Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:07 PM GMT

PDB ID	:	4BHT
Title	:	Structural Determinants of Cofactor Specificity and Domain Flexibility in Bacterial Glutamate Dehydrogenases
Authors	:	Oliveira, T.; Sharkey, M.; Engel, P.; Khan, A.
Deposited on	:	2013-04-06
Resolution	:	2.50 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:

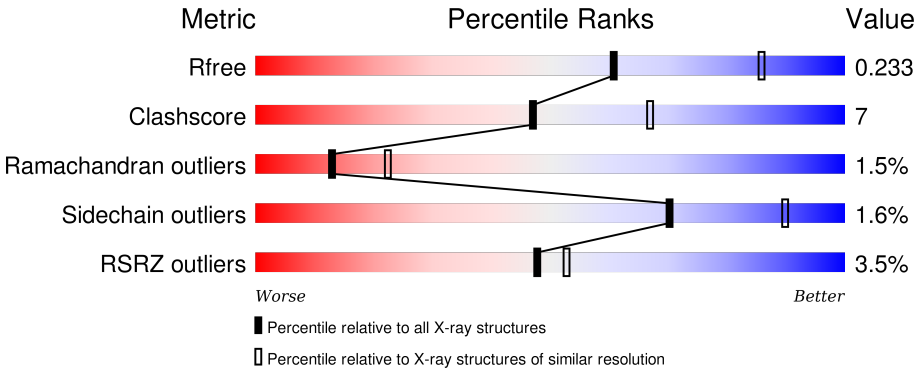
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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.



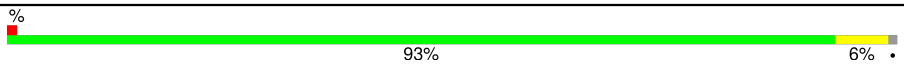
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	447	90% 9%
1	B	447	91% 8%
1	C	447	90% 9%
1	D	447	17% 72% 19% 5%
1	E	447	2% 88% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	447	

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	GOL	A	1450	-	-	-	X
2	GOL	A	1451	-	-	-	X
2	GOL	A	1452	-	-	-	X
2	GOL	A	1453	-	-	-	X
2	GOL	A	1454	-	-	X	X
2	GOL	D	1448	-	-	-	X
2	GOL	D	1449	-	-	-	X
2	GOL	E	1448	-	-	-	X
2	GOL	E	1449	-	-	-	X
2	GOL	E	1450	-	-	-	X
2	GOL	F	1448	-	-	-	X
3	EPE	C	1451	-	-	X	X
4	PG4	E	1451	-	-	X	X

2 Entry composition

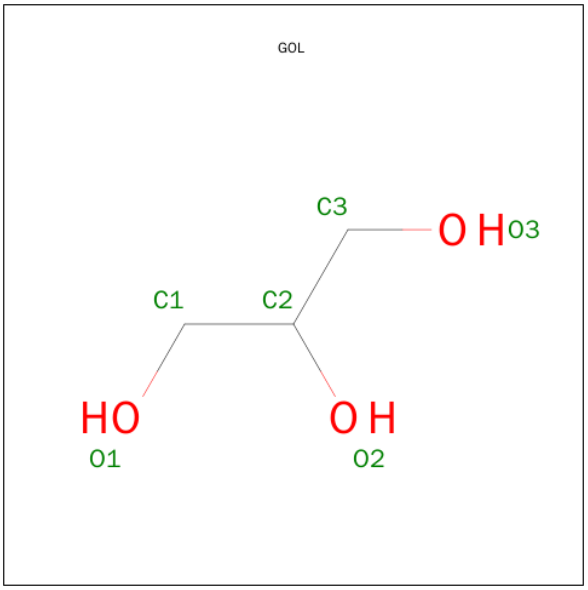
There are 5 unique types of molecules in this entry. The entry contains 41397 atoms, of which 20253 are hydrogens and 0 are deuteriums.

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 NADP-SPECIFIC GLUTAMATE DEHYDROGENASE.

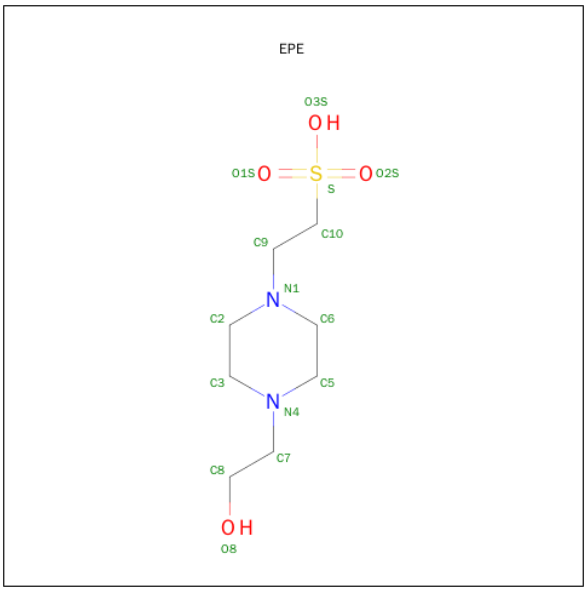
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	442	Total	C	H	N	O	S	0	4	0
			6752	2136	3362	597	636	21			
1	B	442	Total	C	H	N	O	S	0	1	0
			6719	2125	3346	595	632	21			
1	C	442	Total	C	H	N	O	S	0	1	0
			6717	2124	3345	595	632	21			
1	D	439	Total	C	H	N	O	S	0	1	0
			6684	2113	3330	594	626	21			
1	E	442	Total	C	H	N	O	S	0	0	0
			6706	2121	3339	594	631	21			
1	F	442	Total	C	H	N	O	S	0	2	0
			6732	2129	3353	597	632	21			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



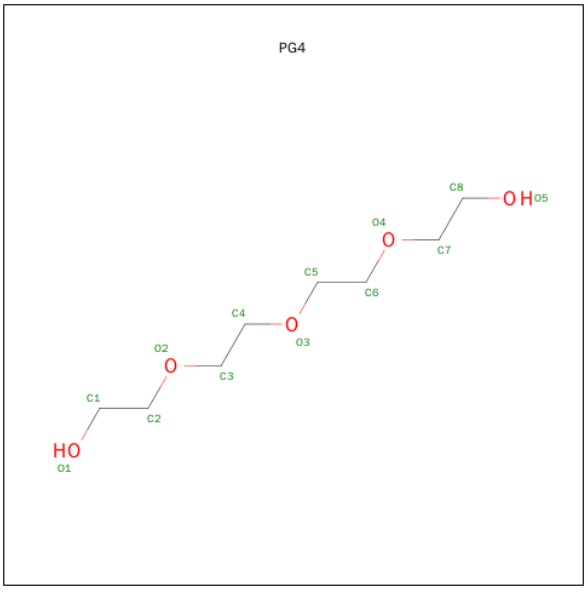
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C H O 14 3 8 3	0	0
2	A	1	Total C H O 14 3 8 3	0	0
2	A	1	Total C H O 14 3 8 3	0	0
2	A	1	Total C H O 14 3 8 3	0	0
2	A	1	Total C H O 14 3 8 3	0	0
2	A	1	Total C H O 14 3 8 3	0	0
2	A	1	Total C H O 14 3 8 3	0	0
2	C	1	Total C H O 14 3 8 3	0	0
2	C	1	Total C H O 14 3 8 3	0	0
2	C	1	Total C H O 14 3 8 3	0	0
2	D	1	Total C H O 14 3 8 3	0	0
2	D	1	Total C H O 14 3 8 3	0	0
2	D	1	Total C H O 14 3 8 3	0	0
2	E	1	Total C H O 14 3 8 3	0	0
2	E	1	Total C H O 14 3 8 3	0	0
2	E	1	Total C H O 14 3 8 3	0	0
2	F	1	Total C H O 14 3 8 3	0	0
2	F	1	Total C H O 13 3 7 3	0	0

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	C	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	1	Total	C	H	O	0	0
			31	8	18	5		

- Molecule 5 is water.

