

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	4RV1
Title	:	Crystal Structure of Engineered Protein. Northeast Structural Genomics Con-
		sortium (NESG) Target OR497.
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		T.B.; Baker, D.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural
		Genomics Consortium (NESG)
Deposited on	:	2014-11-24
Resolution	:	2.57 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity Mogul	:	4.02b-467 1.8.5 (274361) CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\;DIFFRACTION$

The reported resolution of this entry is 2.57 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.



Motria	Whole archive	Similar resolution		
	$(\# {\rm Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$		
R _{free}	130704	3676 (2.60-2.56)		
Clashscore	141614	4049 (2.60-2.56)		
Ramachandran outliers	138981	3979 (2.60-2.56)		
Sidechain outliers	138945	3979 (2.60-2.56)		
RSRZ outliers	127900	3614 (2.60-2.56)		

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	А	420	73%	25%	.		
1	В	420	71%	26%	••		
1	С	420	% 77%	21%	.		
1	D	420	73%	25%	••		



Mol	Chain	Length	Quality of chain				
			14%				
1	E	420		53%	43%	• •	
			15%				
1	F	420		52%	44%	• •	



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 18115 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.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	А	413	Total C N O S 2931 1815 496 619 1	0	0	0
1	В	414	Total C N O 2950 1826 500 624	0	0	0
1	С	412	Total C N O 2925 1811 496 618	0	0	0
1	D	415	Total C N O S 2954 1828 500 625 1	0	0	0
1	Е	412	Total C N O S 2931 1814 496 620 1	0	0	0
1	F	411	Total C N O S 2917 1803 494 619 1	0	0	0

• Molecule 1 is a protein called Engineered Protein OR497.

• Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
2	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	104	Total O 104 104	0	0
3	В	104	Total O 104 104	0	0
3	С	110	Total O 110 110	0	0
3	D	93	Total O 93 93	0	0
3	Е	35	$\begin{array}{cc} \text{Total} & \text{O} \\ 35 & 35 \end{array}$	0	0
3	F	53	$\begin{array}{cc} \text{Total} & \text{O} \\ 53 & 53 \end{array}$	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Engineered Protein OR497



P327 V17 6 MI A330 L179 M3 K332 E185 M3 V34 L179 M3 V340 R192 M3 V344 A193 L179 V344 A193 K192 V366 V214 D26 A361 V214 L26 V374 K230 K34 V366 L221 W1 V375 L236 E83 L376 L236 L36 V386 L263 E106 K394 K230 L36 L407 K261 V102 E396 C265 P117 L407 K230 L36 K394 K230 L36 K395 K261 L36 K39<

• Molecule 1: Engineered Protein OR497



• Molecule 1: Engineered Protein OR497





W412 LEU GLU HIS HIS HIS HIS HIS

• Molecule 1: Engineered Protein OR497





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants	99.27Å 99.27Å 432.18Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	48.02 - 2.57	Depositor
Resolution (A)	$49.63 \ - \ 2.57$	EDS
% Data completeness	97.5 (48.02-2.57)	Depositor
(in resolution range)	97.9(49.63-2.57)	EDS
R _{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.64 (at 2.58 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
P.P.	0.201 , 0.237	Depositor
n, n_{free}	0.208 , 0.241	DCC
R_{free} test set	3930 reflections $(5.02%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	56.2	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.30 , 59.4	EDS
L-test for twinning ²	$< L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18115	wwPDB-VP
Average B, all atoms $(Å^2)$	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 9.68% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: ACT

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		
	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.35	0/2941	0.57	0/3993	
1	В	0.36	0/2961	0.59	0/4019	
1	С	0.38	0/2935	0.57	1/3984~(0.0%)	
1	D	0.36	0/2965	0.56	0/4025	
1	Е	0.30	0/2941	0.54	0/3991	
1	F	0.29	0/2925	0.53	0/3968	
All	All	0.34	0/17668	0.56	1/23980~(0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	С	393	ASP	N-CA-C	-5.09	97.27	111.00

There are no chirality outliers.

There are no planarity outliers.

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	А	2931	0	3050	78	0
1	В	2950	0	3066	96	0
1	С	2925	0	3045	64	0
1	D	2954	0	3067	93	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Е	2931	0	3054	178	0
1	F	2917	0	3044	195	0
2	А	4	0	3	1	0
2	С	4	0	3	0	0
3	А	104	0	0	12	0
3	В	104	0	0	11	0
3	С	110	0	0	4	0
3	D	93	0	0	6	0
3	Е	35	0	0	1	0
3	F	53	0	0	16	0
All	All	18115	0	18332	681	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 (681) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:24:ARG:HG2	1:F:63:GLU:HG2	1.38	1.03
1:F:26:LEU:HD23	1:F:29:ILE:HD12	1.48	0.94
1:F:100:SER:HA	1:F:103:GLN:HE21	1.32	0.92
1:F:351:ASP:HB3	1:F:354:VAL:HG12	1.52	0.90
1:B:57:ASP:HB2	1:B:60:VAL:HG12	1.54	0.89
1:D:104:LYS:HD2	1:D:143:GLU:HG2	1.54	0.89
1:F:17:GLU:HA	1:F:20:LYS:HD2	1.55	0.87
1:B:382:VAL:O	1:B:386:GLN:HG2	1.75	0.85
1:E:214:VAL:O	1:E:218:VAL:HG23	1.77	0.85
1:E:53:LEU:HB3	1:E:94:LEU:HD11	1.57	0.84
1:E:408:LYS:HD3	1:E:409:SER:N	1.92	0.84
1:F:290:LYS:HG2	1:F:294:ASP:OD2	1.79	0.83
1:F:110:LEU:HA	1:F:113:ILE:HD12	1.61	0.82
1:C:393:ASP:O	1:C:396:VAL:HG12	1.80	0.81
1:F:367:SER:HB3	1:F:406:ASN:ND2	1.93	0.81
1:B:393:ASP:OD2	1:B:395:GLU:HG2	1.81	0.80
1:A:328:ASP:OD2	1:A:369:PRO:HD3	1.81	0.80
1:E:37:ILE:HD11	1:E:71:ILE:HA	1.63	0.80
1:C:340:VAL:O	1:C:344:VAL:HG23	1.81	0.79
1:F:68:LEU:HB2	3:F:547:HOH:O	1.81	0.79
1:B:15:ASP:HB2	1:B:18:THR:HG22	1.63	0.79
1:D:69:ALA:HB3	1:D:108:ARG:HH21	1.48	0.78
1:E:88:VAL:O	1:E:92:VAL:HG23	1.83	0.78



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:328:ASP:OD2	1:D:369:PRO:HD3	1.84	0.77
1:A:46:VAL:O	1:A:50:VAL:HG23	1.85	0.77
1:F:340:VAL:O	1:F:344:VAL:HG23	1.84	0.77
1:D:367:SER:HB2	1:D:414:GLU:HG3	1.68	0.76
1:F:88:VAL:O	1:F:92:VAL:HG23	1.85	0.76
1:C:214:VAL:O	1:C:218:VAL:HG23	1.86	0.76
1:F:290:LYS:HA	1:F:293:VAL:HG22	1.68	0.76
1:F:130:VAL:O	1:F:134:VAL:HG23	1.86	0.76
1:D:104:LYS:HB3	1:D:144:VAL:HG12	1.66	0.76
1:F:360:ARG:HA	1:F:399:GLU:OE1	1.87	0.75
1:A:276:ARG:HG3	1:A:315:GLU:OE2	1.86	0.75
1:B:2:ASN:HB3	1:B:5:GLU:CD	2.06	0.75
1:B:11:LEU:HB3	1:B:52:LEU:HD11	1.67	0.74
1:F:141:ASP:O	1:F:144:VAL:HG12	1.86	0.74
1:E:341:GLU:HG3	3:E:525:HOH:O	1.86	0.74
1:D:1:MET:HB3	1:D:6:LYS:HE3	1.69	0.74
1:A:244:ASP:OD2	1:A:285:PRO:HD3	1.88	0.74
1:D:20:LYS:HG2	1:D:60:VAL:HG22	1.69	0.74
1:F:272:LYS:HD2	1:F:311:GLU:HB3	1.68	0.73
1:F:141:ASP:HB2	1:F:144:VAL:CG1	2.18	0.73
1:E:87:GLY:O	1:E:91:LEU:HB2	1.90	0.72
1:E:355:GLN:HE21	1:E:396:VAL:HG11	1.53	0.72
1:F:109:ALA:O	1:F:113:ILE:HG13	1.89	0.72
1:F:58:SER:HA	1:F:61:GLN:OE1	1.89	0.72
1:E:34:ALA:HA	1:E:37:ILE:HG22	1.71	0.72
1:E:141:ASP:HB3	1:E:144:VAL:HG12	1.71	0.72
1:F:101:GLU:HA	1:F:104:LYS:NZ	2.05	0.71
1:B:374:LYS:HG2	1:B:378:ASP:OD2	1.89	0.71
1:D:172:VAL:O	1:D:176:VAL:HG23	1.90	0.71
1:D:17:GLU:OE2	1:D:21:GLU:HG3	1.91	0.70
1:F:152:LEU:HA	3:F:548:HOH:O	1.92	0.70
1:A:269:GLU:HG2	1:D:227:GLU:HG3	1.73	0.70
1:F:7:LEU:O	1:F:11:LEU:HD23	1.91	0.70
1:E:225:ASP:OD2	1:E:228:VAL:HG23	1.91	0.69
1:F:177:LYS:O	1:F:180:THR:HG22	1.92	0.69
1:D:21:GLU:HA	1:D:24:ARG:HD2	1.74	0.69
1:E:24:ARG:HH12	1:F:394:SER:HB2	1.56	0.69
1:F:177:LYS:HB3	3:F:508:HOH:O	1.91	0.69
1:D:109:ALA:O	1:D:113:ILE:HG13	1.93	0.69
1:D:356:LYS:HD3	1:D:395:GLU:HB3	1.74	0.69
1:E:19:GLN:HG2	1:E:52:LEU:HD21	1.74	0.69



