



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:00 PM GMT

PDB ID : 3SC6
Title : 2.65 Angstrom resolution crystal structure of dTDP-4-dehydrorhamnose reductase (rfbD) from Bacillus anthracis str. Ames in complex with NADP
Authors : Halavaty, A.S.; Kuhn, M.; Shuvalova, L.; Minasov, G.; Peterson, S.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2011-06-07
Resolution : 2.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

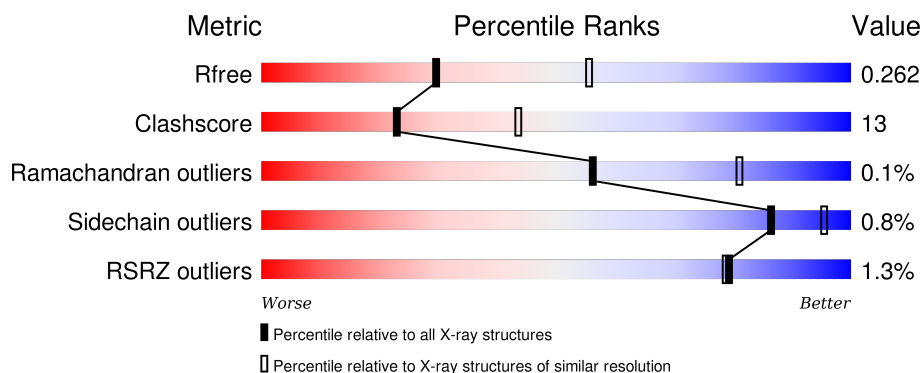
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	287	<div> <div>3%</div> <div>70%</div> <div>28%</div> <div>.</div> </div>
1	B	287	<div> <div>70%</div> <div>26%</div> <div>..</div> </div>
1	C	287	<div> <div>76%</div> <div>22%</div> <div>.</div> </div>
1	D	287	<div> <div>3%</div> <div>69%</div> <div>29%</div> <div>..</div> </div>
1	E	287	<div> <div>%</div> <div>70%</div> <div>26%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	287	<div> <div></div> <div>%</div> <div>70%</div> <div>27%</div> <div>..</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	B	288	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14334 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called dTDP-4-dehydrorhamnose reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	3	0
			2288	1470	386	425	7			
1	B	280	Total	C	N	O	S	0	1	0
			2260	1451	383	418	8			
1	C	281	Total	C	N	O	S	0	3	0
			2296	1474	391	423	8			
1	D	283	Total	C	N	O	S	0	2	0
			2293	1472	387	426	8			
1	E	278	Total	C	N	O	S	0	1	0
			2261	1455	381	418	7			
1	F	281	Total	C	N	O	S	0	1	0
			2274	1462	383	421	8			

There are 18 discrepancies between the modelled and reference sequences:

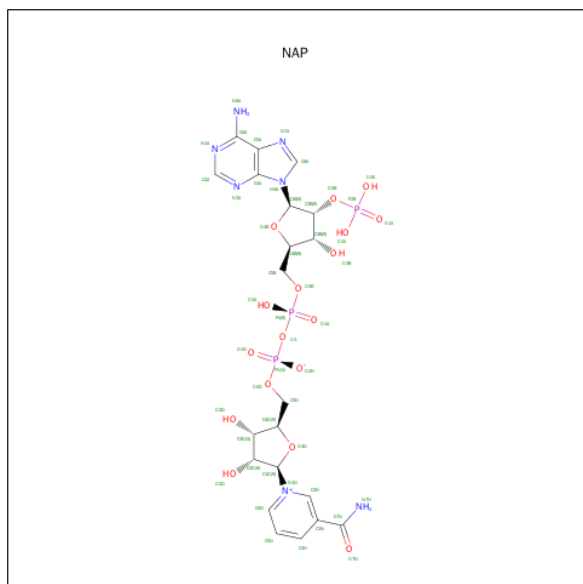
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q81TN9
A	-1	ASN	-	EXPRESSION TAG	UNP Q81TN9
A	0	ALA	-	EXPRESSION TAG	UNP Q81TN9
B	-2	SER	-	EXPRESSION TAG	UNP Q81TN9
B	-1	ASN	-	EXPRESSION TAG	UNP Q81TN9
B	0	ALA	-	EXPRESSION TAG	UNP Q81TN9
C	-2	SER	-	EXPRESSION TAG	UNP Q81TN9
C	-1	ASN	-	EXPRESSION TAG	UNP Q81TN9
C	0	ALA	-	EXPRESSION TAG	UNP Q81TN9
D	-2	SER	-	EXPRESSION TAG	UNP Q81TN9
D	-1	ASN	-	EXPRESSION TAG	UNP Q81TN9
D	0	ALA	-	EXPRESSION TAG	UNP Q81TN9
E	-2	SER	-	EXPRESSION TAG	UNP Q81TN9
E	-1	ASN	-	EXPRESSION TAG	UNP Q81TN9
E	0	ALA	-	EXPRESSION TAG	UNP Q81TN9
F	-2	SER	-	EXPRESSION TAG	UNP Q81TN9
F	-1	ASN	-	EXPRESSION TAG	UNP Q81TN9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	ALA	-	EXPRESSION TAG	UNP Q81TN9