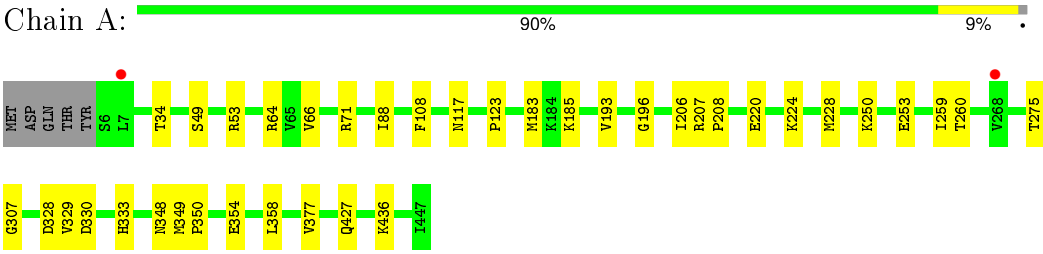
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	160	Total O 160 160	0	0
5	B	151	Total O 151 151	0	0
5	C	160	Total O 160 160	0	0
5	D	103	Total O 103 103	0	0
5	E	93	Total O 93 93	0	0
5	F	106	Total O 106 106	0	0

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.

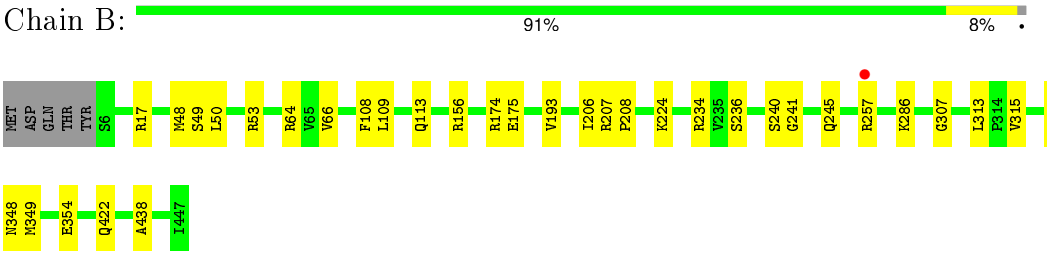
- Molecule 1: NADP-SPECIFIC GLUTAMATE DEHYDROGENASE

Chain A:



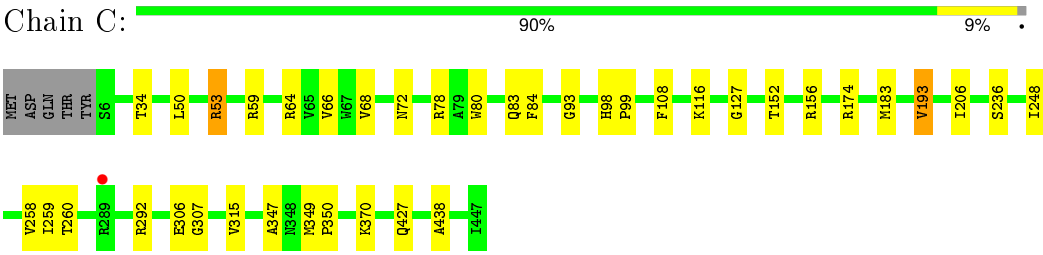
- Molecule 1: NADP-SPECIFIC GLUTAMATE DEHYDROGENASE

Chain B:



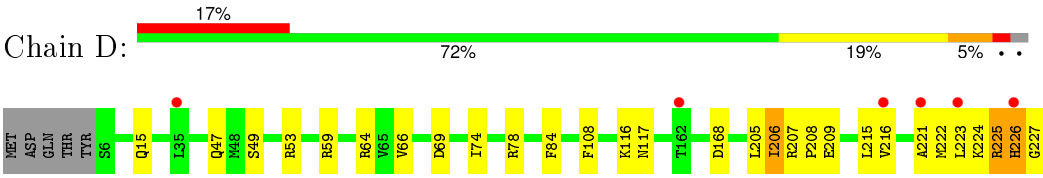
- Molecule 1: NADP-SPECIFIC GLUTAMATE DEHYDROGENASE

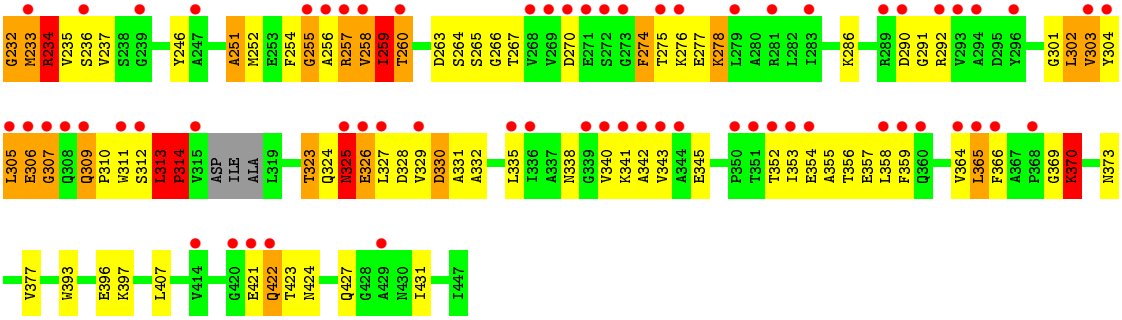
Chain C:



- Molecule 1: NADP-SPECIFIC GLUTAMATE DEHYDROGENASE

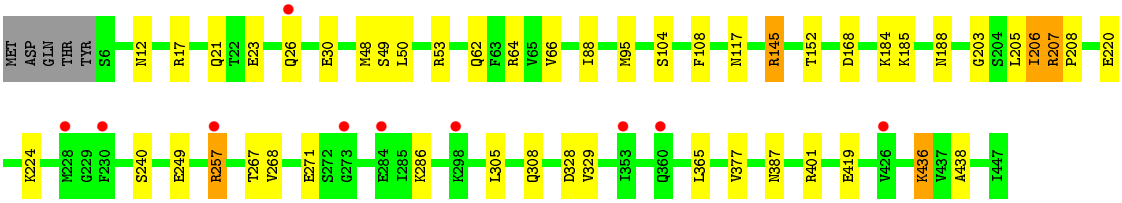
Chain D:





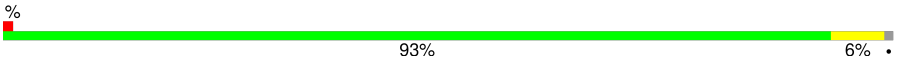
• Molecule 1: NADP-SPECIFIC GLUTAMATE DEHYDROGENASE

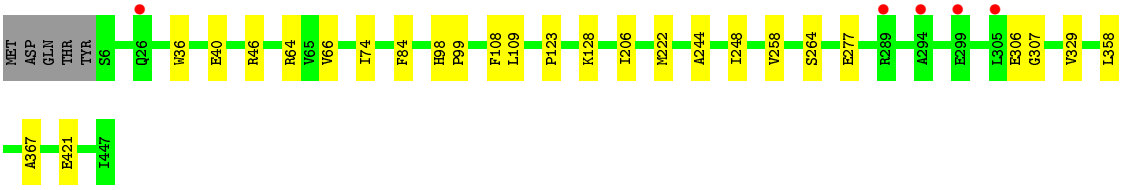
Chain E:



• Molecule 1: NADP-SPECIFIC GLUTAMATE DEHYDROGENASE

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	100.97Å 152.86Å 169.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.90 – 2.50 46.90 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.90-2.50) 99.9 (46.90-2.50)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.22 (at 2.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, R_{free}	0.159 , 0.227 0.174 , 0.233	Depositor DCC
R_{free} test set	4557 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	34.9	Xtriage
Anisotropy	0.662	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 47.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 91084 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	41397	wwPDB-VP
Average B, all atoms (Å^2)	44.0	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 24.39 % 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 3.8687e-03.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, 0.375 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: GOL, PG4, EPE

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	0.73	0/3468	0.79	2/4680 (0.0%)
1	B	0.71	0/3441	0.79	1/4643 (0.0%)
1	C	0.74	1/3440 (0.0%)	0.80	2/4642 (0.0%)
1	D	0.73	0/3421	0.85	8/4613 (0.2%)
1	E	0.70	0/3432	0.75	3/4631 (0.1%)
1	F	0.70	0/3451	0.78	0/4657
All	All	0.72	1/20653 (0.0%)	0.79	16/27866 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	4
1	F	0	1
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	193	VAL	CB-CG2	-6.73	1.38	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	326	GLU	C-N-CA	8.10	141.95	121.70
1	A	71	ARG	NE-CZ-NH1	7.36	123.98	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	69	ASP	CB-CG-OD1	6.74	124.37	118.30
1	B	193	VAL	CG1-CB-CG2	6.64	121.52	110.90
1	D	309	GLN	C-N-CD	6.33	141.68	128.40
1	D	59	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	D	259	ILE	CG1-CB-CG2	-5.94	98.34	111.40
1	D	313	LEU	C-N-CD	5.73	140.44	128.40
1	D	314	PRO	CA-N-CD	-5.60	103.66	111.50
1	D	69	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	C	53	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	C	174	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	E	17	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	E	145	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	E	257	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	71	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	306	GLU	Peptide
1	C	306	GLU	Peptide
1	D	226	HIS	Peptide
1	D	230	PHE	Peptide
1	D	257	ARG	Peptide
1	D	312	SER	Peptide
1	F	306	GLU	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	3390	3362	3351	31	0
1	B	3373	3346	3336	32	0
1	C	3372	3345	3334	29	0
1	D	3354	3330	3320	150	0
1	E	3367	3339	3328	42	1
1	F	3379	3353	3341	19	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	42	56	56	7	0
2	C	18	24	24	5	0
2	D	18	24	24	0	0
2	E	18	24	24	0	0
2	F	12	15	16	1	0
3	C	15	17	18	8	0
4	E	13	18	18	11	0
5	A	160	0	0	4	0
5	B	151	0	0	3	0
5	C	160	0	0	4	1
5	D	103	0	0	7	0
5	E	93	0	0	10	1
5	F	106	0	0	2	0
All	All	21144	20253	20190	302	2

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 7.