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:37:ILE:HG23	1:A:71:ILE:HG23	1.74	0.69
1:E:24:ARG:HH22	1:F:394:SER:HB2	1.58	0.69
1:E:57:ASP:HB3	1:E:60:VAL:HG23	1.74	0.69
1:E:405:GLU:O	1:E:408:LYS:HB3	1.93	0.69
1:B:387:LYS:HE2	3:D:580:HOH:O	1.93	0.69
1:E:130:VAL:O	1:E:134:VAL:HG23	1.92	0.69
1:C:298:VAL:O	1:C:302:VAL:HG23	1.93	0.68
1:E:355:GLN:NE2	1:E:396:VAL:HG11	2.08	0.68
1:F:205:ILE:O	1:F:209:VAL:HG23	1.94	0.68
1:F:121:ILE:HG23	1:F:155:ILE:HG23	1.76	0.68
1:D:104:LYS:HD2	1:D:143:GLU:CG	2.24	0.68
1:D:395:GLU:HA	1:D:395:GLU:OE1	1.92	0.68
1:F:318:ARG:HA	1:F:357:GLU:OE1	1.94	0.68
1:E:104:LYS:HE3	1:E:105:GLU:HG3	1.77	0.67
1:F:393:ASP:O	1:F:396:VAL:HG12	1.93	0.67
1:C:314:LYS:HG3	1:C:353:GLU:HB3	1.75	0.67
1:D:412:TRP:HA	1:E:245:GLU:OE1	1.93	0.67
1:F:79:ILE:HD13	1:F:113:ILE:HA	1.77	0.67
1:E:314:LYS:HD3	1:E:353:GLU:CB	2.24	0.67
1:E:361:ALA:O	1:E:365:ILE:HG13	1.93	0.67
3:B:570:HOH:O	1:C:75:PRO:HB2	1.94	0.66
1:F:57:ASP:HB3	1:F:60:VAL:HG23	1.76	0.66
1:F:155:ILE:HB	3:F:548:HOH:O	1.94	0.66
1:A:382:VAL:O	1:A:386:GLN:HG3	1.94	0.66
1:E:104:LYS:HD2	1:E:143:GLU:HG3	1.76	0.66
1:E:389:LEU:HD21	1:E:404:LEU:HD12	1.78	0.66
1:A:164:LYS:HG2	1:A:168:ASP:OD2	1.94	0.66
1:E:15:ASP:HB3	1:E:18:THR:HB	1.78	0.66
1:B:57:ASP:HB2	1:B:60:VAL:CG1	2.25	0.66
1:F:2:ASN:OD1	1:F:5:GLU:HG3	1.95	0.66
1:F:100:SER:HA	1:F:103:GLN:HG2	1.78	0.66
1:F:276:ARG:HA	1:F:315:GLU:HG2	1.78	0.65
1:F:135:LYS:O	1:F:138:THR:HG22	1.96	0.65
1:E:132:VAL:O	1:E:136:LEU:HD23	1.97	0.65
1:E:188:LYS:HZ2	1:F:268:SER:HB3	1.62	0.65
1:F:167:VAL:HG22	1:F:172:VAL:HG21	1.79	0.65
1:A:299:GLU:HG2	1:C:138:THR:O	1.97	0.65
1:B:51:LYS:O	1:B:54:THR:HG22	1.97	0.65
1:D:163:ILE:HG23	1:D:197:ILE:HG23	1.78	0.65
1:B:10:LEU:HD23	1:B:22:ALA:HB2	1.79	0.65
1:C:313:GLN:OE1	1:C:354:VAL:HG21	1.97	0.65



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:95:LEU:HD11	1:D:110:LEU:HD12	1.79	0.65
1:E:46:VAL:HG11	1:E:81:ALA:HB1	1.79	0.64
1:E:79:ILE:O	1:E:83:VAL:HG23	1.97	0.64
1:B:414:GLU:O	1:B:415:HIS:ND1	2.31	0.64
1:E:240:ALA:O	1:E:280:ASN:HB3	1.97	0.64
1:F:100:SER:HA	1:F:103:GLN:NE2	2.09	0.64
1:B:2:ASN:ND2	1:B:5:GLU:H	1.95	0.64
1:C:172:VAL:O	1:C:176:VAL:HG23	1.98	0.64
1:D:27:ALA:HB3	1:D:66:ARG:HH21	1.64	0.63
1:F:121:ILE:CG2	1:F:155:ILE:HG23	2.28	0.63
1:F:214:VAL:O	1:F:218:VAL:HG23	1.98	0.63
1:A:280:ASN:OD1	1:A:318:ARG:NH2	2.32	0.63
1:D:11:LEU:HD12	1:D:22:ALA:HB1	1.80	0.63
1:A:20:LYS:HD3	1:A:59:GLU:OE2	1.99	0.63
1:B:328:ASP:OD1	1:B:369:PRO:HD3	1.97	0.63
1:E:185:GLU:HG3	1:F:311:GLU:OE2	1.99	0.63
1:E:366:ALA:HB1	1:E:406:ASN:HB2	1.79	0.63
1:F:204:ALA:O	1:F:208:ILE:HG13	1.98	0.63
1:A:206:LYS:NZ	3:A:712:HOH:O	2.32	0.62
1:C:395:GLU:O	1:C:399:GLU:HB2	1.99	0.62
1:F:170:GLY:O	1:F:174:VAL:HG23	1.99	0.62
1:A:224:THR:HG22	3:A:717:HOH:O	1.99	0.62
1:D:76:ASP:OD1	1:D:117:PRO:HD3	2.00	0.62
1:E:121:ILE:O	1:E:125:VAL:HG23	2.00	0.62
1:D:285:PRO:HG2	1:D:287:GLU:HG2	1.82	0.62
1:E:19:GLN:CD	1:E:52:LEU:HD11	2.20	0.62
1:E:141:ASP:O	1:E:144:VAL:HG12	1.99	0.62
1:F:20:LYS:HB3	1:F:24:ARG:NH1	2.15	0.62
1:F:50:VAL:HG21	1:F:85:ALA:HB1	1.81	0.62
1:E:245:GLU:CD	1:E:245:GLU:H	2.02	0.61
1:E:185:GLU:OE1	1:F:311:GLU:HG3	2.00	0.61
1:D:104:LYS:CB	1:D:144:VAL:HG12	2.30	0.61
1:E:24:ARG:NH1	1:F:394:SER:HB2	2.14	0.61
1:B:57:ASP:C	1:B:59:GLU:H	2.02	0.61
1:D:38:LYS:HE3	1:D:75:PRO:HG3	1.83	0.61
1:F:167:VAL:HG22	1:F:172:VAL:CG2	2.31	0.61
1:F:384:VAL:HG23	1:F:387:LYS:HZ3	1.66	0.61
1:F:389:LEU:HD11	1:F:404:LEU:HD12	1.83	0.61
1:A:24:ARG:HG3	1:A:63:GLU:HG2	1.82	0.61
1:E:46:VAL:O	1:E:50:VAL:HG23	2.01	0.61
1:A:14:THR:HG23	3:A:787:HOH:O	1.99	0.60