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	1
			96	42	14	34	6		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

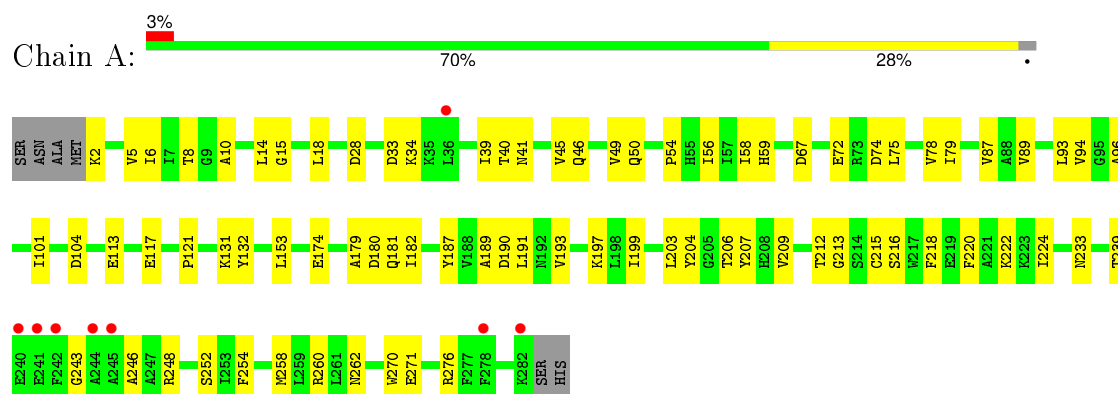
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	33	Total	O	0	0
			33	33		
4	B	50	Total	O	0	1
			50	50		
4	C	46	Total	O	0	0
			46	46		
4	D	32	Total	O	0	0
			32	32		
4	E	32	Total	O	0	0
			32	32		
4	F	47	Total	O	0	1
			48	48		

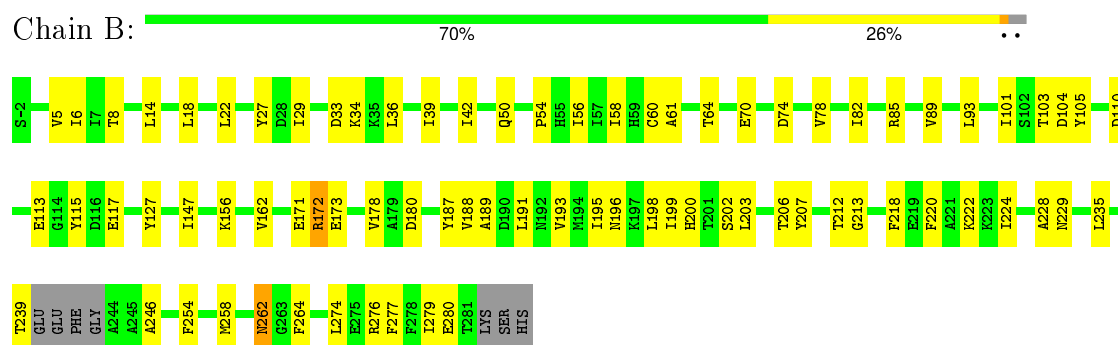
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