All (302) 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:D:230:PHE:CD1	1:D:256:ALA:HB2	1.72	1.25
1:B:234:ARG:HD2	1:B:257:ARG:NH2	1.54	1.21
1:B:234:ARG:CG	1:B:257:ARG:HH21	1.56	1.19
1:B:234:ARG:CD	1:B:257:ARG:HH21	1.55	1.18
1:D:230:PHE:CE1	1:D:256:ALA:HB2	1.80	1.15
1:D:230:PHE:HA	1:D:232:GLY:H	1.04	1.12
1:B:234:ARG:CG	1:B:257:ARG:NH2	2.24	0.98
1:D:309:GLN:HE22	1:D:326:GLU:HG2	1.24	0.97
1:B:234:ARG:CD	1:B:257:ARG:NH2	2.19	0.97
1:D:233:MET:SD	1:D:234:ARG:NH1	2.38	0.96
1:D:313:LEU:HD13	1:D:314:PRO:HD3	1.51	0.92
1:D:236:SER:CA	1:D:260:THR:OG1	2.17	0.92
1:D:258:VAL:HG21	1:D:274:PHE:H	1.34	0.91
1:D:309:GLN:NE2	1:D:326:GLU:HG2	1.85	0.91
1:A:328[A]:ASP:OD1	5:A:2133:HOH:O	1.88	0.90
1:D:313:LEU:HD13	1:D:314:PRO:CD	2.02	0.89
1:A:220:GLU:O	1:A:224:LYS:HG2	1.71	0.89
1:D:236:SER:HA	1:D:260:THR:OG1	1.73	0.88
1:D:230:PHE:HA	1:D:232:GLY:N	1.89	0.88
1:B:234:ARG:HG2	1:B:257:ARG:HH21	1.39	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:ARG:HA	1:D:258:VAL:HG23	1.58	0.85
1:C:183:MET:HG2	1:C:193:VAL:HG21	1.58	0.84
1:D:302:LEU:HD23	1:D:303:VAL:HG23	1.58	0.83
1:D:236:SER:HA	1:D:260:THR:HG1	1.43	0.83
1:D:223:LEU:HD23	1:D:228:MET:HB3	1.61	0.83
1:D:304:TYR:O	1:D:306:GLU:N	2.12	0.82
1:D:313:LEU:HD22	1:D:314:PRO:HA	1.62	0.81
1:A:348[A]:ASN:ND2	5:A:2059:HOH:O	2.13	0.81
1:B:234:ARG:HD2	1:B:257:ARG:HH22	1.44	0.81
1:D:323:THR:HB	1:D:326:GLU:OE1	1.80	0.81
1:D:258:VAL:HG13	1:D:274:PHE:HD2	1.44	0.81
1:E:387:ASN:HD22	4:E:1451:PG4:H61	1.48	0.77
1:D:309:GLN:HE22	1:D:326:GLU:CG	1.98	0.77
1:D:258:VAL:HG12	1:D:259:ILE:N	2.00	0.77
1:D:305:LEU:O	1:D:307:GLY:N	2.17	0.76
1:D:370:LYS:N	5:D:2088:HOH:O	2.10	0.76
2:A:1451:GOL:O1	5:A:2157:HOH:O	2.06	0.74
1:C:68:VAL:HB	3:C:1451:EPE:H81	1.70	0.74
1:C:116:LYS:HD2	1:C:370:LYS:HA	1.70	0.74
1:D:258:VAL:O	1:D:259:ILE:CD1	2.37	0.73
1:D:258:VAL:CG1	1:D:259:ILE:N	2.51	0.72
1:D:230:PHE:CD1	1:D:256:ALA:CB	2.64	0.72
1:D:236:SER:HB2	1:D:260:THR:OG1	1.89	0.72
1:D:236:SER:CB	1:D:260:THR:OG1	2.36	0.72
5:D:2099:HOH:O	1:E:401:ARG:NH2	2.21	0.71
1:D:259:ILE:O	5:D:2080:HOH:O	2.08	0.70
1:F:264:SER:O	5:F:2081:HOH:O	2.09	0.70
1:D:258:VAL:CG1	1:D:259:ILE:H	2.05	0.69
1:D:236:SER:CA	1:D:260:THR:HG1	2.01	0.69
1:D:251:ALA:O	1:D:254:PHE:HB2	1.92	0.68
3:C:1451:EPE:C7	1:E:145:ARG:HD3	2.23	0.68
1:D:235:VAL:HG13	1:D:258:VAL:H	1.59	0.68
1:D:233:MET:SD	1:D:234:ARG:CZ	2.82	0.68
1:E:419:GLU:OE2	5:E:2089:HOH:O	2.12	0.68
1:D:258:VAL:O	1:D:259:ILE:HD13	1.95	0.67
1:D:258:VAL:HG21	1:D:274:PHE:N	2.09	0.66
1:D:260:THR:HG21	1:D:310:PRO:CB	2.27	0.65
3:C:1451:EPE:H71	1:E:145:ARG:HD3	1.76	0.65
1:D:228:MET:HE2	1:D:341:LYS:HB3	1.77	0.65
1:D:116:LYS:NZ	1:D:373:ASN:OD1	2.23	0.64
1:D:302:LEU:HD23	1:D:303:VAL:H	1.62	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:249:GLU:OE1	5:E:2076:HOH:O	2.15	0.64
1:D:236:SER:HB3	1:D:313:LEU:HD21	1.80	0.64
1:D:258:VAL:C	1:D:259:ILE:HD12	2.18	0.63
1:B:64:ARG:HD3	1:B:66:VAL:CG2	2.28	0.63
1:E:387:ASN:HA	4:E:1451:PG4:H62	1.80	0.63
1:D:263:ASP:O	1:D:265:SER:N	2.32	0.63
1:D:258:VAL:HG22	1:D:274:PHE:HB2	1.81	0.62
1:D:230:PHE:CE1	1:D:256:ALA:CB	2.71	0.62
1:A:277:GLU:H	1:A:277:GLU:CD	2.02	0.62
1:D:275:THR:HB	1:D:277:GLU:O	1.98	0.62
1:D:313:LEU:HD13	1:D:314:PRO:N	2.14	0.61
1:D:266:GLY:HA3	1:D:304:TYR:CE1	2.35	0.61
1:D:258:VAL:O	1:D:259:ILE:CB	2.48	0.61
3:C:1451:EPE:H71	1:E:145:ARG:CZ	2.30	0.61
1:A:275:THR:HB	1:A:277:GLU:OE1	2.00	0.61
2:A:1454:GOL:H32	1:E:188:ASN:HB3	1.83	0.61
1:E:64:ARG:HD3	1:E:66:VAL:CG2	2.30	0.60
1:B:234:ARG:HG3	1:B:257:ARG:NH2	2.16	0.60
1:D:260:THR:HG21	1:D:310:PRO:HB2	1.82	0.60
1:D:237:VAL:N	1:D:260:THR:OG1	2.34	0.60
1:F:36:TRP:O	1:F:40:GLU:HG2	2.02	0.60
1:F:222:MET:HE3	1:F:367:ALA:HB2	1.83	0.60
1:D:225[B]:ARG:HH11	1:D:225[B]:ARG:CB	2.15	0.59
1:D:258:VAL:C	1:D:259:ILE:CD1	2.71	0.59
1:D:258:VAL:CG2	1:D:274:PHE:H	2.12	0.59
1:A:64:ARG:HD3	1:A:66:VAL:CG2	2.33	0.59
4:E:1451:PG4:H31	5:E:2059:HOH:O	2.03	0.59
1:E:387:ASN:ND2	4:E:1451:PG4:H61	2.15	0.59
1:B:234:ARG:HH11	1:B:257:ARG:NH2	2.00	0.59
1:D:310:PRO:O	1:D:313:LEU:HD12	2.02	0.59
1:F:64:ARG:HD3	1:F:66:VAL:CG2	2.33	0.58
1:C:250:LYS:HD3	1:C:253:GLU:OE1	2.04	0.58
1:D:258:VAL:O	1:D:259:ILE:HB	2.02	0.58
1:D:313:LEU:HD22	1:D:314:PRO:CA	2.33	0.58
1:D:260:THR:CG2	1:D:310:PRO:HB3	2.34	0.57
1:B:234:ARG:HG2	1:B:257:ARG:NH2	2.08	0.57
1:D:228:MET:CE	1:D:341:LYS:HB3	2.35	0.57
1:A:250:LYS:NZ	1:A:253:GLU:OE1	2.29	0.56