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:47:GLU:H	1:A:47:GLU:CD	2.05	0.60
1:E:80:LYS:HG2	1:E:84:ASP:OD2	2.00	0.60
1:E:109:ALA:O	1:E:113:ILE:HG13	2.01	0.60
1:C:2:ASN:ND2	1:C:5:GLU:HG3	2.15	0.60
1:A:401:GLN:O	1:A:405:GLU:HG3	2.00	0.60
1:E:314:LYS:HD3	1:E:353:GLU:HB3	1.84	0.60
1:D:23:ALA:HA	1:D:26:LEU:HD12	1.82	0.60
1:E:133:LEU:HA	1:E:136:LEU:HD21	1.82	0.60
1:D:17:GLU:OE1	1:D:20:LYS:HD2	2.01	0.60
1:F:393:ASP:HB3	1:F:396:VAL:HG12	1.84	0.60
1:B:15:ASP:HB2	1:B:18:THR:CG2	2.32	0.60
1:E:227:GLU:HG2	1:F:269:GLU:HG2	1.84	0.60
1:A:373:ILE:O	1:A:377:VAL:HG23	2.02	0.60
1:B:99:ASP:OD2	1:B:102:VAL:HG23	2.02	0.60
1:F:172:VAL:O	1:F:176:VAL:HG23	2.01	0.60
1:B:2:ASN:HD21	1:B:4:VAL:HB	1.67	0.59
1:E:24:ARG:NH2	1:F:394:SER:HB2	2.16	0.59
1:E:188:LYS:HE3	1:F:268:SER:OG	2.02	0.59
1:B:108:ARG:HG3	1:B:147:GLU:OE2	2.01	0.59
1:F:298:VAL:O	1:F:302:VAL:HG23	2.02	0.59
1:D:79:ILE:HG23	1:D:113:ILE:HG23	1.84	0.59
1:F:374:LYS:HE3	3:F:509:HOH:O	2.02	0.59
1:B:413:LEU:HD12	1:B:413:LEU:N	2.17	0.59
1:F:282:ALA:O	1:F:322:ASN:HB3	2.02	0.59
1:B:2:ASN:HD22	1:B:5:GLU:HG2	1.68	0.59
1:B:60:VAL:HG13	1:B:61:GLN:N	2.18	0.59
1:E:172:VAL:O	1:E:176:VAL:HG23	2.03	0.59
1:F:120:ALA:O	1:F:124:ILE:HG13	2.02	0.59
1:F:141:ASP:HB2	1:F:144:VAL:HG12	1.84	0.58
1:F:221:LEU:HD11	1:F:236:LEU:CD1	2.32	0.58
1:B:8:VAL:HG13	1:B:45:GLY:HA2	1.84	0.58
1:F:68:LEU:HA	1:F:71:ILE:HD12	1.85	0.58
1:B:247:ILE:O	1:B:251:VAL:HG23	2.03	0.58
1:E:188:LYS:NZ	1:F:268:SER:HB3	2.18	0.58
1:F:321:ALA:HB3	1:F:360:ARG:NH2	2.18	0.58
1:D:10:LEU:HB3	1:D:22:ALA:HB2	1.85	0.58
1:D:95:LEU:HD11	1:D:110:LEU:CD1	2.33	0.58
1:F:327:PRO:HB2	1:F:329:GLU:OE2	2.04	0.58
1:C:255:GLY:O	1:C:259:LEU:HG	2.04	0.58
1:C:340:VAL:HG11	1:C:376:ILE:HA	1.86	0.58
1:C:361:ALA:O	1:C:365:ILE:HG13	2.03	0.58



		Interatomic	Clash	
Atom-1	Atom-2	distance $(Å)$	overlap (Å)	
1:D:230:LYS:HG2	3:D:546:HOH:O	2.03	0.58	
1:F:114:ALA:O	1:F:154:ASN:HB3	2.03	0.58	
1:F:362:LEU:HD23	1:F:365:ILE:HD12	1.84	0.58	
1:D:6:LYS:O	1:D:10:LEU:HD13	2.03	0.58	
1:D:114:ALA:O	1:D:154:ASN:HB3	2.03	0.58	
1:B:29:ILE:HG22	1:B:36:ALA:HB1	1.86	0.58	
1:F:78:ALA:O	1:F:82:ILE:HG13	2.04	0.58	
1:B:37:ILE:O	1:B:41:VAL:HG23	2.04	0.57	
1:A:184:SER:O	1:A:188:LYS:HG3	2.04	0.57	
1:E:408:LYS:HD3	1:E:409:SER:H	1.66	0.57	
1:F:306:THR:HA	1:F:313:GLN:HE21	1.70	0.57	
1:E:86:GLY:O	1:E:90:VAL:HG12	2.05	0.57	
1:C:108:ARG:HD3	1:C:147:GLU:OE2	2.04	0.57	
1:D:21:GLU:HA	1:D:24:ARG:HB2	1.85	0.57	
1:E:335:VAL:HG22	1:E:340:VAL:HG21	1.86	0.57	
1:E:401:GLN:O	1:E:405:GLU:HG2	2.04	0.57	
1:F:19:GLN:HG2	3:F:546:HOH:O	2.05	0.57	
1:B:341:GLU:OE2	1:B:345:LYS:HE3	2.04	0.57	
1:B:356:LYS:CE	1:B:395:GLU:HB2	2.34	0.57	
1:F:386:GLN:HA	1:F:389:LEU:HD13	1.87	0.57	
1:A:99:ASP:HB3	1:A:102:VAL:HG23	1.85	0.57	
1:F:377:VAL:HG12	1:F:382:VAL:CG2	2.35	0.57	
1:A:88:VAL:O	1:A:92:VAL:HG23	2.05	0.57	
1:C:137:LEU:HD11	1:C:152:LEU:HD12	1.85	0.57	
1:E:335:VAL:HA	1:E:340:VAL:HG23	1.87	0.57	
1:F:369:PRO:O	1:F:373:ILE:HG13	2.04	0.56	
1:A:238:ASN:OD1	1:A:276:ARG:NH2	2.35	0.56	
1:C:37:ILE:O	1:C:41:VAL:HG23	2.06	0.56	
1:B:383:GLU:O	1:B:386:GLN:HB2	2.05	0.56	
1:F:67:ALA:O	1:F:71:ILE:HG13	2.06	0.56	
1:C:263:LEU:HD11	1:C:278:LEU:HD12	1.86	0.56	
1:E:104:LYS:CD	1:E:143:GLU:HG3	2.36	0.56	
1:B:413:LEU:HD21	3:B:586:HOH:O	2.05	0.56	
1:E:24:ARG:HH22	1:F:394:SER:CB	2.19	0.56	
1:E:197:ILE:HG22	1:E:204:ALA:HB1	1.88	0.56	
1:A:344:VAL:HG13	1:A:384:VAL:HG11	1.87	0.56	
1:B:52:LEU:HB3	3:B:593:HOH:O	2.06	0.56	
1:F:57:ASP:HB3	1:F:60:VAL:CG2	2.35	0.56	
1:F:104:LYS:HD2	1:F:143:GLU:CG	2.35	0.56	
1:B:2:ASN:ND2	1:B:5:GLU:HG2	2.21	0.55	
1:D:403:ALA:O	1:D:407:ILE:HG13	2.06	0.55	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:227:GLU:OE1	1:F:227:GLU:N	2.39	0.55
1:F:227:GLU:HB3	3:F:542:HOH:O	2.05	0.55
1:D:20:LYS:CG	1:D:60:VAL:HG22	2.37	0.55
1:E:221:LEU:HD11	1:E:236:LEU:CD1	2.37	0.55
1:F:5:GLU:O	1:F:8:VAL:HB	2.06	0.55
1:F:384:VAL:HG23	1:F:387:LYS:NZ	2.21	0.55
1:C:397:GLN:NE2	3:C:759:HOH:O	2.39	0.55
1:E:152:LEU:HD23	1:E:155:ILE:HD12	1.89	0.55
1:A:332:LYS:HE3	1:C:173:GLU:OE2	2.07	0.55
1:E:57:ASP:HB3	1:E:60:VAL:CG2	2.37	0.55
1:E:318:ARG:HB2	1:E:357:GLU:OE2	2.06	0.55
1:A:405:GLU:HG2	3:A:800:HOH:O	2.07	0.54
1:E:256:VAL:O	1:E:260:VAL:HG23	2.07	0.54
1:F:177:LYS:N	3:F:508:HOH:O	2.41	0.54
1:C:137:LEU:HD11	1:C:152:LEU:CD1	2.36	0.54
1:E:108:ARG:HB2	1:E:147:GLU:HG2	1.89	0.54
1:E:286:ASP:OD1	1:E:327:PRO:HD3	2.07	0.54
1:A:298:VAL:O	1:A:302:VAL:HG23	2.08	0.54
1:B:41:VAL:HG12	1:B:41:VAL:O	2.07	0.54
1:E:304:LEU:HD22	1:E:312:VAL:CG1	2.37	0.54
1:E:406:ASN:N	1:E:406:ASN:HD22	2.05	0.54
1:C:2:ASN:CG	1:C:5:GLU:HG3	2.27	0.54
1:E:301:LEU:O	1:E:305:LEU:HG	2.07	0.54
1:F:15:ASP:OD1	1:F:18:THR:N	2.40	0.54
1:F:377:VAL:HG12	1:F:382:VAL:HG23	1.88	0.54
3:B:563:HOH:O	1:C:142:SER:HB2	2.08	0.54
1:E:298:VAL:O	1:E:302:VAL:HG23	2.08	0.54
1:F:104:LYS:NZ	1:F:104:LYS:HB3	2.23	0.54
1:A:384:VAL:HA	1:A:387:LYS:HE3	1.90	0.54
1:D:69:ALA:HB1	1:D:108:ARG:HE	1.73	0.54
1:D:405:GLU:O	1:D:409:SER:HB3	2.07	0.54
1:E:319:ALA:O	1:E:323:ILE:HG13	2.08	0.54
1:D:104:LYS:HG3	1:D:105:GLU:N	2.23	0.54
1:E:12:THR:HG22	1:E:48:VAL:HG21	1.89	0.54
1:F:20:LYS:HB3	1:F:24:ARG:HH12	1.73	0.54
1:A:67:ALA:O	1:A:71:ILE:HG13	2.07	0.53
1:B:94:LEU:HD22	1:B:102:VAL:HG11	1.90	0.53
1:B:196:ASN:OD1	1:B:234:ARG:NH2	2.37	0.53
1:E:374:LYS:HA	1:E:377:VAL:HG22	1.89	0.53
1:F:100:SER:CA	1:F:103:GLN:HE21	2.15	0.53
1:E:151:ALA:O	1:E:155:ILE:HG13	2.08	0.53