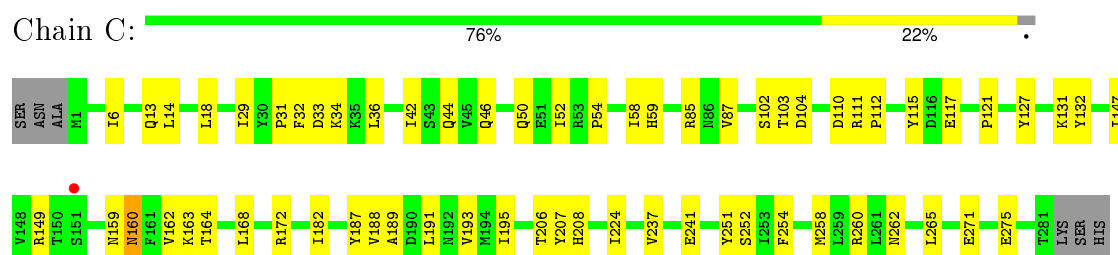
- Molecule 1: dTDP-4-dehydrodharmose reductase



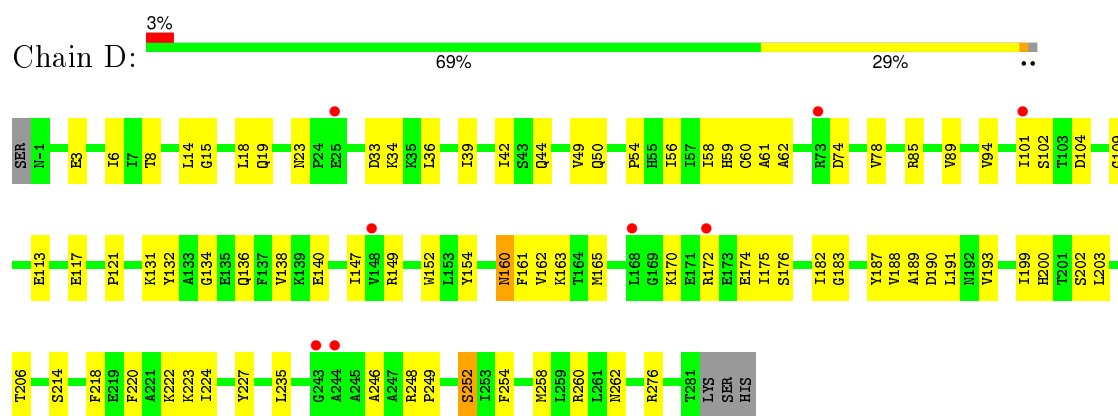
- Molecule 1: dTDP-4-dehydrodharmose reductase



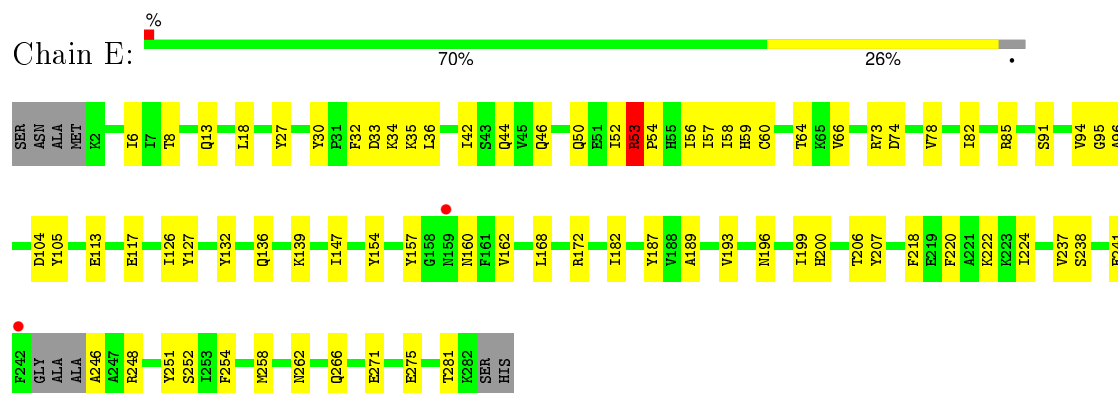
- Molecule 1: dTDP-4-dehydrodharmose reductase