1:C:183:MET:HG2	1:C:193:VAL:CG2	2.35	0.56
1:D:223:LEU:HB3	1:D:228:MET:HB2	1.87	0.56
1:A:123:PRO:HB3	4:E:1451:PG4:H52	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:64:ARG:HD3	1:E:66:VAL:HG23	1.86	0.56
1:A:207:ARG:HB3	1:A:208:PRO:HD3	1.87	0.56
1:D:230:PHE:HD1	1:D:256:ALA:HB2	1.55	0.56
1:A:220:GLU:OE2	1:A:224:LYS:HD3	2.04	0.56
1:D:369:GLY:O	1:D:370:LYS:HB2	2.06	0.56
1:D:259:ILE:HG22	1:D:260:THR:N	2.21	0.56
1:D:327:LEU:HD23	1:D:327:LEU:C	2.26	0.56
1:D:236:SER:CB	1:D:260:THR:HG1	2.16	0.55
1:E:12:ASN:ND2	5:E:2004:HOH:O	2.29	0.55
1:C:64:ARG:HD3	1:C:66:VAL:CG2	2.37	0.55
1:E:48:MET:HA	1:F:74:ILE:HD12	1.89	0.55
2:C:1448:GOL:O3	5:C:2141:HOH:O	2.11	0.55
1:E:26:GLN:HG3	1:E:30:GLU:OE2	2.06	0.55
1:D:311:TRP:CD1	1:D:327:LEU:HA	2.42	0.55
1:C:292:ARG:NH1	5:C:2117:HOH:O	2.41	0.54
1:D:225[B]:ARG:NH2	1:D:422:GLN:HA	2.23	0.54
1:D:311:TRP:HA	1:D:311:TRP:CE3	2.43	0.54
4:E:1451:PG4:H11	5:E:2060:HOH:O	2.07	0.54
1:D:222:MET:HG2	1:D:365:LEU:HD23	1.90	0.54
1:D:230:PHE:HB3	1:D:255:GLY:C	2.28	0.53
1:E:305:LEU:HB3	1:E:308:GLN:HG3	1.90	0.53
1:D:64:ARG:HD3	1:D:66:VAL:CG2	2.38	0.53
1:E:50:LEU:HD21	1:E:438:ALA:HB1	1.89	0.53
1:D:230:PHE:CE2	1:D:254:PHE:HD2	2.27	0.53
1:C:64:ARG:HD3	1:C:66:VAL:HG23	1.91	0.53
1:D:343:VAL:HG21	1:D:359:PHE:CE2	2.43	0.53
1:D:230:PHE:CD2	1:D:254:PHE:HB3	2.43	0.53
1:B:236:SER:HB3	1:B:315:VAL:HG11	1.90	0.53
3:C:1451:EPE:H71	1:E:145:ARG:CD	2.39	0.52
1:D:258:VAL:HG13	1:D:274:PHE:CD2	2.35	0.52
1:B:66:VAL:HG11	1:D:53:ARG:HD3	1.90	0.52
1:D:353:ILE:O	1:D:355:ALA:N	2.42	0.52
1:D:260:THR:HG21	1:D:310:PRO:HB3	1.91	0.52
1:F:64:ARG:HD3	1:F:66:VAL:HG23	1.92	0.52
1:C:250:LYS:NZ	1:C:253:GLU:OE1	2.36	0.52
1:E:257:ARG:HD3	1:E:271:GLU:O	2.10	0.52
1:D:270:ASP:OD2	1:D:278:LYS:NZ	2.30	0.51
1:E:53:ARG:HD3	1:F:66:VAL:HG11	1.92	0.51
1:B:48:MET:HA	1:D:74:ILE:HD12	1.93	0.51
2:A:1454:GOL:O2	1:C:156:ARG:NH1	2.42	0.51
1:B:49:SER:O	1:B:53:ARG:HG3	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ARG:HD3	1:A:66:VAL:HG23	1.92	0.51
1:E:387:ASN:HD22	4:E:1451:PG4:C6	2.18	0.51
1:F:222:MET:CE	1:F:367:ALA:HB2	2.41	0.51
1:D:258:VAL:HG13	1:D:259:ILE:H	1.76	0.51
2:A:1454:GOL:C3	1:E:188:ASN:HB3	2.40	0.51
2:C:1450:GOL:H11	5:C:2012:HOH:O	2.10	0.51
1:D:356:THR:HG22	1:D:359:PHE:H	1.76	0.50
1:D:314:PRO:HB3	1:D:335:LEU:HD23	1.94	0.50
1:D:311:TRP:HE3	1:D:311:TRP:HA	1.76	0.50
1:A:224:LYS:HD2	1:A:228:MET:O	2.12	0.50
1:A:196:GLY:HA2	1:A:207:ARG:HD2	1.94	0.50
1:D:221:ALA:HB2	1:D:407:LEU:CD2	2.41	0.50
1:A:66:VAL:HG11	1:C:53:ARG:HD3	1.93	0.49
2:A:1454:GOL:C2	1:C:156:ARG:HH11	2.23	0.49
1:D:266:GLY:HA3	1:D:304:TYR:CZ	2.47	0.49
1:D:277:GLU:O	1:D:278:LYS:CB	2.60	0.49
1:C:250:LYS:CD	1:C:253:GLU:OE1	2.61	0.49
1:D:225[B]:ARG:HB2	1:D:225[B]:ARG:HH11	1.76	0.49
1:A:329:VAL:HG23	1:A:330:ASP:N	2.28	0.49
1:B:234:ARG:HG2	1:B:257:ARG:HE	1.78	0.49
1:E:267:THR:HG22	1:E:268:VAL:N	2.28	0.49
1:B:207:ARG:HB3	1:B:208:PRO:HD3	1.94	0.49
1:D:257:ARG:HA	1:D:258:VAL:CG2	2.37	0.49
1:A:123:PRO:HB3	4:E:1451:PG4:C5	2.43	0.49
1:A:277:GLU:OE1	1:A:277:GLU:N	2.26	0.48
1:D:277:GLU:O	1:D:278:LYS:HB2	2.13	0.48
1:B:113:GLN:OE1	5:B:2057:HOH:O	2.20	0.48
1:B:64:ARG:HD3	1:B:66:VAL:HG23	1.96	0.48
1:D:225[B]:ARG:HH21	1:D:423:THR:H	1.62	0.48
1:D:236:SER:C	1:D:260:THR:OG1	2.52	0.47
1:D:311:TRP:HB3	1:D:331:ALA:HB2	1.96	0.47
4:E:1451:PG4:H82	5:E:2066:HOH:O	2.15	0.47
1:E:220:GLU:O	1:E:224:LYS:HG2	2.15	0.47
1:D:263:ASP:C	1:D:265:SER:H	2.18	0.47
1:A:333:HIS:CD2	1:A:358:LEU:HD21	2.49	0.47
1:A:49:SER:O	1:A:53:ARG:HG3	2.15	0.47
1:C:50:LEU:HD21	1:C:438:ALA:HB1	1.96	0.47
1:D:235:VAL:CG1	1:D:258:VAL:H	2.26	0.47
1:A:123:PRO:CB	4:E:1451:PG4:H51	2.45	0.47
1:E:23:GLU:OE2	5:E:2014:HOH:O	2.19	0.47
1:C:68:VAL:HB	3:C:1451:EPE:C8	2.43	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1451:EPE:H71	1:E:145:ARG:NE	2.29	0.47
1:D:263:ASP:C	1:D:265:SER:N	2.68	0.46
1:D:209:GLU:HG3	1:D:246:TYR:CD1	2.50	0.46
1:D:216:VAL:HG12	1:D:254:PHE:HE2	1.81	0.46
1:D:313:LEU:CD2	1:D:314:PRO:HA	2.42	0.46
1:A:275:THR:CB	1:A:277:GLU:OE1	2.63	0.46
1:C:152:THR:HG22	1:E:185:LYS:HE3	1.97	0.46
2:A:1454:GOL:C3	1:E:188:ASN:HD22	2.29	0.46
1:B:53:ARG:HD3	1:D:66:VAL:HG11	1.98	0.46
1:D:309:GLN:HB3	1:D:310:PRO:CD	2.46	0.46
1:C:34:THR:CG2	1:C:427:GLN:HA	2.46	0.46
1:E:184:LYS:CE	4:E:1451:PG4:H12	2.46	0.45
1:E:48:MET:CA	1:F:74:ILE:HD12	2.46	0.45
1:E:21:GLN:HG2	1:E:104:SER:HB2	1.99	0.45