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:370:THR:HA	1:F:373:ILE:HD12	1.90	0.53
1:F:83:VAL:HG13	1:F:88:VAL:HG11	1.90	0.53
1:B:20:LYS:NZ	1:B:59:GLU:HB2	2.22	0.53
1:E:79:ILE:CG2	1:E:113:ILE:HG23	2.39	0.53
1:F:8:VAL:O	1:F:11:LEU:HB2	2.09	0.53
1:F:374:LYS:CE	3:F:509:HOH:O	2.56	0.53
1:E:37:ILE:HD11	1:E:71:ILE:CA	2.37	0.53
1:B:356:LYS:HE3	1:B:395:GLU:HB2	1.90	0.53
1:C:272:LYS:CD	1:C:311:GLU:HB3	2.38	0.53
1:C:263:LEU:HB3	1:C:304:LEU:HD11	1.91	0.53
1:B:146:LYS:HG2	3:B:587:HOH:O	2.08	0.53
1:D:11:LEU:O	1:D:19:GLN:HG2	2.09	0.53
1:E:91:LEU:HD21	1:E:109:ALA:CB	2.38	0.53
1:E:164:LYS:O	1:E:167:VAL:HG12	2.09	0.53
1:D:90:VAL:O	1:D:93:LYS:HB3	2.09	0.52
1:E:7:LEU:HD22	1:E:26:LEU:HG	1.91	0.52
1:F:179:LEU:HD11	1:F:194:LEU:CD1	2.40	0.52
1:C:3:ASP:O	1:C:7:LEU:HG	2.08	0.52
1:D:24:ARG:HG3	1:D:24:ARG:HH11	1.75	0.52
1:D:341:GLU:OE1	1:D:379:ALA:HB2	2.10	0.52
1:F:299:GLU:HB2	3:F:520:HOH:O	2.09	0.52
1:F:328:ASP:OD2	1:F:369:PRO:HD3	2.09	0.52
1:A:384:VAL:O	1:A:387:LYS:HG2	2.09	0.52
1:C:192:ARG:HA	1:C:231:GLU:OE1	2.09	0.52
1:B:256:VAL:O	1:B:260:VAL:HG23	2.09	0.52
1:C:163:ILE:O	1:C:167:VAL:HG23	2.10	0.52
1:D:49:LEU:HD21	1:D:67:ALA:CB	2.40	0.52
1:E:38:LYS:HG3	1:E:42:ASP:OD2	2.10	0.52
1:E:380:GLY:O	1:E:384:VAL:HG23	2.10	0.52
1:F:118:ASP:HB3	1:F:159:PRO:HD3	1.91	0.52
1:D:163:ILE:CG2	1:D:197:ILE:HG23	2.38	0.52
1:F:37:ILE:CG2	1:F:71:ILE:HG23	2.40	0.52
1:C:53:LEU:HD11	1:C:68:LEU:CD1	2.40	0.52
1:D:8:VAL:HG21	1:D:43:ALA:HB1	1.92	0.52
1:E:355:GLN:HE21	1:E:396:VAL:HG21	1.74	0.52
1:F:49:LEU:HD11	1:F:67:ALA:HB1	1.91	0.52
1:A:122:LYS:HG2	1:A:126:ASP:OD2	2.10	0.52
1:C:221:LEU:HD11	1:C:236:LEU:HD12	1.92	0.52
1:C:374:LYS:HG2	1:C:378:ASP:OD2	2.10	0.51
1:B:329:GLU:CD	1:B:329:GLU:H	2.14	0.51
1:D:11:LEU:HD12	1:D:22:ALA:CB	2.40	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:122:LYS:HD3	3:F:535:HOH:O	2.09	0.51
1:A:25:ASP:O	1:A:29:ILE:HG13	2.10	0.51
1:E:136:LEU:HD23	1:E:136:LEU:H	1.75	0.51
1:C:314:LYS:HD3	1:C:353:GLU:CD	2.31	0.51
1:E:340:VAL:O	1:E:344:VAL:HG13	2.10	0.51
1:E:24:ARG:HG3	1:E:63:GLU:HG2	1.93	0.51
1:E:314:LYS:HD3	1:E:353:GLU:HB2	1.93	0.51
1:F:363:ALA:HB3	1:F:402:ARG:NH2	2.25	0.51
1:B:66:ARG:HG3	1:B:105:GLU:OE2	2.11	0.51
1:E:37:ILE:O	1:E:41:VAL:HG23	2.10	0.51
1:E:121:ILE:HG23	1:E:155:ILE:HG23	1.92	0.51
1:F:45:GLY:O	1:F:49:LEU:HB2	2.11	0.51
1:B:205:ILE:O	1:B:209:VAL:HG23	2.11	0.51
1:B:59:GLU:HA	1:B:62:LYS:HE3	1.92	0.51
1:D:231:GLU:OE1	1:D:231:GLU:HA	2.11	0.51
1:F:152:LEU:HD23	3:F:548:HOH:O	2.11	0.51
1:E:185:GLU:N	1:E:185:GLU:OE2	2.42	0.50
1:E:121:ILE:CG2	1:E:155:ILE:HG23	2.41	0.50
1:F:4:VAL:HG11	1:F:40:ILE:HD13	1.93	0.50
1:A:340:VAL:O	1:A:344:VAL:HG23	2.11	0.50
1:E:11:LEU:O	1:E:19:GLN:HG3	2.10	0.50
1:F:386:GLN:O	1:F:389:LEU:HD13	2.11	0.50
1:F:306:THR:HA	1:F:313:GLN:NE2	2.26	0.50
1:B:60:VAL:CG1	1:B:61:GLN:N	2.75	0.50
1:D:374:LYS:HG2	1:D:378:ASP:OD2	2.11	0.50
1:E:20:LYS:O	1:E:24:ARG:HG3	2.11	0.50
1:F:4:VAL:CG1	1:F:40:ILE:HD13	2.41	0.50
1:E:194:LEU:HA	1:E:197:ILE:HD12	1.94	0.50
1:F:131:GLU:H	1:F:131:GLU:CD	2.15	0.50
1:A:221:LEU:HB3	1:A:262:LEU:HD11	1.94	0.50
1:A:381:GLY:HA2	1:A:384:VAL:HG12	1.92	0.50
1:B:286:ASP:OD2	1:B:327:PRO:HD3	2.11	0.50
1:C:272:LYS:HD2	1:C:311:GLU:HB3	1.94	0.50
1:D:88:VAL:O	1:D:92:VAL:HG23	2.12	0.50
1:A:24:ARG:HG3	1:A:63:GLU:CG	2.42	0.50
1:B:57:ASP:O	1:B:61:GLN:HG2	2.12	0.50
1:C:20:LYS:HE2	1:C:59:GLU:HB3	1.94	0.50
1:E:383:GLU:CD	1:E:383:GLU:H	2.14	0.50
1:D:108:ARG:HG3	1:D:147:GLU:OE2	2.12	0.50
1:F:145:GLN:HG3	1:F:146:LYS:N	2.27	0.50
1:F:218:VAL:HA	1:F:221:LEU:HD12	1.94	0.50