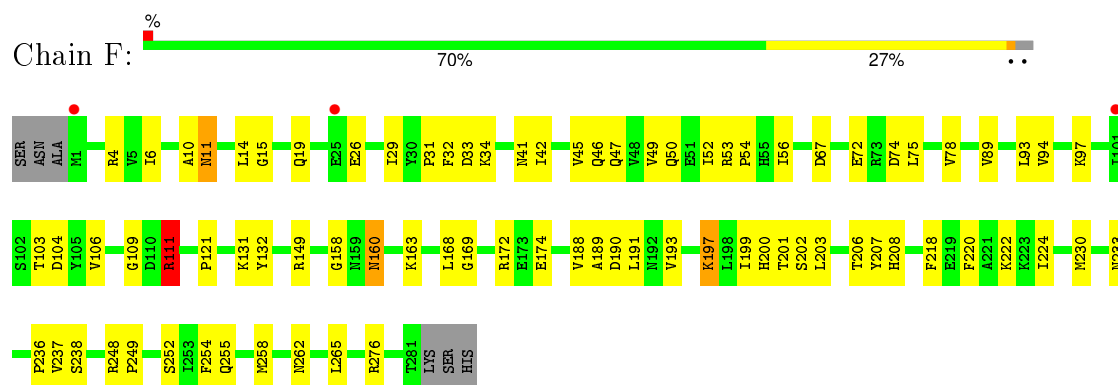
- Molecule 1: dTDP-4-dehydrodharmose reductase



• Molecule 1: dTDP-4-dehydrorhamnose reductase



• Molecule 1: dTDP-4-dehydrorhamnose reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.45Å 113.34Å 144.95Å 90.00° 91.18° 90.00°	Depositor
Resolution (Å)	29.90 – 2.65 29.90 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.90-2.65) 99.9 (29.90-2.65)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.64Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.215 , 0.258 0.219 , 0.262	Depositor DCC
R_{free} test set	3745 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	56.4	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 45.7	EDS
Estimated twinning fraction	0.044 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 74606 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14334	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: NAP, 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	0.32	0/2342	0.62	0/3171
1	B	0.35	0/2312	0.66	1/3130 (0.0%)
1	C	0.34	0/2350	0.62	0/3180
1	D	0.34	0/2347	0.63	0/3179
1	E	0.34	0/2314	0.63	1/3131 (0.0%)
1	F	0.34	0/2328	0.67	2/3152 (0.1%)
All	All	0.34	0/13993	0.64	4/18943 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	255	GLN	N-CA-C	-5.40	96.42	111.00
1	B	172	ARG	N-CA-C	5.25	125.17	111.00
1	E	53	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	F	111	ARG	NE-CZ-NH1	5.13	122.87	120.30

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	A	2288	0	2253	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2260	0	2232	74	0
1	C	2296	0	2265	56	0
1	D	2293	0	2257	72	0
1	E	2261	0	2228	63	0
1	F	2274	0	2241	62	0
2	A	48	0	25	3	0
2	B	96	0	50	5	0
2	C	48	0	25	2	0
2	D	48	0	25	0	0
2	E	48	0	25	0	0
2	F	48	0	25	1	0
3	A	10	0	0	0	0
3	B	20	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	1	0
3	E	20	0	0	0	0
3	F	15	0	0	0	0
4	A	33	0	0	0	0
4	B	50	0	0	2	0
4	C	46	0	0	1	0
4	D	32	0	0	2	0
4	E	32	0	0	4	0
4	F	48	0	0	2	0
All	All	14334	0	13651	374	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 13.

