Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 08:17 PM EDT

PDB ID	:	4ZHS
Title	:	Crystal Structure of Aspartate Semialdehyde Dehydrogenase from Trichophyton rubrum
Authors	:	Li, Q.; Cui, S.
Deposited on	:	2015-04-27
Resolution	:	2.60 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 (i)) were used in the production of this report:

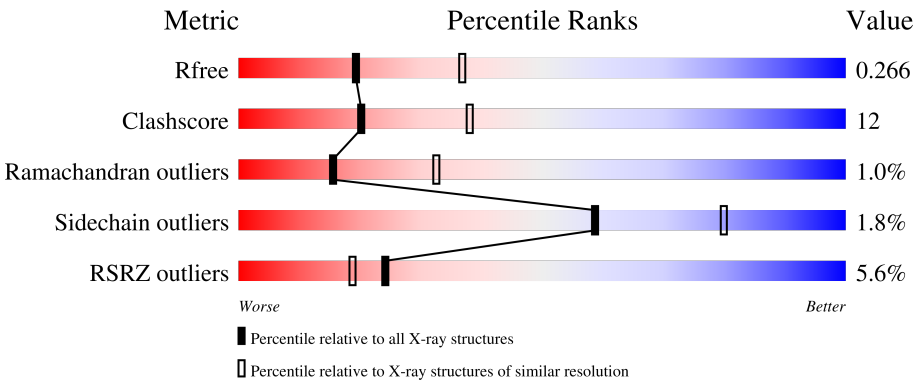
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	A	379	4% 77% 16% • 7%
1	B	379	4% 74% 17% • 8%
1	C	379	6% 73% 20% • 6%
1	D	379	4% 74% 19% • 6%
1	E	379	5% 72% 19% • 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	379	7% 67% 23% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	F	401	-	-	X	-

2 Entry composition (i)

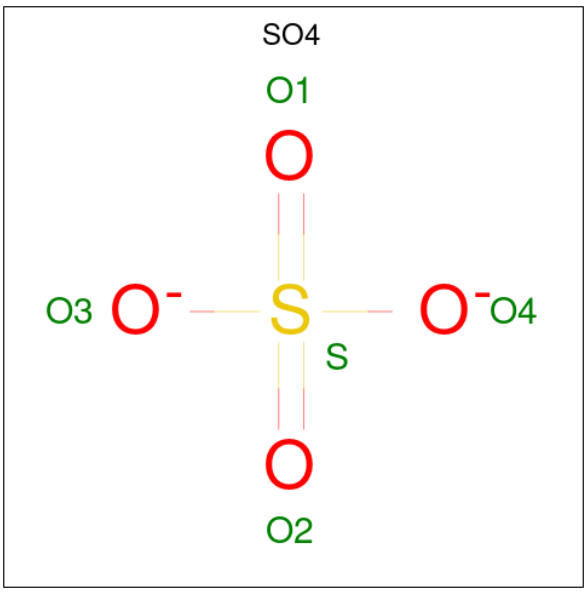
There are 3 unique types of molecules in this entry. The entry contains 32241 atoms, of which 15998 are hydrogens and 0 are deuteriums.

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 Aspartate Semialdehyde Dehydrogenase.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S	Se			
1	D	356	5365	1681	2697	464	504	10	9	0	0	0
1	C	355	5352	1677	2692	463	501	10	9	0	0	0
1	B	349	5278	1656	2653	459	491	10	9	0	0	0
1	E	348	5253	1650	2641	454	489	10	9	0	0	0
1	A	354	5341	1674	2687	462	499	10	9	0	0	0
1	F	346	5221	1637	2628	452	485	10	9	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is water.

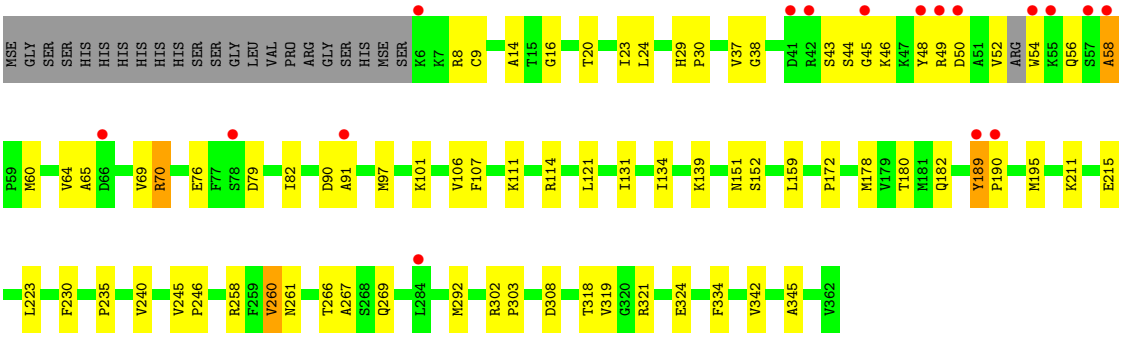
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	D	81	81	81	0	0
			Total	O		
3	C	66	66	66	0	0
			Total	O		
3	B	67	67	67	0	0
			Total	O		
3	E	66	66	66	0	0
			Total	O		
3	A	84	84	84	0	0
			Total	O		
3	F	37	37	37	0	0

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.

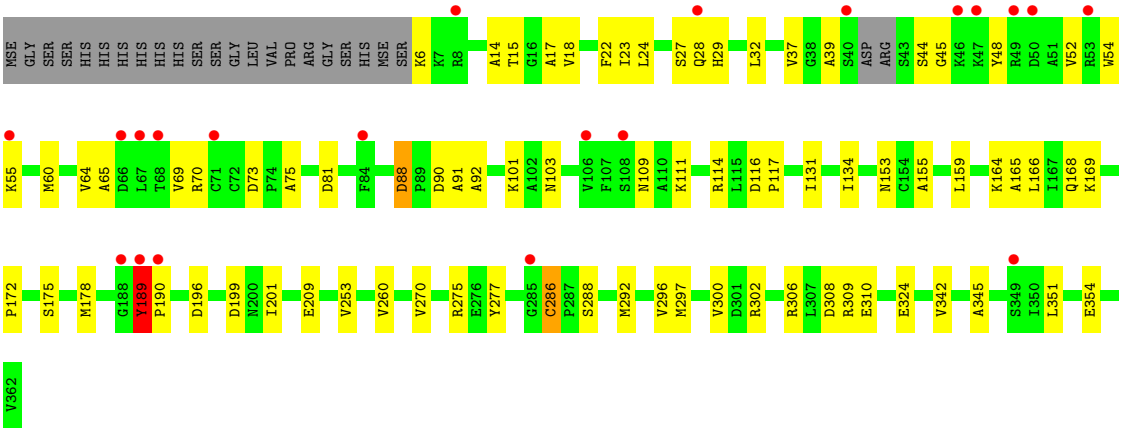
• Molecule 1: Aspartate Semialdehyde Dehydrogenase

Chain D:



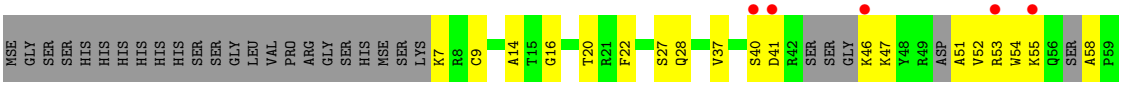
• Molecule 1: Aspartate Semialdehyde Dehydrogenase

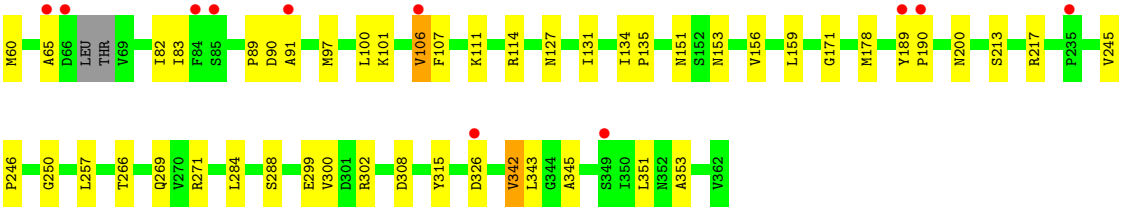
Chain C:



• Molecule 1: Aspartate Semialdehyde Dehydrogenase

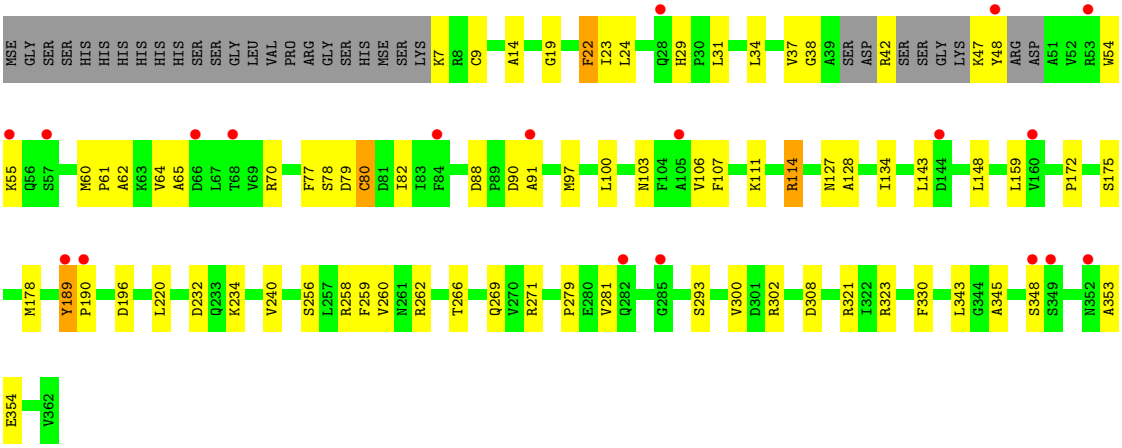
Chain B:





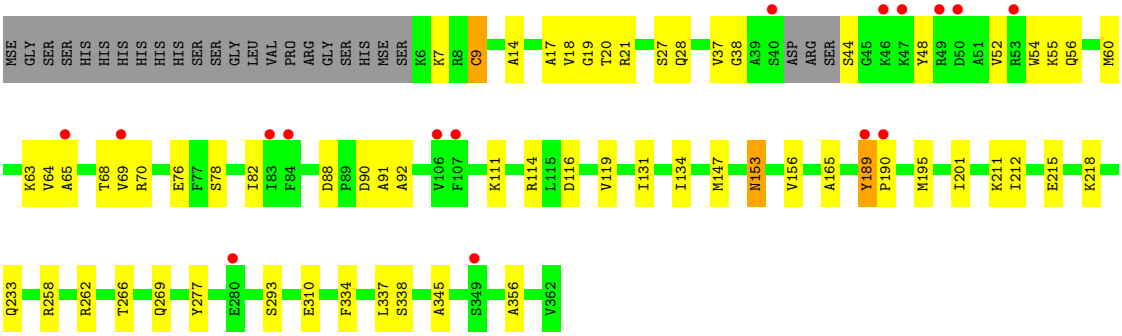
• Molecule 1: Aspartate Semialdehyde Dehydrogenase

Chain E:



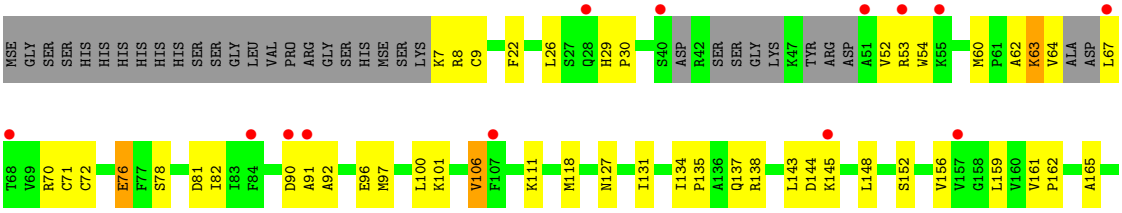
• Molecule 1: Aspartate Semialdehyde Dehydrogenase

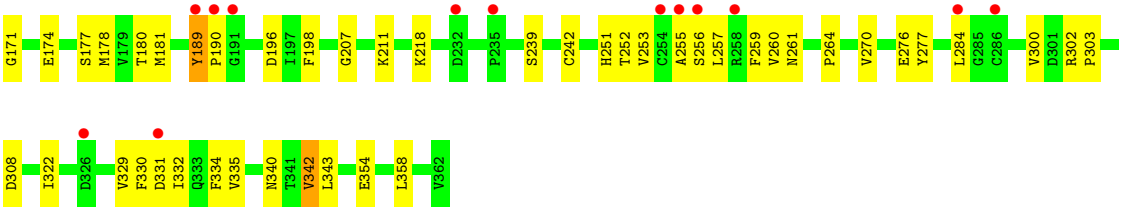
Chain A:



• Molecule 1: Aspartate Semialdehyde Dehydrogenase

Chain F:




G171
E174
S177
M178
V179
T180
M181
Y189
P190
G191
D196
I197
F198
G207
K211
K218
D232
P235
S239
C242
H251
T252
V253
C254
A255
S256
L257
R258
F259
V260
N261
P264
V270
E276
Y277
L284
G285
C286
V300
D301
R302
P303
D308
I322
D326
V329
F330
D331
I332
Q333
F334
V335
N340
T341
V342
L343
E354
L358
V362

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	157.50Å 157.50Å 188.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.62 – 2.60 27.62 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (27.62-2.60) 99.7 (27.62-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.90 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, R_{free}	0.214 , 0.257 0.225 , 0.266	Depositor DCC
R_{free} test set	4138 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	48.2	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 40.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	32241	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.72 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.5282e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.38	0/2695	0.54	0/3640
1	B	0.37	0/2663	0.52	0/3592
1	C	0.38	0/2701	0.54	0/3648
1	D	0.39	0/2709	0.55	0/3659
1	E	0.35	0/2651	0.52	0/3580
1	F	0.34	0/2630	0.53	0/3549
All	All	0.37	0/16049	0.53	0/21668

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	171	GLY	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	2654	2687	2681	54	0
1	B	2625	2653	2647	54	0
1	C	2660	2692	2686	62	0
1	D	2668	2697	2690	78	0
1	E	2612	2641	2636	70	1
1	F	2593	2628	2622	86	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	2	0
3	A	84	0	0	15	0
3	B	67	0	0	15	0
3	C	66	0	0	14	0
3	D	81	0	0	9	0
3	E	66	0	0	17	1
3	F	37	0	0	15	0
All	All	16243	15998	15962	397	1

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 12.