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Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:67:ALA:O	1:B:71:ILE:HG13	2.11	0.49
1:B:285:PRO:HB2	1:B:287:GLU:OE1	2.11	0.49
1:B:380:GLY:O	1:B:384:VAL:HG23	2.12	0.49
1:B:80:LYS:HG2	1:B:84:ASP:OD1	2.12	0.49
1:F:188:LYS:CG	1:F:228:VAL:HG22	2.42	0.49
1:E:24:ARG:CG	1:E:63:GLU:HG2	2.42	0.49
1:A:47:GLU:CD	1:A:47:GLU:N	2.65	0.49
1:A:160:ASP:OD2	1:A:201:PRO:HD3	2.12	0.49
1:B:11:LEU:HD11	1:B:26:LEU:HD12	1.94	0.49
1:C:185:GLU:O	1:C:189:GLU:HG2	2.12	0.49
1:E:104:LYS:CE	1:E:105:GLU:HG3	2.42	0.49
1:A:302:VAL:O	1:A:305:LEU:HB2	2.12	0.49
1:B:10:LEU:HD23	1:B:22:ALA:CB	2.42	0.49
1:E:155:ILE:HG22	1:E:162:ALA:HB1	1.93	0.49
1:E:363:ALA:HB2	1:E:403:ALA:HB2	1.95	0.49
1:A:11:LEU:O	1:A:19:GLN:HG3	2.12	0.49
1:A:172:VAL:HG11	1:A:208:ILE:HA	1.94	0.49
1:C:373:ILE:O	1:C:377:VAL:HG22	2.12	0.49
1:E:152:LEU:HA	1:E:155:ILE:HD12	1.95	0.49
1:E:287:GLU:HG3	1:E:288:ALA:N	2.27	0.49
1:F:69:ALA:HB1	1:F:108:ARG:CZ	2.42	0.49
1:B:11:LEU:HD23	1:B:22:ALA:HB3	1.94	0.49
1:E:179:LEU:HD22	1:E:220:LEU:CD1	2.42	0.49
1:E:179:LEU:HB3	1:E:220:LEU:HD11	1.95	0.49
1:F:30:ALA:O	1:F:37:ILE:HD11	2.13	0.49
1:D:15:ASP:HB3	1:D:18:THR:OG1	2.13	0.49
1:F:79:ILE:CG2	1:F:113:ILE:HG23	2.43	0.49
1:F:83:VAL:HG13	1:F:88:VAL:CG1	2.43	0.49
1:A:147:GLU:HA	1:A:147:GLU:OE1	2.12	0.48
1:B:2:ASN:HD22	1:B:5:GLU:CG	2.26	0.48
1:B:292:ILE:HG21	1:B:323:ILE:HD11	1.94	0.48
1:D:382:VAL:O	1:D:386:GLN:HG3	2.13	0.48
1:E:263:LEU:HD21	1:E:278:LEU:HD12	1.95	0.48
1:A:244:ASP:CG	1:A:285:PRO:HD3	2.34	0.48
1:A:121:ILE:O	1:A:125:VAL:HG23	2.13	0.48
1:E:5:GLU:O	1:E:9:LYS:HG2	2.13	0.48
1:E:374:LYS:O	1:E:378:ASP:HB2	2.13	0.48
1:F:290:LYS:CA	1:F:293:VAL:HG22	2.41	0.48
1:A:185:GLU:HG3	1:D:311:GLU:HG2	1.94	0.48
1:F:122:LYS:HG3	1:F:126:ASP:OD2	2.13	0.48
1:F:290:LYS:HA	1:F:293:VAL:CG2	2.42	0.48



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:192:ARG:HA	1:A:231:GLU:OE1	2.14	0.48	
1:D:10:LEU:HB3	1:D:22:ALA:CB	2.43	0.48	
1:E:29:ILE:HB	1:E:40:ILE:HD11	1.94	0.48	
1:E:321:ALA:HB3	1:E:360:ARG:NH2	2.28	0.48	
1:E:343:LEU:HD22	1:E:358:ALA:HA	1.96	0.48	
1:F:188:LYS:HG2	1:F:228:VAL:HG22	1.96	0.48	
1:A:256:VAL:O	1:A:260:VAL:HG23	2.14	0.48	
1:E:99:ASP:HB2	1:E:102:VAL:HB	1.96	0.48	
1:F:155:ILE:HD12	3:F:548:HOH:O	2.14	0.48	
1:A:367:SER:HB3	1:A:406:ASN:ND2	2.29	0.47	
1:D:399:GLU:OE1	1:D:399:GLU:HA	2.13	0.47	
1:A:394:SER:O	1:A:398:LYS:HG3	2.14	0.47	
1:D:59:GLU:HA	1:D:59:GLU:OE1	2.14	0.47	
1:E:389:LEU:HD21	1:E:404:LEU:CD1	2.44	0.47	
1:F:272:LYS:CD	1:F:311:GLU:HB3	2.40	0.47	
1:A:263:LEU:HD11	1:A:278:LEU:CD1	2.44	0.47	
1:A:315:GLU:OE1	1:A:315:GLU:HA	2.15	0.47	
1:D:384:VAL:O	1:D:388:LEU:HD13	2.14	0.47	
1:E:90:VAL:HG13	1:E:91:LEU:N	2.30	0.47	
1:F:225:ASP:OD2	1:F:227:GLU:HG2	2.14	0.47	
1:B:109:ALA:O	1:B:113:ILE:HG13	2.14	0.47	
1:E:122:LYS:HE2	1:E:126:ASP:OD2	2.14	0.47	
1:A:331:ILE:HG23	1:A:365:ILE:HG23	1.95	0.47	
1:F:104:LYS:HB3	1:F:104:LYS:HZ3	1.79	0.47	
1:F:341:GLU:N	3:F:523:HOH:O	2.47	0.47	
1:A:332:LYS:HZ3	1:A:336:ASP:CG	2.18	0.47	
1:B:13:SER:OG	1:B:18:THR:HG21	2.14	0.47	
1:B:24:ARG:HG3	1:B:63:GLU:CG	2.45	0.47	
1:C:176:VAL:O	1:C:179:LEU:HB2	2.15	0.47	
1:D:21:GLU:CA	1:D:24:ARG:HB2	2.45	0.47	
1:D:33:PRO:HG2	1:D:36:ALA:HB2	1.97	0.47	
1:D:87:GLY:O	1:D:91:LEU:HG	2.15	0.47	
1:E:30:ALA:C	1:E:32:GLY:H	2.17	0.47	
1:E:299:GLU:O	1:E:302:VAL:HB	2.15	0.47	
1:F:151:ALA:O	1:F:155:ILE:HG13	2.14	0.47	
1:B:261:LYS:NZ	3:B:537:HOH:O	2.47	0.47	
1:E:2:ASN:OD1	1:E:5:GLU:HG3	2.15	0.47	
1:E:188:LYS:NZ	1:E:225:ASP:OD2	2.43	0.47	
1:F:39:ALA:O	1:F:42:ASP:HB3	2.15	0.47	
1:F:356:LYS:HD2	1:F:356:LYS:O	2.14	0.47	
1:F:174:VAL:C	3:F:508:HOH:O	2.53	0.47	



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:E:34:ALA:O	1:E:37:ILE:HG22	2.15	0.47	
1:A:332:LYS:HD3	3:A:785:HOH:O	2.15	0.46	
1:B:78:ALA:O	1:B:81:ALA:HB3	2.15	0.46	
1:B:216:VAL:O	1:B:220:LEU:HD13	2.15	0.46	
1:C:105:GLU:OE1	1:C:108:ARG:NH2	2.46	0.46	
1:E:24:ARG:CZ	1:F:394:SER:HB2	2.45	0.46	
1:A:94:LEU:HA	3:A:792:HOH:O	2.16	0.46	
1:B:2:ASN:HB3	1:B:5:GLU:OE1	2.15	0.46	
1:F:403:ALA:O	1:F:407:ILE:HG13	2.14	0.46	
1:E:360:ARG:HG2	1:E:360:ARG:HH11	1.81	0.46	
1:F:61:GLN:HG2	3:F:530:HOH:O	2.13	0.46	
1:A:361:ALA:O	1:A:365:ILE:HG13	2.15	0.46	
1:C:332:LYS:HE2	1:C:336:ASP:OD1	2.16	0.46	
1:F:33:PRO:O	1:F:36:ALA:HB3	2.16	0.46	
1:F:88:VAL:HG11	1:F:123:ALA:HB1	1.96	0.46	
1:D:45:GLY:O	1:D:49:LEU:HB2	2.15	0.46	
1:E:304:LEU:HD22	1:E:312:VAL:HG12	1.97	0.46	
1:F:175:LEU:O	1:F:179:LEU:HG	2.16	0.46	
1:B:366:ALA:O	1:B:406:ASN:HB3	2.16	0.46	
1:F:121:ILE:HA	1:F:124:ILE:HD12	1.97	0.46	
1:E:289:ILE:O	1:E:293:VAL:HG23	2.15	0.46	
1:A:327:PRO:HB2	1:A:329:GLU:OE1	2.16	0.46	
1:C:314:LYS:CG	1:C:353:GLU:HB3	2.45	0.46	
1:D:49:LEU:HD21	1:D:67:ALA:HB1	1.96	0.46	
1:A:230:LYS:HD2	1:D:227:GLU:OE2	2.15	0.46	
1:B:42:ASP:C	1:B:44:GLY:H	2.19	0.46	
1:D:4:VAL:O	1:D:8:VAL:HG23	2.16	0.46	
1:F:276:ARG:HA	1:F:315:GLU:CG	2.46	0.46	
1:B:24:ARG:HG3	1:B:63:GLU:HG2	1.98	0.46	
1:C:374:LYS:O	1:C:377:VAL:HG23	2.15	0.46	
1:D:304:LEU:HD22	1:D:312:VAL:HG11	1.97	0.46	
1:E:70:ASN:HD22	1:E:70:ASN:N	2.13	0.46	
1:E:408:LYS:HD3	1:E:409:SER:OG	2.16	0.46	
1:D:227:GLU:HA	1:D:230:LYS:HE2	1.98	0.45	
1:E:153:ALA:HB2	1:E:193:ALA:HB2	1.98	0.45	
1:E:394:SER:O	1:E:398:LYS:HG3	2.16	0.45	
1:F:179:LEU:HD11	1:F:194:LEU:HD12	1.98	0.45	
1:F:230:LYS:HD3	1:F:269:GLU:HB3	1.98	0.45	
1:A:95:LEU:HD11	1:A:110:LEU:CD1	2.46	0.45	
1:C:332:LYS:HE2	1:C:336:ASP:OD2	2.16	0.45	
1:F:60:VAL:HG12	1:F:60:VAL:O	2.16	0.45	