All (374) 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:A:104:ASP:OD1	1:A:252:SER:HB2	1.63	0.97
1:F:104:ASP:OD1	1:F:252:SER:HB2	1.80	0.81
1:E:281:THR:O	1:E:281:THR:HG22	1.84	0.75
1:F:160:ASN:ND2	1:F:163:LYS:H	1.85	0.75
1:C:160:ASN:ND2	1:C:163:LYS:H	1.83	0.75
1:A:39:ILE:HG22	2:A:285:NAP:N6A	2.02	0.74
1:E:220:PHE:O	1:E:224:ILE:HG13	1.87	0.74
1:C:160:ASN:C	1:C:160:ASN:HD22	1.91	0.74
1:D:147:ILE:HB	1:D:206:THR:HG22	1.70	0.73
1:E:73:ARG:NH2	1:E:126:ILE:HD11	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:LEU:HD23	1:D:188:VAL:HG13	1.72	0.72
1:E:53:ARG:HH11	1:E:53:ARG:CG	2.02	0.72
1:A:182:ILE:HG23	1:A:215:CYS:O	1.90	0.71
1:B:117:GLU:N	1:B:117:GLU:OE1	2.19	0.71
1:C:187:TYR:CE2	1:C:189:ALA:HB3	2.27	0.70
1:F:111:ARG:CG	1:F:111:ARG:HH11	2.04	0.70
1:D:190:ASP:OD1	1:D:276:ARG:NH1	2.25	0.69
1:A:207:TYR:OH	1:A:262:ASN:ND2	2.25	0.69
1:A:2:LYS:HE3	1:A:28:ASP:OD1	1.92	0.69
1:B:178:VAL:HG23	4:B:326:HOH:O	1.91	0.68
1:A:260:ARG:NH2	1:B:74:ASP:OD2	2.26	0.68
1:C:260:ARG:NH2	4:C:331:HOH:O	2.27	0.68
1:F:189:ALA:O	1:F:193:VAL:HG23	1.94	0.68
1:C:160:ASN:HD21	1:C:163:LYS:H	1.40	0.67
1:D:161:PHE:CE1	1:D:165:MET:HE2	2.30	0.67
1:C:14:LEU:HD23	1:C:188:VAL:HG13	1.77	0.67
1:D:104:ASP:HB3	1:D:254:PHE:CZ	2.29	0.67
1:F:14:LEU:HD23	1:F:188:VAL:HG13	1.76	0.66
1:E:237:VAL:CG1	1:E:241:GLU:HB2	2.25	0.66
1:B:56:ILE:HD13	1:B:199:ILE:HB	1.78	0.66
1:B:189:ALA:O	1:B:193:VAL:HG23	1.96	0.66
1:C:104:ASP:HB3	1:C:254:PHE:CZ	2.31	0.66
1:D:56:ILE:HD13	1:D:199:ILE:HB	1.78	0.65
1:D:117:GLU:N	1:D:117:GLU:OE1	2.27	0.65
1:A:67:ASP:OD2	1:A:248:ARG:NH1	2.29	0.65
1:F:26:GLU:OE2	1:F:200:HIS:NE2	2.22	0.65
1:D:74:ASP:O	1:D:78:VAL:HG23	1.96	0.65
1:F:89:VAL:O	1:F:93:LEU:HD13	1.97	0.65
1:A:39:ILE:HG22	2:A:285:NAP:C6A	2.27	0.65
1:A:218:PHE:CE2	1:A:222:LYS:HE2	2.32	0.64
1:B:218:PHE:CZ	1:B:222:LYS:HE3	2.32	0.64
1:B:189:ALA:HB1	1:B:276:ARG:HH12	1.61	0.64
2:B:285[A]:NAP:O1N	2:B:285[A]:NAP:N7N	2.30	0.64
1:B:191:LEU:HD21	1:B:195:ILE:HD11	1.79	0.64
1:B:191:LEU:CD2	1:B:195:ILE:HD11	2.28	0.64
1:F:160:ASN:HD22	1:F:160:ASN:C	2.00	0.64
1:B:82:ILE:HG23	1:B:85:ARG:HH12	1.62	0.63
1:E:18:LEU:HD21	1:E:58:ILE:HG21	1.81	0.63
1:C:191:LEU:HD21	1:C:195:ILE:HD11	1.80	0.63
