC	C12-C11	2.31	1.42	1.37
3	B	9003	NSC	C12-C11	2.33	1.42	1.37
3	B	9003	NSC	C9-C10	2.35	1.41	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	9003	NSC	C17-C16	2.42	1.42	1.37
3	A	9002	NSC	C17-C16	2.44	1.42	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	9002	NSC	C23-C21-N22	-3.04	120.07	122.69
3	A	9002	NSC	C7-C6-N5	-2.99	120.11	122.69
3	B	9003	NSC	C3-C4-N5	-2.90	120.07	122.90
3	B	9003	NSC	C23-C21-N22	-2.87	120.22	122.69
3	A	9002	NSC	C3-C4-N5	-2.86	120.10	122.90
3	B	9003	NSC	C7-C6-N5	-2.82	120.26	122.69
3	B	9003	NSC	C18-C19-N22	-2.81	120.16	122.90
3	A	9002	NSC	C18-C19-N22	-2.70	120.27	122.90

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	9003	NSC	C6
3	B	9003	NSC	C24
3	B	9003	NSC	C18
3	B	9003	NSC	C19
3	B	9003	NSC	C16
3	B	9003	NSC	C21
3	A	9002	NSC	C6
3	A	9002	NSC	C24
3	A	9002	NSC	C18
3	A	9002	NSC	C19
3	A	9002	NSC	C16
3	A	9002	NSC	C21

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	9002	NSC	8	0
3	B	9003	NSC	7	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

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, 95^{th} 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	732/776 (94%)	0.16	51 (6%) 19 13	8, 39, 94, 125	0
1	B	743/776 (95%)	0.18	56 (7%) 17 11	9, 37, 91, 101	0
All	All	1475/1552 (95%)	0.17	107 (7%) 18 12	8, 39, 92, 125	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	319	LEU	6.2
1	B	352	GLU	6.2
1	B	349	LEU	5.7
1	B	358	ASN	5.6
1	B	37	LYS	5.4
1	A	365	SER	5.1
1	B	364	SER	4.9
1	B	114	LEU	4.9
1	B	353	GLU	4.9
1	B	356	LEU	4.8
1	B	363	ASP	4.8
1	B	48	VAL	4.6
1	A	320	LYS	4.5
1	A	308	ILE	4.4
1	A	33	GLU	4.4
1	A	54	VAL	4.3
1	B	97	LEU	4.3
1	B	54	VAL	4.3
1	B	115	HIS	4.2
1	A	367	PRO	4.2
1	A	703	ASN	4.1
1	B	366	ASN	4.1
1	B	359	ARG	4.1
1	A	324	ILE	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	34	GLU	4.0
1	B	348	SER	3.9
1	A	318	LEU	3.8
1	A	321	ARG	3.8
1	A	309	HIS	3.8
1	A	310	SER	3.7
1	B	355	GLU	3.6
1	B	367	PRO	3.6
1	B	49	LYS	3.6
1	A	346	ARG	3.6
1	A	341	LEU	3.5
1	A	322	ILE	3.4
1	A	347	ASP	3.4
1	A	317	GLU	3.4
1	B	51	GLU	3.4
1	B	52	GLU	3.4
1	A	330	LEU	3.4
1	B	354	LYS	3.3
1	A	316	LYS	3.3
1	A	368	LEU	3.2
1	A	34	GLU	3.2
1	A	32	GLN	3.2
1	B	35	HIS	3.2
1	A	344	ASP	3.1
1	A	48	VAL	3.1
1	B	365	SER	3.1
1	B	59	ALA	3.0
1	B	33	GLU	3.0
1	B	44	VAL	3.0
1	B	324	ILE	3.0
1	A	53	ALA	3.0
1	B	135	GLU	3.0
1	A	348	SER	2.9
1	B	345	ILE	2.9
1	A	311	LEU	2.9
1	B	84	VAL	2.8
1	A	31	THR	2.8
1	A	36	LEU	2.8
1	B	703	ASN	2.8
1	A	579	TYR	2.8
1	B	56	LYS	2.8
1	A	312	SER	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	49	LYS	2.7
1	A	345	ILE	2.7
1	B	357	LEU	2.6
1	B	329	PHE	2.6
1	A	704	GLN	2.6
1	A	306	ASP	2.6
1	B	321	ARG	2.5
1	A	305	ASP	2.5
1	B	351	GLU	2.5
1	B	94	LEU	2.5
1	B	31	THR	2.5
1	B	91	HIS	2.5
1	A	303	LYS	2.5
1	B	32	GLN	2.5
1	A	100	ASP	2.5
1	B	50	GLY	2.4
1	B	133	SER	2.4
1	B	83	ILE	2.4
1	A	329	PHE	2.4
1	B	350	SER	2.4
1	A	307	ILE	2.4
1	B	368	LEU	2.3
1	B	53	ALA	2.3
1	B	60	GLU	2.3
1	A	372	GLU	2.3
1	A	30	LYS	2.3
1	A	90	LYS	2.3
1	B	702	LYS	2.3
1	A	52	GLU	2.2
1	A	349	LEU	2.2
1	B	92	ILE	2.2
1	A	55	LYS	2.2
1	A	327	SER	2.2
1	B	134	SER	2.1
1	B	46	ILE	2.1
1	B	346	ARG	2.1
1	B	136	ASP	2.1
1	A	314	GLU	2.1
1	A	337	PHE	2.0
1	B	182	ASP	2.0
1	A	315	GLU	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, 95^{th} 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	NSC	B	9003	28/28	0.70	0.51	7.85	76,80,88,88	0
3	NSC	A	9002	28/28	0.78	0.40	3.00	75,80,87,87	0
2	ZN	A	9001	1/1	1.00	0.20	1.81	37,37,37,37	0
2	ZN	B	9002	1/1	1.00	0.14	-1.31	27,27,27,27	0

6.5 Other polymers (i)

There are no such residues in this entry.