All (397) 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:E:55:LYS:NZ	1:F:196:ASP:OD1	1.89	1.04
1:A:18:VAL:N	3:A:501:HOH:O	1.90	1.03
1:B:55:LYS:HE2	3:B:501:HOH:O	1.63	0.99
1:E:38:GLY:O	3:E:501:HOH:O	1.85	0.94
1:E:240:VAL:O	3:E:502:HOH:O	1.90	0.88
1:D:54:TRP:NE1	1:D:56:GLN:O	2.07	0.88
1:C:199:ASP:OD2	3:C:501:HOH:O	1.92	0.87
1:F:329:VAL:HG12	1:F:330:PHE:CD1	2.11	0.85
1:E:47:LYS:NZ	3:E:507:HOH:O	2.09	0.85
1:E:42:ARG:NH2	3:E:506:HOH:O	2.09	0.84
1:A:233:GLN:O	3:A:502:HOH:O	1.93	0.84
1:D:139:LYS:NZ	3:D:503:HOH:O	2.12	0.82
1:C:90:ASP:OD2	3:C:502:HOH:O	1.98	0.82
1:A:17:ALA:C	3:A:501:HOH:O	2.16	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:VAL:N	3:C:504:HOH:O	2.12	0.80
1:C:45:GLY:N	3:C:505:HOH:O	2.14	0.79
1:A:56:GLN:O	3:A:503:HOH:O	2.01	0.79
1:D:180:THR:CG2	1:D:182:GLN:HG3	2.14	0.77
1:F:64:VAL:O	3:F:501:HOH:O	2.03	0.77
1:F:54:TRP:N	3:F:505:HOH:O	2.18	0.76
1:D:235:PRO:O	3:D:501:HOH:O	2.03	0.76
1:E:232:ASP:OD1	3:E:504:HOH:O	2.03	0.76
1:D:261:ASN:O	3:D:502:HOH:O	2.04	0.75
1:D:54:TRP:CZ2	1:D:58:ALA:O	2.40	0.75
1:E:196:ASP:OD2	3:E:503:HOH:O	2.03	0.75
1:C:172:PRO:O	3:C:503:HOH:O	2.06	0.73
1:F:322:ILE:O	3:F:502:HOH:O	2.07	0.72
1:C:189:TYR:HB3	1:C:190:PRO:CD	2.19	0.72
1:E:54:TRP:N	3:E:511:HOH:O	2.22	0.72
1:E:61:PRO:O	3:E:505:HOH:O	2.05	0.72
1:D:54:TRP:CH2	1:D:56:GLN:HB2	2.25	0.72
1:C:189:TYR:CG	1:C:190:PRO:HD3	2.25	0.71
1:A:310:GLU:OE1	3:A:504:HOH:O	2.08	0.71
1:A:18:VAL:HA	3:A:501:HOH:O	1.88	0.71
1:E:189:TYR:HB3	1:E:190:PRO:CD	2.20	0.71
1:F:189:TYR:CB	1:F:190:PRO:CD	2.68	0.70
1:A:90:ASP:OD2	3:A:505:HOH:O	2.08	0.70
1:E:48:TYR:HH	1:E:54:TRP:HZ3	1.39	0.70
1:F:70:ARG:NH1	1:F:76:GLU:O	2.25	0.70
1:C:302:ARG:NH1	1:C:308:ASP:OD1	2.25	0.69
1:A:18:VAL:CA	3:A:501:HOH:O	2.31	0.69
1:D:43:SER:HB2	1:D:44:SER:HA	1.74	0.69
1:D:195:MSE:O	1:C:306:ARG:NH2	2.26	0.69
1:B:53:ARG:O	3:B:501:HOH:O	2.12	0.68
1:C:196:ASP:OD1	1:A:55:LYS:NZ	2.24	0.68
1:C:14:ALA:CB	1:C:37:VAL:HG13	2.24	0.68
1:F:111:LYS:HE2	2:F:401:SO4:S	2.33	0.68
1:D:189:TYR:CB	1:D:190:PRO:CD	2.71	0.67
1:B:55:LYS:CE	3:B:501:HOH:O	2.31	0.67
1:B:299:GLU:OE1	3:B:502:HOH:O	2.13	0.67
1:E:7:LYS:N	3:E:515:HOH:O	2.28	0.67
1:F:52:VAL:HG23	3:F:505:HOH:O	1.95	0.67
1:C:60:MSE:HE2	1:C:65:ALA:HB2	1.77	0.66
1:F:276:GLU:OE1	3:F:503:HOH:O	2.14	0.66
1:F:264:PRO:HG3	1:F:331:ASP:OD2	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:ALA:N	1:D:324:GLU:OE1	2.29	0.66
1:E:103:ASN:OD1	3:E:508:HOH:O	2.13	0.66
1:A:189:TYR:HB3	1:A:190:PRO:CD	2.26	0.66
1:E:189:TYR:CG	1:E:190:PRO:HD3	2.30	0.66
1:F:111:LYS:HE2	2:F:401:SO4:O3	1.94	0.66
1:E:14:ALA:N	3:E:516:HOH:O	2.28	0.65
1:A:189:TYR:CG	1:A:190:PRO:HD3	2.32	0.65
1:F:152:SER:OG	3:F:504:HOH:O	2.14	0.65
1:F:54:TRP:HB2	3:F:505:HOH:O	1.98	0.64
1:E:159:LEU:HD22	1:E:178:MSE:SE	2.48	0.64
1:A:17:ALA:O	1:A:20:THR:N	2.29	0.63
1:E:7:LYS:N	1:E:31:LEU:O	2.32	0.63
1:F:189:TYR:HB3	1:F:190:PRO:HD3	1.80	0.63
1:D:302:ARG:NH1	1:D:308:ASP:OD1	2.33	0.62
1:C:189:TYR:CB	1:C:190:PRO:CD	2.78	0.62
1:F:189:TYR:HB3	1:F:190:PRO:CD	2.30	0.62
1:C:18:VAL:CA	3:C:504:HOH:O	2.45	0.61
1:B:55:LYS:CD	3:B:501:HOH:O	2.48	0.61
1:A:60:MSE:SE	1:A:65:ALA:HB2	2.50	0.61
1:D:8:ARG:NH1	1:D:79:ASP:O	2.34	0.61
1:C:18:VAL:HA	3:C:504:HOH:O	2.00	0.61
1:E:189:TYR:CB	1:E:190:PRO:CD	2.80	0.60
1:F:189:TYR:HB2	1:F:190:PRO:HD2	1.83	0.60
1:B:271:ARG:NE	3:B:511:HOH:O	2.35	0.60
1:F:218:LYS:HD2	3:F:511:HOH:O	2.00	0.60
1:B:7:LYS:HE2	1:B:7:LYS:N	2.16	0.60
1:B:58:ALA:N	3:B:510:HOH:O	2.34	0.59
1:E:172:PRO:HG2	1:E:260:VAL:HG11	1.84	0.59
1:F:264:PRO:CB	1:F:331:ASP:OD2	2.50	0.59
1:C:24:LEU:HD11	1:C:54:TRP:CZ2	2.37	0.59
1:D:90:ASP:O	1:D:91:ALA:HB3	2.02	0.59
1:B:217:ARG:NH1	3:B:512:HOH:O	2.36	0.59
1:B:54:TRP:CZ2	1:B:60:MSE:HA	2.37	0.59
1:E:7:LYS:N	1:E:7:LYS:HE2	2.18	0.59
1:F:165:ALA:HA	1:F:277:TYR:CD2	2.36	0.58
1:D:54:TRP:CE2	1:D:56:GLN:O	2.56	0.58
1:D:54:TRP:CZ2	1:D:56:GLN:HB2	2.38	0.58
1:D:189:TYR:HB3	1:D:190:PRO:HD3	1.85	0.58
1:D:44:SER:HB2	1:D:45:GLY:HA2	1.85	0.57
1:C:111:LYS:HA	1:C:114:ARG:HG3	1.86	0.57
1:C:189:TYR:HB3	1:C:190:PRO:HD2	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:TYR:HB3	1:D:190:PRO:CD	2.34	0.57
1:A:14:ALA:CB	1:A:37:VAL:HG13	2.34	0.57
1:A:189:TYR:CB	1:A:190:PRO:CD	2.81	0.57
1:A:134:ILE:HD11	1:A:147:MSE:HE3	1.85	0.57