1:D:230:PHE:HB2	1:D:254:PHE:HB3	1.98	0.45
1:D:323:THR:HB	1:D:326:GLU:CD	2.36	0.45
1:B:241:GLY:O	1:B:245:GLN:HG3	2.16	0.45
1:D:49:SER:O	1:D:53:ARG:HG3	2.16	0.45
5:E:2091:HOH:O	1:F:64:ARG:HD2	2.16	0.45
1:B:324:GLN:NE2	1:B:349:MET:SD	2.90	0.45
1:C:72:ASN:HD22	2:C:1449:GOL:H12	1.81	0.45
1:D:352:THR:O	1:D:355:ALA:HB2	2.17	0.45
1:D:329:VAL:O	1:D:330:ASP:HB3	2.17	0.45
1:C:349:MET:N	1:C:350:PRO:HD3	2.32	0.45
1:A:88:ILE:HD11	1:A:436:LYS:HG3	1.98	0.45
1:D:234:ARG:HD3	1:D:340:VAL:HA	1.98	0.44
1:F:277:GLU:OE1	1:F:277:GLU:N	2.47	0.44
1:B:17:ARG:HB3	1:D:78:ARG:NH1	2.33	0.44
1:F:329:VAL:HG13	1:F:358:LEU:CD1	2.47	0.44
1:F:46:ARG:NE	2:F:1449:GOL:H11	2.33	0.44
1:E:88:ILE:CD1	1:E:436:LYS:HD2	2.47	0.44
1:D:356:THR:HG21	1:D:359:PHE:CD2	2.53	0.44
1:B:348:ASN:C	1:B:349:MET:HG2	2.36	0.44
1:D:260:THR:HG22	1:D:310:PRO:HB3	1.99	0.44
3:C:1451:EPE:H71	1:E:145:ARG:NH1	2.31	0.44
1:D:233:MET:HB2	1:D:234:ARG:H	1.39	0.44
1:D:274:PHE:HE2	5:D:2080:HOH:O	2.01	0.44
1:D:117:ASN:OD1	1:D:377:VAL:HG21	2.16	0.44
1:B:174:ARG:HD2	1:B:175:GLU:OE2	2.18	0.44
1:D:324:GLN:O	1:D:325:ASN:HB2	2.17	0.44
1:A:34:THR:HG21	1:A:427:GLN:HA	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:356:THR:C	1:D:358:LEU:H	2.20	0.43
1:C:59:ARG:HD2	1:C:83:GLN:OE1	2.18	0.43
1:D:230:PHE:CA	1:D:232:GLY:H	1.97	0.43
1:D:257:ARG:NH2	5:D:2078:HOH:O	2.50	0.43
1:D:216:VAL:HG12	1:D:254:PHE:CE2	2.53	0.43
1:D:233:MET:SD	1:D:234:ARG:NH2	2.92	0.43
1:B:324:GLN:HG3	1:B:349:MET:HG3	1.99	0.43
1:E:49:SER:O	1:E:53:ARG:HG3	2.19	0.43
1:D:332:ALA:HB1	1:D:356:THR:HG23	2.00	0.43
1:D:359:PHE:HB3	1:D:364:VAL:HB	2.00	0.43
1:F:244:ALA:O	1:F:248:ILE:HG13	2.18	0.43
1:D:205:LEU:O	1:D:206:ILE:HB	2.17	0.43
1:A:117:ASN:OD1	1:A:377:VAL:HG21	2.18	0.43
1:A:349:MET:N	1:A:350:PRO:CD	2.82	0.43
1:A:259:ILE:HG13	1:A:260:THR:HG23	2.00	0.43
1:D:327:LEU:HD23	1:D:327:LEU:O	2.18	0.43
1:F:329:VAL:HG13	1:F:358:LEU:HD11	2.01	0.43
1:D:223:LEU:HD11	1:D:342:ALA:CB	2.49	0.43
1:A:34:THR:CG2	1:A:427:GLN:HA	2.49	0.43
5:B:2028:HOH:O	1:D:64:ARG:NH2	2.52	0.42
1:C:93:GLY:HA3	1:C:127:GLY:O	2.18	0.42
1:D:314:PRO:HG3	1:D:335:LEU:N	2.34	0.42
1:A:53:ARG:HD3	1:C:66:VAL:HG11	2.01	0.42
1:D:15:GLN:HG3	1:D:15:GLN:O	2.18	0.42
1:E:205:LEU:O	1:E:206:ILE:HB	2.19	0.42
1:D:252:MET:C	1:D:254:PHE:H	2.23	0.42
1:D:311:TRP:CE3	1:D:311:TRP:CA	3.03	0.42
1:D:207:ARG:HB3	1:D:208:PRO:HD3	2.00	0.42
1:E:117:ASN:OD1	1:E:377:VAL:HG21	2.18	0.42
1:F:98:HIS:CG	1:F:99:PRO:HD2	2.55	0.42
1:A:183:MET:HG2	1:A:193:VAL:HG11	2.02	0.42
1:D:256:ALA:C	1:D:257:ARG:HG3	2.38	0.42
2:A:1452:GOL:O3	5:A:2157:HOH:O	2.20	0.42
1:C:78:ARG:CD	1:C:80:TRP:CZ2	3.02	0.42
1:E:240:SER:OG	1:E:286:LYS:HE3	2.20	0.42
1:C:248:ILE:HG12	1:C:258:VAL:HG11	2.02	0.42
1:D:231:GLU:HA	1:D:255:GLY:O	2.19	0.42
1:F:109:LEU:HB2	1:F:128:LYS:HG2	2.02	0.42
1:D:313:LEU:HD22	1:D:313:LEU:C	2.41	0.41
1:E:207:ARG:HB3	1:E:208:PRO:HD3	2.02	0.41
1:D:421:GLU:O	1:D:422:GLN:CB	2.67	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:MET:HE1	1:D:365:LEU:C	2.41	0.41
2:C:1448:GOL:H32	1:F:123:PRO:HB3	2.01	0.41
1:D:64:ARG:HD3	1:D:66:VAL:HG23	2.02	0.41
1:B:109:LEU:O	1:B:113:GLN:HB2	2.21	0.41
1:D:222:MET:HE3	1:D:366:PHE:O	2.21	0.41
1:D:215:LEU:HD13	1:D:345:GLU:O	2.20	0.41
1:A:185:LYS:O	1:B:156:ARG:NH2	2.54	0.41
1:E:62:GLN:NE2	5:E:2033:HOH:O	2.53	0.41
1:C:347:ALA:HB3	1:C:350:PRO:HG3	2.03	0.41
1:D:256:ALA:C	1:D:257:ARG:CG	2.89	0.41
1:D:259:ILE:HG22	1:D:260:THR:H	1.84	0.41
1:D:260:THR:HG22	1:D:267:THR:CG2	2.50	0.41
2:C:1450:GOL:C1	5:C:2012:HOH:O	2.68	0.41
1:B:50:LEU:HD21	1:B:438:ALA:HB1	2.02	0.41
1:D:258:VAL:CG2	1:D:274:PHE:HB2	2.47	0.41
1:E:328:ASP:OD1	1:E:329:VAL:N	2.49	0.41
1:D:393:TRP:HB3	1:D:397:LYS:HD3	2.01	0.41
1:B:329:VAL:CG1	1:B:354:GLU:HG2	2.51	0.41
1:D:427:GLN:HG2	1:D:431:ILE:HD12	2.03	0.41
1:B:240:SER:OG	1:B:286:LYS:HE2	2.21	0.41
1:D:311:TRP:HB3	1:D:331:ALA:CB	2.51	0.41
1:D:329:VAL:O	1:D:330:ASP:CB	2.69	0.41
1:F:258:VAL:N	5:F:2079:HOH:O	2.43	0.41
1:B:422:GLN:O	5:B:2143:HOH:O	2.22	0.41
1:D:266:GLY:CA	1:D:304:TYR:CE1	3.02	0.40
1:C:236:SER:HB3	1:C:315:VAL:HG11	2.02	0.40
1:D:230:PHE:CD2	1:D:254:PHE:CD2	3.10	0.40
1:E:203:GLY:O	5:E:2066:HOH:O	2.22	0.40
1:C:98:HIS:CG	1:C:99:PRO:HD2	2.55	0.40
1:E:95:MET:O	1:E:168:ASP:HB3	2.21	0.40
1:D:310:PRO:O	1:D:313:LEU:HB3	2.22	0.40
1:C:250:LYS:HA	1:C:250:LYS:HD3	1.91	0.40
1:C:259:ILE:HG13	1:C:260:THR:HG23	2.03	0.40