1:B:196:ASN:O	1:B:200:HIS:ND1	2.32	0.62
1:F:193:VAL:HG12	1:F:197:LYS:HE2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:160:ASN:HD21	1:F:163:LYS:H	1.44	0.62
1:B:74:ASP:O	1:B:78:VAL:HG23	1.98	0.62
1:B:50:GLN:NE2	1:B:93:LEU:CD2	2.63	0.62
1:D:160:ASN:ND2	1:D:163:LYS:H	1.97	0.62
1:D:248:ARG:NH2	3:D:287:SO4:O1	2.32	0.62
1:F:207:TYR:OH	1:F:262:ASN:ND2	2.34	0.61
1:C:191:LEU:HD23	1:C:195:ILE:HG13	1.83	0.61
1:D:203:LEU:HD23	1:E:42:ILE:HD12	1.82	0.61
1:F:131:LYS:NZ	2:F:285:NAP:O3D	2.29	0.61
1:D:147:ILE:HD12	1:D:206:THR:HG22	1.82	0.61
1:D:189:ALA:O	1:D:193:VAL:HG23	2.00	0.61
1:F:104:ASP:HB3	1:F:254:PHE:CZ	2.37	0.60
1:F:74:ASP:O	1:F:78:VAL:HG23	2.01	0.60
1:A:206:THR:O	1:A:258:MET:HG3	2.02	0.60
1:C:147:ILE:HB	1:C:206:THR:HG22	1.84	0.60
1:E:53:ARG:HH11	1:E:53:ARG:HG3	1.65	0.60
1:A:74:ASP:O	1:A:78:VAL:HG23	2.02	0.60
1:C:237:VAL:HG13	1:C:241:GLU:OE1	2.02	0.60
1:A:180:ASP:OD2	1:A:239:THR:HG23	2.02	0.59
1:D:160:ASN:C	1:D:160:ASN:HD22	2.06	0.59
1:E:206:THR:O	1:E:258:MET:HG3	2.03	0.59
1:E:207:TYR:OH	1:E:262:ASN:ND2	2.34	0.59
1:F:103:THR:O	1:F:106:VAL:HG22	2.02	0.59
1:B:147:ILE:HD12	1:B:206:THR:HG22	1.84	0.59
1:E:266:GLN:NE2	4:E:321:HOH:O	2.35	0.59
1:A:203:LEU:HD22	1:B:85:ARG:HH21	1.67	0.59
1:C:191:LEU:CD2	1:C:195:ILE:HD11	2.33	0.59
1:F:29:ILE:HD12	1:F:29:ILE:N	2.18	0.59
1:A:189:ALA:O	1:A:193:VAL:HG23	2.03	0.59
1:D:182:ILE:HD12	1:D:182:ILE:N	2.18	0.59
1:F:14:LEU:HD21	1:F:191:LEU:HD23	1.84	0.58
1:A:5:VAL:HG12	1:A:56:ILE:HB	1.85	0.58
1:A:104:ASP:HB3	1:A:254:PHE:CZ	2.38	0.58
1:F:206:THR:O	1:F:258:MET:HG3	2.03	0.58
1:A:6:ILE:HD12	1:A:54:PRO:HG3	1.85	0.58
1:E:196:ASN:O	1:E:200:HIS:CD2	2.57	0.58
1:B:27:TYR:OH	1:B:200:HIS:NE2	2.36	0.57
1:C:110:ASP:OD2	1:C:115:TYR:OH	2.23	0.57
1:B:147:ILE:HB	1:B:206:THR:HG22	1.87	0.57
1:B:198:LEU:HD23	1:B:264:PHE:CZ	2.38	0.57
1:D:101:ILE:N	1:D:101:ILE:HD12	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:ALA:HB3	1:D:248:ARG:NH1	2.19	0.57
1:A:49:VAL:HG12	1:A:94:VAL:HG11	1.87	0.57
1:B:189:ALA:CB	1:B:276:ARG:HH12	2.18	0.57
1:B:64:THR:HG22	2:B:285[B]:NAP:H2D	1.86	0.56
1:B:18:LEU:HD21	1:B:58:ILE:HD13	1.86	0.56
1:D:220:PHE:O	1:D:224:ILE:HG13	2.04	0.56
1:B:14:LEU:HD12	1:B:188:VAL:HG13	1.87	0.56