1:E:19:GLY:O	1:E:22:PHE:HB2	2.05	0.57
1:A:63:LYS:NZ	3:A:518:HOH:O	2.38	0.57
1:C:101:LYS:O	1:C:103:ASN:ND2	2.38	0.56
1:F:180:THR:OG1	1:F:242:CYS:HA	2.04	0.56
1:A:334:PHE:O	3:A:506:HOH:O	2.18	0.56
1:E:258:ARG:NH1	1:E:262:ARG:CZ	2.68	0.56
1:D:8:ARG:HD2	1:D:79:ASP:O	2.05	0.56
1:D:14:ALA:HB3	1:D:37:VAL:HG13	1.86	0.56
1:F:255:ALA:HB3	1:F:334:PHE:CE1	2.41	0.56
1:B:60:MSE:CE	1:B:65:ALA:HB2	2.36	0.56
1:D:189:TYR:HB2	1:D:190:PRO:HD2	1.89	0.55
1:D:60:MSE:HE2	1:D:65:ALA:HB2	1.88	0.55
1:C:172:PRO:HG2	1:C:260:VAL:HG11	1.88	0.55
1:B:46:LYS:HD2	1:B:51:ALA:HB2	1.88	0.55
1:C:109:ASN:ND2	3:C:510:HOH:O	2.35	0.55
1:E:64:VAL:N	3:E:505:HOH:O	2.40	0.55
1:F:62:ALA:O	1:F:64:VAL:N	2.40	0.55
1:F:90:ASP:O	1:F:91:ALA:HB3	2.06	0.55
1:C:292:MSE:SE	3:C:563:HOH:O	2.75	0.54
1:D:9:CYS:HB3	1:D:82:ILE:HB	1.89	0.54
1:C:60:MSE:SE	3:C:564:HOH:O	2.75	0.54
1:B:97:MSE:HE3	1:B:100:LEU:HB3	1.89	0.54
1:E:47:LYS:N	1:E:47:LYS:HZ2	2.05	0.54
1:D:50:ASP:HB3	3:D:505:HOH:O	2.07	0.54
1:E:88:ASP:OD1	3:E:509:HOH:O	2.19	0.54
1:F:264:PRO:HB3	1:F:331:ASP:OD2	2.08	0.54
1:F:264:PRO:CG	1:F:331:ASP:OD2	2.56	0.54
1:C:168:GLN:NE2	3:C:512:HOH:O	2.38	0.54
1:F:165:ALA:CB	1:F:277:TYR:CD2	2.90	0.54
1:F:165:ALA:HB2	1:F:277:TYR:CD2	2.43	0.54
1:C:288:SER:HB2	1:C:351:LEU:HD13	1.90	0.53
1:B:40:SER:O	1:B:41:ASP:HB2	2.08	0.53
1:E:271:ARG:NH1	3:E:513:HOH:O	2.28	0.53
1:B:7:LYS:N	1:B:7:LYS:CE	2.71	0.53
1:A:90:ASP:O	1:A:91:ALA:HB3	2.08	0.53
1:D:48:TYR:O	1:D:52:VAL:HG13	2.08	0.53
1:A:189:TYR:CD2	1:A:190:PRO:HD3	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:VAL:O	1:A:65:ALA:HB3	2.08	0.53
1:E:9:CYS:HB3	1:E:82:ILE:HB	1.90	0.53
1:E:302:ARG:NH1	1:E:308:ASP:OD2	2.41	0.53
1:D:303:PRO:HB3	1:D:318:THR:HG21	1.91	0.53
1:F:174:GLU:HB2	1:F:260:VAL:CG1	2.38	0.53
1:F:261:ASN:ND2	3:F:507:HOH:O	2.34	0.53
1:C:48:TYR:CZ	1:C:52:VAL:HG11	2.45	0.52
1:F:52:VAL:CG2	3:F:505:HOH:O	2.55	0.52
1:F:260:VAL:N	3:F:510:HOH:O	2.42	0.52
1:F:329:VAL:HG12	1:F:330:PHE:CE1	2.44	0.52
1:D:48:TYR:CE2	1:D:52:VAL:HG11	2.45	0.52
1:C:172:PRO:HG2	1:C:260:VAL:CG1	2.39	0.52
1:B:271:ARG:HD2	3:B:511:HOH:O	2.09	0.52
1:A:21:ARG:NE	3:A:516:HOH:O	2.34	0.52
1:A:258:ARG:NE	3:A:509:HOH:O	2.26	0.52
1:F:159:LEU:HD22	1:F:178:MSE:SE	2.59	0.52
1:D:258:ARG:NH2	3:D:511:HOH:O	2.38	0.52
1:D:14:ALA:CB	1:D:37:VAL:HG13	2.39	0.52
1:B:266:THR:HG22	1:B:269:GLN:HG3	1.92	0.52
1:D:43:SER:CB	1:D:44:SER:HA	2.40	0.52
1:A:156:VAL:CG2	1:A:212:ILE:HA	2.40	0.52
1:B:89:PRO:HG2	1:B:189:TYR:HE2	1.75	0.51
1:E:48:TYR:OH	1:E:54:TRP:HZ3	1.93	0.51
1:B:27:SER:O	1:B:28:GLN:CB	2.58	0.51
1:E:302:ARG:NH1	1:E:308:ASP:OD1	2.43	0.51
1:D:60:MSE:CE	1:D:65:ALA:HA	2.41	0.51
1:B:54:TRP:CE2	1:B:60:MSE:HB2	2.45	0.51
1:B:250:GLY:O	3:B:505:HOH:O	2.19	0.51
1:C:14:ALA:HB2	1:C:37:VAL:HG13	1.92	0.51
1:E:62:ALA:C	3:E:505:HOH:O	2.49	0.51
1:E:220:LEU:O	3:E:510:HOH:O	2.20	0.50
1:B:54:TRP:NE1	1:B:60:MSE:HB2	2.26	0.50
1:F:118:MSE:HE2	1:F:137:GLN:HA	1.93	0.50
1:C:15:THR:HA	1:C:52:VAL:HG12	1.94	0.50
1:B:111:LYS:HA	1:B:114:ARG:HG3	1.92	0.50
1:A:9:CYS:HB3	1:A:82:ILE:HB	1.94	0.50
1:F:251:HIS:CD2	1:F:340:ASN:HB3	2.47	0.50
1:F:261:ASN:HB3	3:F:507:HOH:O	2.11	0.50
1:F:284:LEU:HD21	1:F:358:LEU:HB2	1.93	0.50
1:B:14:ALA:CB	1:B:37:VAL:HG13	2.42	0.50
1:B:153:ASN:O	1:B:156:VAL:HG12	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:LEU:HD21	1:D:54:TRP:HH2	1.77	0.50
1:E:29:HIS:NE2	1:E:354:GLU:OE2	2.44	0.50
1:E:343:LEU:O	1:E:348:SER:OG	2.22	0.50
1:D:14:ALA:HB3	1:D:37:VAL:CG1	2.41	0.50
1:C:286:CYS:HB3	1:C:354:GLU:HB3	1.94	0.50
1:E:14:ALA:HB3	1:E:37:VAL:HG13	1.93	0.50
1:F:92:ALA:O	1:F:96:GLU:HG3	2.12	0.50
1:C:159:LEU:HD22	1:C:178:MSE:SE	2.61	0.49
1:B:302:ARG:NH2	1:B:308:ASP:OD1	2.45	0.49
1:E:90:ASP:O	1:E:91:ALA:HB3	2.11	0.49
1:D:321:ARG:HD2	3:D:563:HOH:O	2.12	0.49
1:E:189:TYR:HB3	1:E:190:PRO:HD2	1.93	0.49
1:A:88:ASP:O	1:A:92:ALA:HB2	2.12	0.49
1:D:180:THR:HG21	1:D:182:GLN:HG3	1.94	0.49
1:E:106:VAL:CG2	1:E:148:LEU:HD13	2.42	0.49
1:E:172:PRO:HG2	1:E:260:VAL:CG1	2.41	0.49
1:F:54:TRP:CZ2	1:F:60:MSE:HA	2.48	0.49
1:F:284:LEU:HD21	1:F:358:LEU:CB	2.42	0.49
1:C:88:ASP:O	1:C:92:ALA:HB2	2.12	0.49
1:B:90:ASP:O	1:B:91:ALA:HB3	2.13	0.49
1:E:258:ARG:NH1	1:E:259:PHE:O	2.46	0.49
1:F:97:MSE:HE2	1:F:101:LYS:CE	2.42	0.49