All (2) 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)
5:C:2125:HOH:O	5:E:2030:HOH:O[4_545]	2.12	0.08
1:E:224:LYS:HZ3	1:F:421:GLU:OE2[1_455]	1.55	0.05

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	444/447 (99%)	435 (98%)	7 (2%)	2 (0%)	34	55
1	B	441/447 (99%)	432 (98%)	7 (2%)	2 (0%)	34	55
1	C	441/447 (99%)	432 (98%)	7 (2%)	2 (0%)	34	55
1	D	436/447 (98%)	363 (83%)	43 (10%)	30 (7%)	1	1
1	E	440/447 (98%)	429 (98%)	10 (2%)	1 (0%)	52	75
1	F	442/447 (99%)	434 (98%)	6 (1%)	2 (0%)	34	55
All	All	2644/2682 (99%)	2525 (96%)	80 (3%)	39 (2%)	13	22

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	ILE
1	B	206	ILE
1	C	206	ILE
1	D	206	ILE
1	D	226	HIS
1	D	228	MET
1	D	234	ARG
1	D	258	VAL
1	D	259	ILE
1	D	264	SER
1	D	276	LYS
1	D	305	LEU
1	D	306	GLU
1	D	330	ASP
1	E	206	ILE
1	F	206	ILE
1	F	307	GLY
1	A	307	GLY
1	B	307	GLY
1	C	307	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	168	ASP
1	D	224	LYS
1	D	278	LYS
1	D	291	GLY
1	D	325	ASN
1	D	370	LYS
1	D	424	ASN
1	D	292	ARG
1	D	303	VAL
1	D	307	GLY
1	D	314	PRO
1	D	354	GLU
1	D	232	GLY
1	D	251	ALA
1	D	255	GLY
1	D	422	GLN
1	D	365	LEU
1	D	301	GLY
1	D	227	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	350/351 (100%)	349 (100%)	1 (0%)	94 99
1	B	347/351 (99%)	344 (99%)	3 (1%)	84 95
1	C	347/351 (99%)	345 (99%)	2 (1%)	90 97
1	D	345/351 (98%)	324 (94%)	21 (6%)	23 42
1	E	346/351 (99%)	341 (99%)	5 (1%)	74 91
1	F	348/351 (99%)	346 (99%)	2 (1%)	90 97
All	All	2083/2106 (99%)	2049 (98%)	34 (2%)	70 90

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	PHE
1	B	108	PHE
1	B	224	LYS
1	B	313	LEU
1	C	84	PHE
1	C	108	PHE
1	D	47	GLN
1	D	84	PHE
1	D	108	PHE
1	D	225[A]	ARG
1	D	225[B]	ARG
1	D	228	MET
1	D	233	MET
1	D	234	ARG
1	D	260	THR
1	D	274	PHE
1	D	286	LYS
1	D	290	ASP
1	D	302	LEU
1	D	313	LEU
1	D	323	THR
1	D	325	ASN
1	D	328	ASP
1	D	338	ASN
1	D	357	GLU
1	D	370	LYS
1	D	396	GLU
1	E	108	PHE
1	E	152	THR
1	E	207	ARG
1	E	365	LEU
1	E	436	LYS
1	F	84	PHE
1	F	108	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	ASN
1	A	333	HIS
1	B	324	GLN
1	C	72	ASN
1	C	73	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	309	GLN
1	E	62	GLN
1	E	188	ASN
1	E	242	ASN
1	E	387	ASN
1	F	334	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

20 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	GOL	A	1448	-	5,5,5	0.69	0	5,5,5	0.96	0
2	GOL	A	1449	-	5,5,5	0.38	0	5,5,5	0.95	0
2	GOL	A	1450	-	5,5,5	0.33	0	5,5,5	0.58	0
2	GOL	A	1451	-	5,5,5	0.53	0	5,5,5	1.43	1 (20%)
2	GOL	A	1452	-	5,5,5	0.41	0	5,5,5	0.42	0
2	GOL	A	1453	-	5,5,5	0.41	0	5,5,5	0.51	0
2	GOL	A	1454	-	5,5,5	0.67	0	5,5,5	1.27	0
2	GOL	C	1448	-	5,5,5	0.66	0	5,5,5	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GOL	C	1449	-	5,5,5	0.49	0	5,5,5	0.91	0
2	GOL	C	1450	-	5,5,5	0.22	0	5,5,5	0.72	0
3	EPE	C	1451	-	14,15,15	1.54	4 (28%)	18,20,20	3.11	8 (44%)
2	GOL	D	1448	-	5,5,5	0.34	0	5,5,5	0.38	0
2	GOL	D	1449	-	5,5,5	0.44	0	5,5,5	0.50	0
2	GOL	D	1450	-	5,5,5	0.38	0	5,5,5	0.73	0
2	GOL	E	1448	-	5,5,5	0.45	0	5,5,5	0.92	0
2	GOL	E	1449	-	5,5,5	0.46	0	5,5,5	0.54	0
2	GOL	E	1450	-	5,5,5	0.57	0	5,5,5	0.95	0
4	PG4	E	1451	-	12,12,12	0.97	1 (8%)	11,11,11	0.68	0
2	GOL	F	1448	-	5,5,5	0.37	0	5,5,5	0.42	0
2	GOL	F	1449	-	5,5,5	0.44	0	5,5,5	0.77	0