	loue page	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:F:288:ALA:O	1:F:291:ALA:HB3	2.17	0.45	
1:B:57:ASP:C	1:B:59:GLU:N	2.69	0.45	
1:F:118:ASP:OD1	1:F:158:GLY:HA2	2.16	0.45	
1:B:2:ASN:O	1:B:6:LYS:HG2	2.16	0.45	
1:C:66:ARG:NH2	3:C:745:HOH:O	2.48	0.45	
1:C:396:VAL:CG1	1:C:397:GLN:N	2.79	0.45	
1:F:197:ILE:HG22	1:F:208:ILE:HD11	1.98	0.45	
1:A:287:GLU:O	1:A:290:LYS:HB3	2.17	0.45	
1:B:55:SER:OG	1:B:60:VAL:HG11	2.17	0.45	
1:B:327:PRO:O	1:B:330:ALA:HB3	2.16	0.45	
1:D:21:GLU:C	1:D:24:ARG:HB2	2.37	0.45	
1:D:305:LEU:HD11	1:D:320:LEU:HD12	1.99	0.45	
1:E:408:LYS:CD	1:E:409:SER:N	2.74	0.45	
1:B:55:SER:OG	1:B:56:THR:N	2.47	0.45	
1:E:332:LYS:HG2	1:E:336:ASP:OD2	2.17	0.45	
1:E:34:ALA:HA	1:E:37:ILE:CG2	2.42	0.45	
1:E:45:GLY:O	1:E:49:LEU:HD13	2.17	0.45	
1:E:91:LEU:HD21	1:E:109:ALA:HB3	1.97	0.45	
1:F:221:LEU:O	1:F:262:LEU:HD11	2.16	0.45	
1:A:114:ALA:HB1	1:A:155:ILE:HG13	1.98	0.45	
1:B:114:ALA:O	1:B:154:ASN:HB3	2.16	0.45	
1:F:351:ASP:HB3	1:F:354:VAL:CG1	2.36	0.45	
1:A:341:GLU:O	1:A:345:LYS:HG2	2.16	0.45	
1:A:388:LEU:HD22	1:A:396:VAL:HG11	1.99	0.45	
1:C:327:PRO:O	1:C:330:ALA:HB3	2.17	0.45	
1:E:137:LEU:HD22	1:E:178:LEU:CD2	2.47	0.45	
1:F:256:VAL:O	1:F:260:VAL:HG23	2.16	0.45	
1:B:15:ASP:CB	1:B:18:THR:HG22	2.42	0.44	
1:C:406:ASN:N	1:C:406:ASN:HD22	2.15	0.44	
1:E:108:ARG:CB	1:E:147:GLU:HG2	2.47	0.44	
1:E:289:ILE:HG23	1:E:323:ILE:HG23	1.99	0.44	
1:C:11:LEU:HD11	1:C:26:LEU:CD1	2.48	0.44	
1:C:403:ALA:O	1:C:407:ILE:HG13	2.17	0.44	
1:E:347:LEU:HD21	1:E:362:LEU:HD12	1.99	0.44	
1:F:135:LYS:C	1:F:137:LEU:H	2.21	0.44	
1:C:99:ASP:HB3	1:C:102:VAL:HG23	1.98	0.44	
1:D:122:LYS:HG3	1:D:161:GLU:OE1	2.17	0.44	
1:D:163:ILE:O	1:D:167:VAL:HG23	2.17	0.44	
1:F:57:ASP:CB	1:F:60:VAL:HG23	2.46	0.44	
1:F:361:ALA:O	1:F:365:ILE:HG13	2.18	0.44	
1:B:121:ILE:HG23	1:B:155:ILE:HG23	1.99	0.44	