1:D:172:PRO:HG2	1:D:260:VAL:HG11	1.93	0.49
1:B:54:TRP:N	3:B:518:HOH:O	2.45	0.49
1:F:257:LEU:O	1:F:330:PHE:HB3	2.13	0.49
1:C:164:LYS:NZ	3:C:514:HOH:O	2.39	0.49
1:D:303:PRO:HB3	1:D:318:THR:CG2	2.43	0.49
1:A:266:THR:HG22	1:A:269:GLN:HG3	1.94	0.48
1:A:14:ALA:HB3	1:A:37:VAL:HG13	1.95	0.48
1:D:97:MSE:HE2	1:D:101:LYS:HE3	1.94	0.48
1:E:175:SER:HB2	1:E:258:ARG:HB3	1.94	0.48
1:A:218:LYS:NZ	3:A:521:HOH:O	2.46	0.48
1:D:16:GLY:O	1:D:20:THR:HG23	2.13	0.48
1:F:161:VAL:N	1:F:162:PRO:HD2	2.29	0.48
1:F:189:TYR:HB2	1:F:190:PRO:CD	2.38	0.48
1:D:189:TYR:HB2	1:D:190:PRO:CD	2.41	0.48
1:C:29:HIS:CE1	1:C:32:LEU:HD12	2.48	0.48
1:C:166:LEU:HD21	1:C:270:VAL:HG13	1.94	0.48
1:E:127:ASN:OD1	1:E:127:ASN:N	2.46	0.48
1:B:131:ILE:O	1:B:134:ILE:HG12	2.14	0.48
1:D:45:GLY:O	1:D:46:LYS:HG3	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:TRP:CE2	1:D:58:ALA:O	2.66	0.48
1:D:292:MSE:SE	3:D:580:HOH:O	2.81	0.48
1:B:288:SER:HB2	1:B:351:LEU:HD13	1.96	0.48
1:E:189:TYR:HB3	1:E:190:PRO:HD3	1.96	0.48
1:F:138:ARG:HG2	1:F:143:LEU:HD12	1.94	0.48
1:B:60:MSE:HE2	1:B:65:ALA:HB2	1.95	0.48
1:F:7:LYS:HE2	1:F:7:LYS:N	2.29	0.48
1:F:144:ASP:O	1:F:145:LYS:HB2	2.14	0.48
1:D:49:ARG:HA	1:D:60:MSE:SE	2.64	0.47
1:C:60:MSE:CE	1:C:65:ALA:HB2	2.44	0.47
1:C:189:TYR:CG	1:C:190:PRO:CD	2.95	0.47
1:B:326:ASP:OD1	1:B:326:ASP:O	2.32	0.47
1:F:270:VAL:HG21	1:F:332:ILE:CD1	2.44	0.47
1:B:16:GLY:O	1:B:20:THR:HG23	2.14	0.47
1:C:55:LYS:HD3	1:A:195:MSE:HB3	1.96	0.47
1:F:9:CYS:HB3	1:F:82:ILE:HB	1.96	0.47
1:A:27:SER:O	1:A:28:GLN:HB2	2.15	0.47
1:A:293:SER:N	3:A:515:HOH:O	2.33	0.47
1:B:134:ILE:N	1:B:135:PRO:HD2	2.30	0.47
1:E:97:MSE:HE3	1:E:100:LEU:HB3	1.97	0.47
1:D:180:THR:HG21	1:D:182:GLN:OE1	2.15	0.47
1:D:211:LYS:O	1:D:215:GLU:HG3	2.14	0.47
1:F:127:ASN:OD1	1:F:127:ASN:N	2.48	0.47
1:A:189:TYR:CG	1:A:190:PRO:CD	2.98	0.47
1:A:211:LYS:HG2	1:A:215:GLU:OE2	2.13	0.47
1:C:131:ILE:O	1:C:134:ILE:HG12	2.15	0.47
1:A:153:ASN:HA	2:A:401:SO4:O1	2.15	0.47
1:F:174:GLU:HB2	1:F:260:VAL:HG13	1.97	0.47
1:D:70:ARG:NH1	1:D:76:GLU:O	2.44	0.47
1:E:9:CYS:CB	1:E:82:ILE:HB	2.44	0.47
1:F:131:ILE:O	1:F:134:ILE:HG12	2.15	0.47
1:B:271:ARG:CD	3:B:511:HOH:O	2.63	0.46
1:C:90:ASP:O	1:C:91:ALA:HB3	2.14	0.46
1:E:300:VAL:O	1:E:321:ARG:HD3	2.15	0.46
1:D:8:ARG:CZ	1:D:79:ASP:O	2.64	0.46
1:A:54:TRP:CE3	1:A:60:MSE:HE2	2.50	0.46
1:F:207:GLY:O	1:F:211:LYS:HB2	2.16	0.46
1:D:45:GLY:O	1:D:46:LYS:CG	2.63	0.46
1:F:302:ARG:NH1	1:F:308:ASP:OD1	2.48	0.46
1:D:44:SER:CB	1:D:45:GLY:HA2	2.44	0.46
1:C:275:ARG:HG2	1:C:292:MSE:HE1	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:VAL:HG22	1:B:53:ARG:N	2.29	0.46
1:E:24:LEU:HD21	1:E:54:TRP:CZ2	2.50	0.46
1:D:50:ASP:N	3:D:505:HOH:O	2.26	0.46
1:B:189:TYR:N	1:B:190:PRO:HD2	2.30	0.46
1:F:256:SER:HB3	1:F:330:PHE:CG	2.51	0.46
1:C:39:ALA:HB3	1:C:69:VAL:HG11	1.98	0.46
1:C:165:ALA:HB2	1:C:277:TYR:CD1	2.51	0.46
1:E:60:MSE:CE	1:E:65:ALA:HB2	2.46	0.46
1:A:165:ALA:HB2	1:A:277:TYR:CD1	2.51	0.46
1:C:24:LEU:HD11	1:C:54:TRP:CH2	2.50	0.46
1:C:60:MSE:HE3	1:C:64:VAL:HG13	1.98	0.46
1:F:67:LEU:N	3:F:501:HOH:O	2.49	0.45
1:E:266:THR:HG22	1:E:269:GLN:CG	2.46	0.45
1:A:48:TYR:CZ	1:A:52:VAL:HG11	2.51	0.45
1:D:60:MSE:HE1	1:D:65:ALA:HA	1.98	0.45
1:C:45:GLY:CA	3:C:505:HOH:O	2.60	0.45
1:A:189:TYR:HB3	1:A:190:PRO:HD2	1.97	0.45
1:B:14:ALA:HB3	1:B:37:VAL:HG13	1.98	0.45
1:E:55:LYS:HA	1:E:55:LYS:HD3	1.81	0.45
1:F:8:ARG:O	1:F:81:ASP:N	2.42	0.45
1:E:234:LYS:C	3:E:530:HOH:O	2.54	0.45
1:A:111:LYS:HA	1:A:114:ARG:HG3	1.99	0.45
1:D:23:ILE:HD13	1:D:64:VAL:HG21	1.98	0.45
1:D:90:ASP:O	1:D:91:ALA:CB	2.64	0.45
1:E:266:THR:HG22	1:E:269:GLN:HG3	1.99	0.45
1:F:302:ARG:HB3	1:F:303:PRO:HA	1.99	0.45
1:F:329:VAL:CG1	1:F:330:PHE:CD1	2.94	0.45
1:D:54:TRP:CZ3	1:D:56:GLN:OE1	2.70	0.45
1:D:54:TRP:CZ2	1:D:56:GLN:CB	3.00	0.44
1:D:114:ARG:HD3	1:D:151:ASN:O	2.17	0.44
1:A:14:ALA:HB3	1:A:37:VAL:CG1	2.48	0.44
1:D:107:PHE:CD1	1:D:107:PHE:N	2.85	0.44
1:D:258:ARG:NE	3:D:511:HOH:O	2.44	0.44
1:A:134:ILE:HD11	1:A:147:MSE:CE	2.46	0.44
1:E:77:PHE:O	1:E:79:ASP:N	2.51	0.44
1:F:165:ALA:HA	1:F:277:TYR:CE2	2.53	0.44
1:E:14:ALA:HA	1:E:19:GLY:HA3	2.00	0.44
1:F:29:HIS:NE2	1:F:354:GLU:OE2	2.50	0.44
1:D:29:HIS:HA	1:D:30:PRO:HD3	1.90	0.44
1:D:121:LEU:HD11	1:D:152:SER:HA	2.00	0.44