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
2	GOL	A	1448	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1449	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1450	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1451	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1452	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1453	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1454	-	-	0/4/4/4	0/0/0/0
2	GOL	C	1448	-	-	0/4/4/4	0/0/0/0
2	GOL	C	1449	-	-	0/4/4/4	0/0/0/0
2	GOL	C	1450	-	-	0/4/4/4	0/0/0/0
3	EPE	C	1451	-	-	0/9/19/19	0/1/1/1
2	GOL	D	1448	-	-	0/4/4/4	0/0/0/0
2	GOL	D	1449	-	-	0/4/4/4	0/0/0/0
2	GOL	D	1450	-	-	0/4/4/4	0/0/0/0
2	GOL	E	1448	-	-	0/4/4/4	0/0/0/0
2	GOL	E	1449	-	-	0/4/4/4	0/0/0/0
2	GOL	E	1450	-	-	0/4/4/4	0/0/0/0
4	PG4	E	1451	-	-	0/10/10/10	0/0/0/0
2	GOL	F	1448	-	-	0/4/4/4	0/0/0/0
2	GOL	F	1449	-	-	0/4/4/4	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1451	EPE	C7-N4	-2.82	1.40	1.47
3	C	1451	EPE	C7-C8	2.10	1.60	1.51
4	E	1451	PG4	O2-C2	2.20	1.51	1.42
3	C	1451	EPE	O1S-S	2.45	1.52	1.45
3	C	1451	EPE	O3S-S	2.63	1.53	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1451	EPE	O3S-S-O1S	-3.73	102.92	111.61
2	A	1451	GOL	O2-C2-C1	2.00	117.83	108.65
3	C	1451	EPE	C9-N1-C2	2.16	116.81	111.27
3	C	1451	EPE	C8-C7-N4	2.96	124.41	113.41
3	C	1451	EPE	C3-C2-N1	2.98	115.96	110.63
3	C	1451	EPE	C7-N4-C5	4.36	122.46	111.27
3	C	1451	EPE	O1S-S-C10	5.13	111.29	106.91
3	C	1451	EPE	C5-N4-C3	5.66	121.17	108.90
3	C	1451	EPE	C6-N1-C2	6.57	123.12	108.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1451	GOL	1	0
2	A	1452	GOL	1	0
2	A	1454	GOL	5	0
2	C	1448	GOL	2	0
2	C	1449	GOL	1	0
2	C	1450	GOL	2	0
3	C	1451	EPE	8	0
4	E	1451	PG4	11	0
2	F	1449	GOL	1	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	442/447 (98%)	-0.05	2 (0%) 91 92	21, 34, 57, 117	0
1	B	442/447 (98%)	-0.10	1 (0%) 95 96	20, 32, 57, 129	0
1	C	442/447 (98%)	-0.08	1 (0%) 95 96	22, 31, 48, 78	0
1	D	439/447 (98%)	0.73	74 (16%) 2 2	21, 44, 104, 149	0
1	E	442/447 (98%)	0.15	10 (2%) 64 67	21, 39, 75, 116	0
1	F	442/447 (98%)	0.05	5 (1%) 82 84	20, 36, 68, 120	0
All	All	2649/2682 (98%)	0.12	93 (3%) 48 53	20, 34, 79, 149	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	226	HIS	10.4
1	D	353	ILE	6.6
1	F	289	ARG	6.3
1	D	279	LEU	6.2
1	D	365	LEU	6.0
1	D	342	ALA	5.7
1	D	306	GLU	5.6
1	D	260	THR	5.6
1	D	329	VAL	5.5
1	D	223	LEU	5.2
1	D	229	GLY	5.0
1	D	308	GLN	5.0
1	D	352	THR	4.9
1	D	304	TYR	4.3
1	D	230	PHE	4.3
1	D	255	GLY	4.2
1	D	273	GLY	4.2
1	D	294	ALA	4.2
1	D	344	ALA	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	327	LEU	4.1
1	D	269	VAL	4.0
1	D	268	VAL	4.0
1	D	290	ASP	3.9
1	D	303	VAL	3.8
1	D	326	GLU	3.7
1	D	341	LYS	3.5
1	D	340	VAL	3.5
1	D	343	VAL	3.5
1	D	275	THR	3.4
1	D	272	SER	3.4
1	D	354	GLU	3.3
1	D	359	PHE	3.3
1	F	26	GLN	3.2
1	D	256	ALA	3.1
1	D	336	ILE	3.1
1	D	257	ARG	3.1
1	D	420	GLY	3.1
1	D	364	VAL	3.1
1	D	307	GLY	3.0
1	D	289	ARG	3.0
1	D	233	MET	2.9
1	D	422	GLN	2.9
1	D	239	GLY	2.9
1	D	312	SER	2.9
1	D	421	GLU	2.9
1	D	339	GLY	2.8
1	E	26	GLN	2.8
1	D	311	TRP	2.8
1	D	335	LEU	2.8
1	E	284	GLU	2.7
1	D	292	ARG	2.7
1	F	299	GLU	2.7
1	D	351	THR	2.7
1	D	309	GLN	2.7
1	D	236	SER	2.6
1	D	366	PHE	2.6
1	D	281	ARG	2.6
1	D	270	ASP	2.6
1	D	221	ALA	2.6
1	A	7	LEU	2.5
1	D	315	VAL	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	230	PHE	2.5
1	B	257	ARG	2.5
1	D	325	ASN	2.4
1	D	276	LYS	2.4
1	D	296	TYR	2.4
1	D	247	ALA	2.3
1	D	216	VAL	2.3
1	C	289	ARG	2.3
1	D	429	ALA	2.3
1	F	305	LEU	2.3
1	D	350	PRO	2.3
1	D	305	LEU	2.3
1	D	258	VAL	2.3
1	D	360	GLN	2.3
1	F	294	ALA	2.2
1	D	293	VAL	2.2
1	E	298	LYS	2.2
1	E	228	MET	2.2
1	D	358	LEU	2.2
1	D	283	ILE	2.2
1	D	368	PRO	2.2
1	D	414	VAL	2.1
1	D	271	GLU	2.1
1	E	360	GLN	2.1
1	E	353	ILE	2.1
1	E	273	GLY	2.1
1	E	257	ARG	2.1
1	E	426	VAL	2.1
1	D	228	MET	2.1
1	D	162	THR	2.1
1	A	268	VAL	2.0
1	D	35	LEU	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

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
2	GOL	A	1452	6/6	0.93	0.40	10.41	48,64,77,83	0
2	GOL	A	1453	6/6	0.89	0.41	10.34	55,66,75,79	0
2	GOL	A	1450	6/6	0.90	0.34	9.99	47,57,64,65	0
2	GOL	F	1448	6/6	0.93	0.36	9.57	53,64,68,69	0
2	GOL	E	1449	6/6	0.92	0.38	8.80	46,58,69,70	0
2	GOL	A	1451	6/6	0.89	0.33	5.42	40,49,65,66	0
2	GOL	D	1449	6/6	0.91	0.31	3.79	30,43,53,57	0
3	EPE	C	1451	15/15	0.93	0.26	3.27	37,52,73,83	0
4	PG4	E	1451	13/13	0.87	0.24	2.71	43,59,71,77	0
2	GOL	A	1454	6/6	0.87	0.29	2.65	58,69,82,82	0
2	GOL	E	1448	6/6	0.95	0.29	2.36	32,46,59,64	0
2	GOL	D	1448	6/6	0.94	0.22	2.13	30,41,49,52	0
2	GOL	E	1450	6/6	0.93	0.24	2.03	48,59,63,75	0
2	GOL	C	1449	6/6	0.92	0.19	1.37	37,54,65,69	0
2	GOL	C	1448	6/6	0.95	0.18	1.24	42,52,68,82	0
2	GOL	A	1449	6/6	0.90	0.18	1.02	48,58,69,73	0
2	GOL	D	1450	6/6	0.91	0.15	0.46	42,55,70,70	0
2	GOL	A	1448	6/6	0.88	0.21	0.32	47,62,71,79	0
2	GOL	F	1449	6/6	0.87	0.21	0.15	43,63,86,86	0
2	GOL	C	1450	6/6	0.90	0.16	0.11	47,64,77,77	0

6.5 Other polymers

There are no such residues in this entry.