1:C:46:GLN:O	1:C:50:GLN:HG2	2.05	0.56
1:E:56:ILE:HD13	1:E:199:ILE:HB	1.85	0.56
1:E:237:VAL:HG11	1:E:241:GLU:HB2	1.87	0.56
1:E:187:TYR:CE2	1:E:189:ALA:HB3	2.39	0.56
1:D:117:GLU:HG2	1:D:258:MET:HG3	1.87	0.56
1:B:180:ASP:OD1	1:B:239:THR:HG22	2.06	0.56
1:C:189:ALA:O	1:C:193:VAL:HG23	2.06	0.56
1:D:39:ILE:HD13	1:D:61:ALA:HB3	1.87	0.56
1:E:182:ILE:HD11	1:E:251:TYR:CD2	2.41	0.55
1:D:202:SER:OG	1:E:42:ILE:HD11	2.04	0.55
1:A:56:ILE:HD13	1:A:199:ILE:HB	1.87	0.55
1:D:191:LEU:HD23	1:D:191:LEU:O	2.06	0.55
1:C:265:LEU:N	1:C:265:LEU:HD12	2.20	0.55
1:B:70:GLU:HG3	1:B:246:ALA:HB2	1.88	0.55
1:D:36:LEU:O	1:D:44:GLN:NE2	2.40	0.55
1:F:149:ARG:HD2	1:F:208:HIS:CE1	2.41	0.55
1:A:117:GLU:N	1:A:117:GLU:OE1	2.35	0.55
1:B:156:LYS:HE3	1:B:280:GLU:HB3	1.88	0.55
1:C:162:VAL:HA	1:C:224:ILE:HD13	1.89	0.55
1:C:18:LEU:HD21	1:C:58:ILE:HG21	1.88	0.55
1:D:218:PHE:CZ	1:D:222:LYS:HE3	2.42	0.55
1:E:104:ASP:OD1	1:E:252:SER:HB3	2.07	0.55
1:D:42:ILE:HG21	1:F:203:LEU:HD21	1.90	0.54
1:C:33:ASP:OD1	1:C:34:LYS:N	2.39	0.54
1:E:33:ASP:OD1	1:E:34:LYS:N	2.40	0.54
1:D:117:GLU:HG2	1:D:258:MET:CG	2.37	0.54
1:B:36:LEU:HD12	4:B:295:HOH:O	2.06	0.54
1:D:23:ASN:N	4:D:317:HOH:O	2.39	0.54
1:E:6:ILE:HD11	1:E:52:ILE:HG21	1.89	0.54
1:A:18:LEU:HD21	1:A:58:ILE:HD13	1.90	0.54
1:D:203:LEU:HD22	1:E:85:ARG:NH2	2.23	0.54
1:C:172[A]:ARG:N	1:C:172[A]:ARG:HD3	2.23	0.54
1:F:11:ASN:O	1:F:11:ASN:ND2	2.41	0.54
1:C:191:LEU:HD23	1:C:191:LEU:C	2.29	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:281:THR:O	1:E:281:THR:CG2	2.55	0.53
1:E:182:ILE:HD11	1:E:251:TYR:HD2	1.73	0.53
1:D:182:ILE:CG2	1:D:214:SER:OG	2.56	0.53
1:B:191:LEU:C	1:B:191:LEU:HD23	2.28	0.53
1:A:220:PHE:O	1:A:224:ILE:HG13	2.09	0.53
1:B:191:LEU:CD2	1:B:195:ILE:CD1	2.87	0.53
1:E:18:LEU:CD2	1:E:58:ILE:HG21	2.39	0.53
1:F:149:ARG:HH11	1:F:208:HIS:HE1	1.55	0.53
1:A:40:THR:CG2	1:A:79:ILE:HD13	2.38	0.53
1:A:33:ASP:OD1	1:A:34:LYS:N	2.35	0.53
1:B:110:ASP:OD2	1:B:115:TYR:OH	2.21	0.53
1:A:46:GLN:O	1:A:50:GLN:HG2	2.08	0.53
1:A:41:ASN:O	1:A:45:VAL:HG23	2.09	0.52
1:F:67:ASP:OD1	1:F:248:ARG:NH1	2.27	0.52
1:B:50:GLN:NE2	1:B:93:LEU:HD21	2.25	0.52
1:D:262:ASN:HD21	1:E:82:ILE:HD12	1.74	0.52
1:D:33:ASP:OD1	1:D:34:LYS:N	2.37	0.52