1:E:97:MSE:HE1	1:E:100:LEU:HD23	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:189:TYR:CB	1:E:190:PRO:HD3	2.46	0.44
1:B:189:TYR:N	1:B:190:PRO:CD	2.80	0.44
1:F:144:ASP:O	1:F:145:LYS:CB	2.66	0.44
1:B:284:LEU:HD22	3:B:515:HOH:O	2.17	0.43
1:D:178:MSE:HG3	1:D:240:VAL:HG23	2.00	0.43
1:D:245:VAL:HG21	1:C:201:ILE:HD11	2.01	0.43
1:C:6:LYS:HE2	1:C:29:HIS:O	2.19	0.43
1:B:9:CYS:HB3	1:B:82:ILE:HB	2.00	0.43
1:B:83:ILE:O	1:B:106:VAL:HA	2.18	0.43
1:B:315:TYR:OH	3:B:504:HOH:O	2.16	0.43
1:F:106:VAL:HG22	1:F:148:LEU:HD13	2.00	0.43
1:F:152:SER:N	3:F:504:HOH:O	2.24	0.43
1:F:284:LEU:CD2	1:F:358:LEU:HD12	2.48	0.43
1:C:153:ASN:OD1	1:C:155:ALA:N	2.51	0.43
1:D:266:THR:HG22	1:D:269:GLN:HG3	2.00	0.43
1:C:23:ILE:HD13	1:C:64:VAL:HG21	2.00	0.43
1:C:73:ASP:OD1	1:C:75:ALA:N	2.52	0.43
1:E:189:TYR:CG	1:E:190:PRO:CD	3.01	0.43
1:D:54:TRP:CH2	1:D:56:GLN:CB	2.99	0.43
1:D:111:LYS:HA	1:D:114:ARG:HG3	2.01	0.43
1:A:337:LEU:HG	1:A:338:SER:N	2.32	0.43
1:F:300:VAL:HG22	1:F:300:VAL:O	2.19	0.43
1:B:159:LEU:HD22	1:B:178:MSE:SE	2.69	0.43
1:F:165:ALA:CA	1:F:277:TYR:CD2	3.00	0.43
1:F:211:LYS:HB2	1:F:211:LYS:HE3	1.85	0.43
1:A:7:LYS:HE2	1:A:7:LYS:N	2.33	0.42
1:A:116:ASP:HB3	1:A:119:VAL:CG2	2.49	0.42
1:F:171:GLY:HA3	1:F:261:ASN:HB2	2.01	0.42
1:C:296:VAL:O	1:C:297:MSE:HE2	2.20	0.42
1:B:97:MSE:HE2	1:B:101:LYS:HG2	2.00	0.42
1:E:107:PHE:CE2	1:E:353:ALA:HA	2.54	0.42
1:D:60:MSE:HE2	1:D:65:ALA:CA	2.50	0.42
1:D:159:LEU:HD22	1:D:178:MSE:SE	2.69	0.42
1:A:70:ARG:HD2	1:A:76:GLU:OE1	2.18	0.42
1:B:189:TYR:H	1:B:190:PRO:HD2	1.84	0.42
1:F:174:GLU:HB2	1:F:260:VAL:HG12	2.00	0.42
1:C:27:SER:O	1:C:28:GLN:HB2	2.19	0.42
1:C:300:VAL:HG22	1:C:300:VAL:O	2.19	0.42
1:B:351:LEU:HD12	1:B:351:LEU:HA	1.90	0.42
1:E:48:TYR:CD1	1:E:64:VAL:HG22	2.55	0.42
1:E:97:MSE:CE	1:E:100:LEU:HD23	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:256:SER:HB3	1:E:330:PHE:CG	2.55	0.42
1:F:181:MSE:HE3	1:F:252:THR:CG2	2.49	0.42
1:F:253:VAL:O	1:F:335:VAL:HA	2.19	0.42
1:D:131:ILE:O	1:D:134:ILE:HG12	2.19	0.42
1:D:172:PRO:HG2	1:D:260:VAL:CG1	2.49	0.42
1:B:342:VAL:HG12	1:B:343:LEU:N	2.34	0.42
1:E:134:ILE:HD13	1:E:134:ILE:HA	1.87	0.42
1:A:60:MSE:SE	1:A:65:ALA:CB	3.17	0.42
1:F:62:ALA:O	1:F:63:LYS:C	2.58	0.42
1:F:329:VAL:CG1	1:F:330:PHE:CE1	3.03	0.42
1:C:17:ALA:C	3:C:504:HOH:O	2.51	0.42
1:C:29:HIS:NE2	1:C:354:GLU:OE2	2.48	0.42
1:C:44:SER:O	1:C:45:GLY:C	2.57	0.42
1:F:161:VAL:N	1:F:162:PRO:CD	2.82	0.42
1:E:262:ARG:HA	1:E:262:ARG:HD2	1.92	0.41
1:A:262:ARG:CZ	3:A:509:HOH:O	2.68	0.41
1:E:111:LYS:HA	1:E:114:ARG:HG3	2.01	0.41
1:A:14:ALA:HA	1:A:19:GLY:HA3	2.02	0.41
1:F:259:PHE:HB3	3:F:510:HOH:O	2.20	0.41
1:A:38:GLY:HA2	1:A:70:ARG:O	2.21	0.41
1:D:211:LYS:HG2	1:D:215:GLU:OE2	2.20	0.41
1:C:302:ARG:NH1	1:C:308:ASP:CG	2.73	0.41
1:C:309:ARG:HG3	1:C:310:GLU:HG2	2.02	0.41
1:D:319:VAL:HG13	1:D:334:PHE:CD1	2.55	0.41
1:C:116:ASP:HA	1:C:117:PRO:HD3	1.96	0.41
1:C:178:MSE:HE3	1:C:253:VAL:HG13	2.02	0.41
1:E:48:TYR:OH	1:E:54:TRP:CZ3	2.70	0.41
1:B:300:VAL:O	1:B:300:VAL:HG22	2.21	0.41
1:F:174:GLU:CA	1:F:260:VAL:HG13	2.51	0.41
1:D:14:ALA:O	1:D:48:TYR:OH	2.27	0.41
1:D:43:SER:HB2	1:D:69:VAL:HG13	2.02	0.41
1:B:245:VAL:HG21	1:A:201:ILE:HD11	2.03	0.41
1:D:321:ARG:NH2	1:C:209:GLU:OE1	2.52	0.41
1:B:55:LYS:CE	3:B:503:HOH:O	2.63	0.41
1:B:107:PHE:CZ	1:B:353:ALA:HA	2.56	0.41
1:B:200:ASN:O	1:B:246:PRO:HG3	2.20	0.41
1:E:38:GLY:HA2	1:E:70:ARG:O	2.21	0.41
1:E:279:PRO:HG3	1:E:293:SER:OG	2.21	0.41
1:F:97:MSE:CE	1:F:100:LEU:HD23	2.51	0.41
1:E:23:ILE:HG23	1:E:34:LEU:CD2	2.51	0.41
1:A:44:SER:HA	1:A:69:VAL:CG1	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:52:VAL:HG23	1:F:53:ARG:N	2.35	0.41
1:F:177:SER:HB2	1:F:330:PHE:CZ	2.56	0.41
1:F:342:VAL:HG12	1:F:343:LEU:N	2.36	0.41
1:A:68:THR:O	1:A:68:THR:HG23	2.21	0.40
1:D:223:LEU:HD13	1:D:230:PHE:CE1	2.57	0.40
1:B:127:ASN:OD1	1:B:127:ASN:N	2.54	0.40
1:E:128:ALA:HB2	1:E:281:VAL:HG13	2.02	0.40
1:A:131:ILE:HD11	1:A:356:ALA:HB2	2.03	0.40
1:F:134:ILE:N	1:F:135:PRO:HD2	2.35	0.40
1:F:22:PHE:O	1:F:26:LEU:N	2.50	0.40
1:F:29:HIS:HA	1:F:30:PRO:HD3	1.89	0.40
1:E:9:CYS:HA	1:E:80:CYS:HB2	2.03	0.40
1:F:284:LEU:HD23	1:F:284:LEU:C	2.42	0.40
1:D:38:GLY:HA2	1:D:70:ARG:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:323:ARG:HH21	3:E:502:HOH:O[4_465]	1.53	0.07