	i i i i i i i i i i i i i i i i i i i	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:272:LYS:HD3	1:C:311:GLU:HB3	2.00	0.44
1:D:164:LYS:HG2	1:D:168:ASP:OD2	2.18	0.44
1:E:19:GLN:OE1	1:E:60:VAL:HG11	2.17	0.44
1:E:406:ASN:N	1:E:406:ASN:ND2	2.65	0.44
1:E:408:LYS:NZ	1:E:409:SER:OG	2.38	0.44
1:F:178:LEU:C	1:F:180:THR:H	2.20	0.44
1:B:20:LYS:HZ1	1:B:59:GLU:HB2	1.82	0.44
1:D:361:ALA:O	1:D:365:ILE:HG13	2.17	0.44
1:E:27:ALA:O	1:E:30:ALA:HB3	2.18	0.44
1:E:141:ASP:HB3	1:E:144:VAL:CG1	2.45	0.44
1:F:110:LEU:HD23	1:F:113:ILE:HD12	1.99	0.44
1:F:129:GLY:O	1:F:132:VAL:HG13	2.18	0.44
1:F:389:LEU:HD11	1:F:404:LEU:CD1	2.48	0.44
1:C:230:LYS:HD2	1:C:269:GLU:HB3	2.00	0.44
1:B:46:VAL:O	1:B:48:VAL:N	2.51	0.44
1:C:305:LEU:HD11	1:C:320:LEU:CD1	2.47	0.44
1:E:311:GLU:OE1	1:F:185:GLU:HG3	2.18	0.44
1:F:235:ALA:O	1:F:239:ILE:HG13	2.18	0.44
1:F:393:ASP:HB3	1:F:396:VAL:CG1	2.46	0.44
1:B:88:VAL:O	1:B:92:VAL:HG23	2.17	0.44
1:D:11:LEU:HD23	1:D:48:VAL:HG12	2.00	0.44
1:E:122:LYS:HE3	1:E:122:LYS:HB2	1.78	0.44
1:B:347:LEU:HD11	1:B:362:LEU:CD1	2.48	0.44
1:D:132:VAL:O	1:D:136:LEU:HD13	2.18	0.44
1:E:177:LYS:HD2	1:E:177:LYS:O	2.18	0.44
1:A:221:LEU:HD22	1:A:262:LEU:CD1	2.49	0.43
1:D:33:PRO:O	1:D:36:ALA:HB3	2.18	0.43
1:E:205:ILE:HG23	1:E:239:ILE:HG23	2.00	0.43
1:E:225:ASP:O	1:E:229:GLN:HG3	2.18	0.43
1:E:356:LYS:HG3	1:E:357:GLU:N	2.33	0.43
1:F:16:SER:O	1:F:20:LYS:HG3	2.19	0.43
1:F:60:VAL:O	1:F:64:ALA:HB2	2.18	0.43
1:B:87:GLY:O	1:B:91:LEU:HD12	2.17	0.43
1:B:257:GLU:HB2	3:B:576:HOH:O	2.18	0.43
1:D:283:SER:HB3	3:D:538:HOH:O	2.18	0.43
1:E:24:ARG:HH12	1:F:394:SER:CB	2.29	0.43
1:E:327:PRO:O	1:E:331:ILE:HG13	2.18	0.43
1:E:334:ILE:HG21	1:E:365:ILE:HD11	2.00	0.43
1:D:293:VAL:HA	3:D:508:HOH:O	2.18	0.43
1:E:324:ALA:O	1:E:364:ASN:HB3	2.18	0.43
1:F:322:ASN:OD1	1:F:360:ARG:NH2	2.50	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:286:ASP:CG	1:C:327:PRO:HD3	2.38	0.43
1:D:21:GLU:HA	1:D:24:ARG:CD	2.46	0.43
1:E:227:GLU:OE2	1:E:230:LYS:HE2	2.18	0.43
1:F:251:VAL:HG22	1:F:256:VAL:HG21	1.99	0.43
1:E:164:LYS:HG2	1:E:168:ASP:OD2	2.18	0.43
1:F:86:GLY:O	1:F:90:VAL:HG23	2.19	0.43
1:F:290:LYS:O	1:F:293:VAL:HG22	2.19	0.43
1:B:50:VAL:HG11	1:B:85:ALA:O	2.18	0.43
1:B:367:SER:HB2	1:B:413:LEU:HD11	2.00	0.43
1:E:189:GLU:OE1	1:E:192:ARG:NH1	2.51	0.43
1:F:327:PRO:O	1:F:331:ILE:HG13	2.18	0.43
1:D:21:GLU:O	1:D:24:ARG:HB2	2.18	0.43
1:D:179:LEU:HB2	1:D:216:VAL:HG11	2.01	0.43
1:F:286:ASP:OD2	1:F:327:PRO:HD3	2.18	0.43
1:E:45:GLY:O	1:E:48:VAL:HG12	2.18	0.43
1:F:143:GLU:HG3	1:F:143:GLU:O	2.18	0.43
1:F:363:ALA:HB1	1:F:402:ARG:CZ	2.49	0.43
1:B:11:LEU:CD2	1:B:22:ALA:HB3	2.49	0.43
1:B:315:GLU:OE1	1:B:315:GLU:HA	2.19	0.43
1:D:18:THR:O	1:D:22:ALA:HB2	2.19	0.43
1:D:134:VAL:O	1:D:137:LEU:HB2	2.19	0.43
1:D:347:LEU:HD11	1:D:362:LEU:CD1	2.49	0.43
1:F:68:LEU:HD23	1:F:71:ILE:HD12	2.00	0.43
1:F:101:GLU:HA	1:F:104:LYS:HZ3	1.84	0.43
1:A:66:ARG:HD3	3:A:768:HOH:O	2.19	0.42
1:B:36:ALA:O	1:B:39:ALA:HB3	2.19	0.42
1:B:70:ASN:O	1:B:73:SER:HB3	2.19	0.42
1:E:133:LEU:HA	1:E:136:LEU:CD2	2.47	0.42
1:E:150:ARG:HG3	1:E:189:GLU:OE1	2.19	0.42
1:E:163:ILE:HG23	1:E:197:ILE:HG23	2.00	0.42
1:E:373:ILE:O	1:E:377:VAL:HG13	2.19	0.42
1:A:401:GLN:OE1	1:A:401:GLN:HA	2.20	0.42
1:A:303:LYS:NZ	3:A:714:HOH:O	2.52	0.42
1:B:46:VAL:O	1:B:47:GLU:C	2.58	0.42
1:B:413:LEU:N	1:B:413:LEU:CD1	2.82	0.42
1:D:99:ASP:OD1	1:D:102:VAL:HB	2.19	0.42
1:E:136:LEU:HD12	1:E:144:VAL:HG22	2.02	0.42
1:A:206:LYS:HE3	3:A:728:HOH:O	2.20	0.42
1:C:117:PRO:HG2	3:C:785:HOH:O	2.19	0.42
1:B:15:ASP:O	1:B:19:GLN:HB2	2.20	0.42
1:B:193:ALA:O	1:B:197:ILE:HG13	2.20	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:57:ASP:CG	1:D:60:VAL:HG23	2.40	0.42
1:E:179:LEU:HD11	1:E:194:LEU:HD12	2.01	0.42
1:F:4:VAL:O	1:F:8:VAL:HG23	2.20	0.42
1:F:53:LEU:HD11	1:F:68:LEU:CD1	2.50	0.42
1:F:195:ALA:HA	1:F:235:ALA:HA	2.02	0.42
1:A:140:THR:HG23	3:A:774:HOH:O	2.19	0.42
1:C:396:VAL:HG13	1:C:397:GLN:N	2.35	0.42
1:F:46:VAL:O	1:F:50:VAL:HG13	2.20	0.42
1:F:314:LYS:HD3	1:F:353:GLU:HB3	2.01	0.42
1:A:157:SER:O	2:A:601:ACT:C	2.68	0.42
1:D:79:ILE:CG2	1:D:113:ILE:HG23	2.49	0.42
1:D:197:ILE:HG22	1:D:204:ALA:HB1	2.01	0.42
1:E:95:LEU:HD21	1:E:110:LEU:HD12	2.01	0.42
1:E:366:ALA:HB1	1:E:406:ASN:CB	2.47	0.42
1:F:11:LEU:HD22	1:F:22:ALA:CB	2.50	0.42
1:F:227:GLU:H	1:F:227:GLU:CD	2.22	0.42
1:A:273:GLU:OE1	1:A:276:ARG:NH1	2.53	0.42
1:B:413:LEU:CD2	3:B:586:HOH:O	2.65	0.42
1:C:245:GLU:CD	1:C:245:GLU:H	2.22	0.42
1:E:289:ILE:CG2	1:E:323:ILE:HG23	2.50	0.42
1:F:91:LEU:O	1:F:94:LEU:HB2	2.20	0.42
1:B:215:GLU:HG3	3:B:599:HOH:O	2.20	0.42
1:C:235:ALA:O	1:C:239:ILE:HG13	2.19	0.42
1:E:305:LEU:O	1:E:313:GLN:NE2	2.52	0.42
1:E:348:THR:O	1:E:348:THR:HG22	2.20	0.42
1:E:205:ILE:O	1:E:209:VAL:HG23	2.20	0.41
1:B:12:THR:HG22	1:B:12:THR:O	2.20	0.41
1:E:13:SER:C	1:E:15:ASP:N	2.74	0.41
1:F:225:ASP:OD2	1:F:228:VAL:HG23	2.21	0.41
1:F:289:ILE:O	1:F:292:ILE:N	2.52	0.41
1:F:390:THR:HG23	1:F:390:THR:O	2.20	0.41
1:D:104:LYS:HE3	1:D:104:LYS:HB2	1.79	0.41
1:D:110:LEU:HD23	1:D:110:LEU:HA	1.89	0.41
1:A:92:VAL:O	1:A:95:LEU:HB2	2.20	0.41
1:B:60:VAL:HG22	3:B:593:HOH:O	2.20	0.41
1:A:1:MET:HG2	1:A:5:GLU:OE1	2.21	0.41
1:D:16:SER:HB2	3:D:574:HOH:O	2.19	0.41
1:F:50:VAL:HG23	1:F:51:LYS:N	2.36	0.41
1:F:279:ALA:HB3	1:F:318:ARG:HH21	1.85	0.41
1:E:248:LYS:HG2	1:E:252:ASP:OD2	2.20	0.41
1:E:310:SER:CB	1:F:146:LYS:HZ2	2.28	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:88:VAL:HG23	1:F:89:GLU:H	1.85	0.41
1:E:260:VAL:O	1:E:263:LEU:HB2	2.20	0.41
1:E:268:SER:HB3	1:F:227:GLU:HG3	2.03	0.41
1:E:279:ALA:HB2	1:E:319:ALA:HB2	2.03	0.41
1:E:301:LEU:HD23	1:E:304:LEU:HD12	2.03	0.41
1:C:24:ARG:HD3	1:C:63:GLU:OE2	2.21	0.41
1:C:331:ILE:HD11	3:C:715:HOH:O	2.20	0.41
1:D:386:GLN:NE2	3:D:509:HOH:O	2.53	0.41
1:F:193:ALA:O	1:F:197:ILE:HG13	2.20	0.41
1:F:398:LYS:O	1:F:401:GLN:HG2	2.21	0.41
1:A:97:SER:N	3:A:792:HOH:O	2.54	0.41
1:A:181:SER:OG	1:A:182:THR:N	2.54	0.41
1:A:219:LYS:NZ	1:B:345:LYS:NZ	2.69	0.41
1:B:382:VAL:HG12	3:B:584:HOH:O	2.21	0.41
1:C:179:LEU:HD22	1:C:220:LEU:CD1	2.50	0.41
1:C:314:LYS:CD	1:C:353:GLU:HB3	2.51	0.41
1:E:18:THR:O	1:E:18:THR:HG22	2.21	0.41
1:E:172:VAL:HG11	1:E:208:ILE:HA	2.02	0.41
1:E:362:LEU:HD23	1:E:365:ILE:HD12	2.03	0.41
1:F:106:ALA:O	1:F:109:ALA:HB3	2.20	0.41
1:F:381:GLY:O	1:F:384:VAL:HG12	2.21	0.41
1:A:206:LYS:CE	3:A:712:HOH:O	2.68	0.41
1:C:151:ALA:O	1:C:155:ILE:HG13	2.21	0.41
1:E:179:LEU:HD22	1:E:220:LEU:HD11	2.02	0.41
1:E:357:GLU:OE1	1:E:357:GLU:HA	2.21	0.41
1:B:156:ALA:O	1:B:196:ASN:HB3	2.20	0.40
1:E:111:ALA:HB2	1:E:151:ALA:HB2	2.03	0.40
1:F:46:VAL:HG11	1:F:82:ILE:HG12	2.03	0.40
1:C:179:LEU:HD11	1:C:194:LEU:CD1	2.51	0.40
1:D:121:ILE:O	1:D:125:VAL:HG23	2.21	0.40
1:E:153:ALA:HB3	1:E:192:ARG:NH1	2.36	0.40
1:E:194:LEU:HD23	1:E:197:ILE:HD12	2.03	0.40
1:F:160:ASP:HA	1:F:163:ILE:HG13	2.04	0.40
1:D:24:ARG:NH1	1:D:63:GLU:HG3	2.37	0.40
1:A:79:ILE:O	1:A:83:VAL:HG23	2.21	0.40
1:A:172:VAL:O	1:A:176:VAL:HG23	2.22	0.40
1:C:63:GLU:HA	1:C:63:GLU:OE1	2.20	0.40
1:E:118:ASP:HA	1:E:121:ILE:HD12	2.03	0.40
1:F:20:LYS:O	1:F:24:ARG:HG3	2.20	0.40
1:F:46:VAL:HG13	1:F:68:LEU:CD2	2.51	0.40
1:F:344:VAL:O	1:F:347:LEU:HB2	2.21	0.40