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	350/379 (92%)	327 (93%)	20 (6%)	3 (1%)	17	35
1	B	339/379 (89%)	323 (95%)	14 (4%)	2 (1%)	25	47
1	C	351/379 (93%)	334 (95%)	14 (4%)	3 (1%)	17	35
1	D	352/379 (93%)	333 (95%)	15 (4%)	4 (1%)	14	30
1	E	341/379 (90%)	325 (95%)	13 (4%)	3 (1%)	17	35

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	338/379 (89%)	310 (92%)	23 (7%)	5 (2%)	10	21
All	All	2071/2274 (91%)	1952 (94%)	99 (5%)	20 (1%)	15	32

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	189	TYR
1	C	189	TYR
1	E	189	TYR
1	A	189	TYR
1	F	189	TYR
1	C	345	ALA
1	E	345	ALA
1	A	345	ALA
1	F	63	LYS
1	D	345	ALA
1	B	345	ALA
1	E	78	SER
1	F	72	CYS
1	A	78	SER
1	D	58	ALA
1	D	342	VAL
1	C	342	VAL
1	B	342	VAL
1	F	156	VAL
1	F	342	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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	292/303 (96%)	290 (99%)	2 (1%)	84	94
1	B	288/303 (95%)	282 (98%)	6 (2%)	53	77
1	C	293/303 (97%)	284 (97%)	9 (3%)	40	66

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	294/303 (97%)	290 (99%)	4 (1%)	67	85
1	E	287/303 (95%)	283 (99%)	4 (1%)	67	85
1	F	286/303 (94%)	280 (98%)	6 (2%)	53	77
All	All	1740/1818 (96%)	1709 (98%)	31 (2%)	59	80

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	70	ARG
1	D	106	VAL
1	D	246	PRO
1	D	260	VAL
1	C	22	PHE
1	C	70	ARG
1	C	81	ASP
1	C	88	ASP
1	C	169	LYS
1	C	175	SER
1	C	189	TYR
1	C	286	CYS
1	C	324	GLU
1	B	22	PHE
1	B	47	LYS
1	B	106	VAL
1	B	151	ASN
1	B	213	SER
1	B	257	LEU
1	E	22	PHE
1	E	80	CYS
1	E	114	ARG
1	E	143	LEU
1	A	9	CYS
1	A	153	ASN
1	F	71	CYS
1	F	76	GLU
1	F	78	SER
1	F	106	VAL
1	F	198	PHE
1	F	239	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such

sidechains are listed below:

Mol	Chain	Res	Type
1	D	56	GLN
1	B	109	ASN
1	B	151	ASN
1	F	109	ASN
1	F	339	HIS

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)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	F	401	-	4,4,4	0.16	0	6,6,6	0.19	0
2	SO4	D	401	-	4,4,4	0.21	0	6,6,6	0.36	0
2	SO4	C	401	-	4,4,4	0.16	0	6,6,6	0.31	0
2	SO4	A	401	-	4,4,4	0.13	0	6,6,6	0.22	0
2	SO4	E	401	-	4,4,4	0.14	0	6,6,6	0.25	0
2	SO4	B	401	-	4,4,4	0.22	0	6,6,6	0.24	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	401	SO4	2	0
2	A	401	SO4	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, 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	345/379 (91%)	0.15	16 (4%)	32	26	25, 45, 86, 115	0
1	B	340/379 (89%)	0.16	16 (4%)	31	25	25, 48, 87, 117	1 (0%)
1	C	346/379 (91%)	0.17	21 (6%)	21	16	24, 48, 90, 121	0
1	D	347/379 (91%)	0.15	17 (4%)	29	23	24, 45, 93, 117	0
1	E	339/379 (89%)	0.23	19 (5%)	24	19	26, 53, 91, 123	0
1	F	337/379 (88%)	0.46	26 (7%)	13	10	36, 62, 92, 118	0
All	All	2054/2274 (90%)	0.22	115 (5%)	24	19	24, 52, 91, 123	1 (0%)

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	189	TYR	7.4
1	D	189	TYR	6.7
1	D	50	ASP	5.8
1	A	53	ARG	5.8
1	F	67	LEU	5.6
1	B	189	TYR	5.5
1	C	67	LEU	5.5
1	A	189	TYR	5.3
1	C	189	TYR	5.3
1	D	41	ASP	5.3
1	E	48	TYR	5.2
1	F	68	THR	4.6
1	D	49	ARG	4.6
1	A	190	PRO	4.4
1	B	41	ASP	4.3
1	B	55	LYS	4.2
1	F	235	PRO	4.0
1	E	53	ARG	4.0
1	E	349	SER	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	285	GLY	3.9
1	D	42	ARG	3.8
1	F	258	ARG	3.7
1	A	50	ASP	3.7
1	C	50	ASP	3.7
1	D	284	LEU	3.6
1	C	47	LYS	3.5
1	F	51	ALA	3.5
1	C	190	PRO	3.4
1	C	28	GLN	3.4
1	A	49	ARG	3.4
1	B	66	ASP	3.4
1	F	55	LYS	3.4
1	E	189	TYR	3.3
1	C	66	ASP	3.2
1	C	349	SER	3.2
1	F	40	SER	3.2
1	D	91	ALA	3.2
1	F	84	PHE	3.1
1	E	55	LYS	3.1
1	D	48	TYR	3.1
1	D	66	ASP	3.1
1	A	349	SER	2.9
1	B	53	ARG	2.9
1	F	90	ASP	2.9
1	A	107	PHE	2.9
1	C	46	LYS	2.9
1	D	57	SER	2.9
1	E	66	ASP	2.9
1	F	28	GLN	2.8
1	A	84	PHE	2.8
1	E	57	SER	2.8
1	C	8	ARG	2.8
1	F	91	ALA	2.8
1	F	331	ASP	2.8
1	D	55	LYS	2.7
1	C	84	PHE	2.7
1	E	105	ALA	2.7
1	C	49	ARG	2.7
1	B	326	ASP	2.7
1	A	106	VAL	2.6
1	C	71	CYS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	69	VAL	2.6
1	B	190	PRO	2.6
1	F	232	ASP	2.5
1	D	58	ALA	2.5
1	F	284	LEU	2.5
1	E	84	PHE	2.5
1	E	190	PRO	2.5
1	F	190	PRO	2.5
1	D	54	TRP	2.5
1	F	145	LYS	2.5
1	B	65	ALA	2.5
1	F	256	SER	2.5
1	E	352	ASN	2.5
1	F	326	ASP	2.4
1	A	65	ALA	2.4
1	B	40	SER	2.4
1	E	91	ALA	2.4
1	D	6	LYS	2.4
1	D	190	PRO	2.4
1	F	191	GLY	2.4
1	F	286	CYS	2.4
1	D	45	GLY	2.4
1	F	53	ARG	2.4
1	E	68	THR	2.3
1	F	107	PHE	2.3
1	B	46	LYS	2.3
1	B	85	SER	2.3
1	C	55	LYS	2.3
1	A	46	LYS	2.3
1	E	28	GLN	2.3
1	A	40	SER	2.3
1	B	84	PHE	2.3
1	A	83	ILE	2.3
1	C	285	GLY	2.2
1	D	78	SER	2.2
1	A	47	LYS	2.2
1	A	280	GLU	2.2
1	B	91	ALA	2.2
1	B	349	SER	2.2
1	C	53	ARG	2.2
1	C	108	SER	2.1
1	E	144	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	106	VAL	2.1
1	E	348	SER	2.1
1	E	160	VAL	2.1
1	B	235	PRO	2.1
1	C	68	THR	2.1
1	F	157	VAL	2.1
1	F	254	CYS	2.1
1	F	255	ALA	2.1
1	E	282	GLN	2.0
1	C	40	SER	2.0
1	C	188	GLY	2.0
1	C	106	VAL	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	E	401	5/5	0.92	0.13	53,60,69,70	0
2	SO4	C	401	5/5	0.93	0.12	43,59,64,68	0
2	SO4	A	401	5/5	0.95	0.12	52,56,61,62	0
2	SO4	F	401	5/5	0.96	0.14	64,67,74,84	0
2	SO4	B	401	5/5	0.97	0.09	47,53,59,64	0
2	SO4	D	401	5/5	0.97	0.13	46,49,53,65	0

6.5 Other polymers (i)

There are no such residues in this entry.