Atom-1	Atom-1 Atom-2		Clash overlap (Å)	
1:F:245:GLU:CD	1:F:245:GLU:H	2.24	0.40	
1:F:251:VAL:HA	1:F:256:VAL:HG23	2.03	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	Perce	ntiles
1	А	411/420~(98%)	399~(97%)	12 (3%)	0	100	100
1	В	412/420~(98%)	390 (95%)	21 (5%)	1 (0%)	47	69
1	C	410/420~(98%)	405 (99%)	5 (1%)	0	100	100
1	D	413/420~(98%)	395~(96%)	18 (4%)	0	100	100
1	E	410/420~(98%)	384 (94%)	24 (6%)	2~(0%)	29	50
1	F	409/420~(97%)	363~(89%)	43 (10%)	3 (1%)	22	41
All	All	2465/2520~(98%)	2336 (95%)	123 (5%)	6 (0%)	47	69

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	54	THR
1	F	136	LEU
1	В	58	SER
1	Е	75	PRO
1	F	33	PRO
1	Е	46	VAL



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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	s
1	А	308/317~(97%)	304 (99%)	4 (1%)	69 85	
1	В	311/317~(98%)	307~(99%)	4 (1%)	69 85	
1	С	307/317~(97%)	306 (100%)	1 (0%)	92 97	
1	D	311/317~(98%)	307~(99%)	4 (1%)	69 85	
1	Е	309/317~(98%)	300 (97%)	9 (3%)	42 66	
1	F	308/317~(97%)	300 (97%)	8 (3%)	46 69	
All	All	1854/1902~(98%)	1824 (98%)	30 (2%)	62 81	

All (30) residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	А	63	GLU
1	А	142	SER
1	А	160	ASP
1	А	178	LEU
1	В	57	ASP
1	В	63	GLU
1	В	84	ASP
1	В	415	HIS
1	С	261	LYS
1	D	24	ARG
1	D	328	ASP
1	D	395	GLU
1	D	409	SER
1	Е	7	LEU
1	Е	96	THR
1	Е	99	ASP
1	Е	136	LEU
1	Е	147	GLU
1	Е	161	GLU
1	Е	267	ASP
1	Е	356	LYS
1	Е	387	LYS



Mol	Chain	Res	Type
1	F	63	GLU
1	F	88	VAL
1	F	227	GLU
1	F	262	LEU
1	F	290	LYS
1	F	328	ASP
1	F	353	GLU
1	F	386	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	В	2	ASN
1	С	406	ASN
1	Е	70	ASN
1	Е	280	ASN
1	Е	355	GLN
1	Е	406	ASN
1	F	103	GLN
1	F	196	ASN
1	F	313	GLN
1	F	386	GLN
1	F	401	GLN
1	F	406	ASN

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 monosaccharides in this entry.



5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Mal Truna Chain I		Pog Link	Bond lengths			Bond angles			
	on Type Chain Res		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2		
2	ACT	С	501	-	3,3,3	1.13	0	3,3,3	0.95	0
2	ACT	А	601	-	3,3,3	0.98	0	3,3,3	0.82	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	601	ACT	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 (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, 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	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	А	413/420~(98%)	-0.05	2 (0%) 91 90	37, 56, 92, 118	0
1	В	414/420~(98%)	-0.07	5 (1%) 79 77	36, 54, 108, 169	0
1	С	412/420~(98%)	-0.07	5 (1%) 79 77	36, 54, 93, 124	0
1	D	415/420 (98%)	0.17	19 (4%) 32 28	35, 63, 127, 176	0
1	Е	412/420~(98%)	0.72	57 (13%) 2 2	56, 103, 152, 196	0
1	F	411/420~(97%)	0.80	65 (15%) 2 1	61, 101, 155, 194	0
All	All	2477/2520 (98%)	0.25	153 (6%) 20 17	35, 71, 135, 196	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Е	396	VAL	11.4
1	F	11	LEU	8.4
1	Е	358	ALA	7.0
1	F	392	THR	5.8
1	Е	393	ASP	5.7
1	Е	397	GLN	5.6
1	Е	6	LYS	5.4
1	F	23	ALA	5.4
1	F	354	VAL	5.4
1	F	25	ASP	5.4
1	Е	10	LEU	5.4
1	D	22	ALA	5.2
1	F	400	ALA	5.1
1	F	21	GLU	4.9
1	Е	102	VAL	4.8
1	Е	30	ALA	4.8
1	Е	391	SER	4.8
1	F	410	GLY	4.7
1	F	18	THR	4.7



Mol	Chain	Res	Type	RSRZ
1	Е	392	THR	4.6
1	D	60	VAL	4.5
1	Е	96	THR	4.5
1	F	362	LEU	4.5
1	D	11	LEU	4.5
1	F	250	ILE	4.4
1	Е	21	GLU	4.4
1	F	19	GLN	4.4
1	F	4	VAL	4.3
1	D	9	LYS	4.1
1	F	101	GLU	4.1
1	F	62	LYS	4.1
1	Е	324	ALA	4.1
1	Е	362	LEU	4.0
1	F	24	ARG	4.0
1	F	22	ALA	3.9
1	D	8	VAL	3.9
1	F	361	ALA	3.8
1	D	23	ALA	3.8
1	F	49	LEU	3.8
1	F	365	ILE	3.7
1	Е	365	ILE	3.7
1	F	393	ASP	3.7
1	Е	22	ALA	3.7
1	F	50	VAL	3.6
1	F	355	GLN	3.6
1	В	23	ALA	3.6
1	F	403	ALA	3.6
1	D	10	LEU	3.6
1	F	352	SER	3.5
1	F	61	GLN	3.5
1	F	57	ASP	3.4
1	Ε	17	GLU	3.4
1	F	366	ALA	3.3
1	Е	400	ALA	3.3
1	Е	16	SER	3.3
1	D	46	VAL	3.3
1	F	60	VAL	3.3
1	F	246	ALA	3.3
1	В	18	THR	3.2
1	Е	37	ILE	3.2
1	F	8	VAL	3.2



4RV1

Mol	Chain	Res	Type	RSRZ
1	Е	40	ILE	3.2
1	Е	405	GLU	3.2
1	F	63	GLU	3.2
1	Е	46	VAL	3.2
1	A	411	GLY	3.1
1	F	26	LEU	3.1
1	Е	11	LEU	3.0
1	Е	14	THR	3.0
1	Е	23	ALA	3.0
1	Е	59	GLU	3.0
1	Е	7	LEU	3.0
1	F	396	VAL	3.0
1	Е	62	LYS	3.0
1	F	52	LEU	3.0
1	Е	83	VAL	2.9
1	Е	110	LEU	2.9
1	F	404	LEU	2.9
1	С	385	LEU	2.9
1	Е	20	LYS	2.9
1	F	7	LEU	2.9
1	F	10	LEU	2.9
1	Е	105	GLU	2.8
1	F	48	VAL	2.8
1	F	320	LEU	2.8
1	F	46	VAL	2.8
1	D	19	GLN	2.7
1	F	6	LYS	2.7
1	А	413	LEU	2.7
1	F	20	LYS	2.7
1	F	104	LYS	2.7
1	F	205	ILE	2.7
1	F	38	LYS	2.7
1	F	53	LEU	2.7
1	С	353	GLU	2.7
1	Е	350	THR	2.6
1	С	396	VAL	2.6
1	F	163	ILE	2.6
1	Е	354	VAL	2.6
1	D	63	GLU	2.5
1	Е	91	LEU	2.5
1	Е	186	VAL	2.5
1	F	323	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	45	GLY	2.5
1	F	102	VAL	2.5
1	D	7	LEU	2.5
1	Е	53	LEU	2.5
1	F	16	SER	2.5
1	F	374	LYS	2.5
1	F	143	GLU	2.4
1	D	12	THR	2.4
1	F	314	LYS	2.4
1	Е	41	VAL	2.4
1	D	64	ALA	2.4
1	Е	343	LEU	2.4
1	F	209	VAL	2.4
1	Е	304	LEU	2.4
1	Е	79	ILE	2.4
1	F	245	GLU	2.3
1	Е	106	ALA	2.3
1	Е	366	ALA	2.3
1	Е	412	TRP	2.3
1	D	52	LEU	2.3
1	Е	355	GLN	2.3
1	Е	407	ILE	2.3
1	Е	312	VAL	2.3
1	В	8	VAL	2.2
1	Е	29	ILE	2.2
1	F	292	ILE	2.2
1	F	397	GLN	2.2
1	В	45	GLY	2.2
1	D	18	THR	2.2
1	D	102	VAL	2.2
1	Е	398	LYS	2.2
1	Е	404	LEU	2.2
1	F	188	LYS	2.1
1	Е	331	ILE	2.1
1	F	346	LEU	2.1
1	Е	409	SER	2.1
1	F	66	ARG	2.1
1	В	52	LEU	2.1
1	Е	137	LEU	2.1
1	D	49	LEU	2.1
1	Е	25	ASP	2.1
1	F	124	ILE	2.0



Mol	Chain	Res	Type	RSRZ
1	С	412	TRP	2.0
1	F	99	ASP	2.0
1	С	395	GLU	2.0
1	D	21	GLU	2.0
1	F	41	VAL	2.0
1	Е	45	GLY	2.0
1	Е	395	GLU	2.0
1	F	1	MET	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
2	ACT	А	601	4/4	0.91	0.14	84,86,87,88	0
2	ACT	С	501	4/4	0.94	0.30	63,69,77,78	0

6.5 Other polymers (i)

There are no such residues in this entry.