1:C:6:ILE:HD12	1:C:54:PRO:HG3	1.92	0.52
1:F:49:VAL:HG12	1:F:94:VAL:HG21	1.92	0.52
1:A:220:PHE:CE2	1:A:224:ILE:HD11	2.45	0.52
1:C:18:LEU:CD2	1:C:58:ILE:HG21	2.40	0.52
1:A:215:CYS:SG	1:A:220:PHE:HB2	2.50	0.52
1:B:5:VAL:HG22	1:B:56:ILE:HB	1.92	0.52
1:D:152:TRP:CZ2	1:D:183:GLY:HA3	2.44	0.52
1:E:94:VAL:O	1:E:94:VAL:CG1	2.58	0.52
1:A:14:LEU:HD21	1:A:153:LEU:HD21	1.91	0.51
1:F:111:ARG:HH11	1:F:111:ARG:HG2	1.74	0.51
1:B:64:THR:CG2	2:B:285[B]:NAP:H2D	2.40	0.51
1:C:271:GLU:O	1:C:275:GLU:HG3	2.09	0.51
1:E:246:ALA:HB3	1:E:248:ARG:NH1	2.26	0.51
1:C:191:LEU:CD2	1:C:195:ILE:CD1	2.88	0.51
1:A:181:GLN:HE21	1:A:239:THR:CG2	2.24	0.51
1:D:85:ARG:O	1:D:89:VAL:HG23	2.10	0.51
1:C:117:GLU:N	1:C:117:GLU:OE1	2.38	0.51
1:C:160:ASN:O	1:C:164:THR:HG23	2.10	0.51
1:D:8:THR:O	1:D:60:CYS:HB2	2.10	0.51
1:B:189:ALA:HB1	1:B:276:ARG:NH1	2.24	0.51
1:E:117:GLU:N	1:E:117:GLU:OE1	2.40	0.51
1:F:111:ARG:HH11	1:F:111:ARG:HG3	1.76	0.50
1:C:237:VAL:CG1	1:C:241:GLU:HB2	2.41	0.50
1:B:70:GLU:CG	1:B:246:ALA:HB2	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:HIS:CE1	1:A:87:VAL:HG21	2.46	0.50
1:C:191:LEU:HD23	1:C:191:LEU:O	2.11	0.50
1:F:218:PHE:CZ	1:F:222:LYS:HE3	2.45	0.50
1:B:220:PHE:O	1:B:224:ILE:HG13	2.12	0.50
1:A:101:ILE:O	1:A:131:LYS:NZ	2.23	0.50
1:D:3:GLU:OE1	1:D:3:GLU:N	2.44	0.50
1:B:104:ASP:HB3	1:B:254:PHE:CZ	2.47	0.50
1:D:8:THR:OG1	1:D:59:HIS:HA	2.11	0.50
1:B:191:LEU:HD23	1:B:195:ILE:HG13	1.93	0.50
1:E:271:GLU:O	1:E:275:GLU:HG3	2.12	0.50
1:D:191:LEU:C	1:D:191:LEU:HD23	2.32	0.49
1:D:223:LYS:HE3	1:D:227:TYR:CE2	2.47	0.49
1:B:113:GLU:OE2	1:B:113:GLU:N	2.41	0.49
1:B:189:ALA:CB	1:B:276:ARG:NH1	2.75	0.49
1:B:202:SER:OG	1:C:42:ILE:HD11	2.12	0.49
1:A:203:LEU:HD22	1:B:85:ARG:NH2	2.27	0.49
1:F:46:GLN:O	1:F:50:GLN:HG2	2.12	0.49
1:A:246:ALA:HB3	1:A:248:ARG:NH1	2.28	0.49
1:D:187:TYR:CE2	1:D:189:ALA:HB3	2.47	0.49
1:E:168:LEU:HD22	1:E:172:ARG:HH22	1.77	0.49
1:D:174:GLU:OE1	1:D:235:LEU:HD11	2.12	0.49
1:E:105:TYR:HD2	1:E:127:TYR:CD2	2.30	0.49
1:D:49:VAL:HG12	1:D:94:VAL:HG11	1.92	0.49
1:B:235:LEU:HD23	1:F:236:PRO:HG3	1.95	0.49
1:B:206:THR:O	1:B:258:MET:HG3	2.12	0.49
1:B:33:ASP:OD1	1:B:34:LYS:N	2.44	0.49
1:C:237:VAL:HG13	1:C:241:GLU:HB2	1.95	0.49
1:D:154:TYR:CD2	1:D:162:VAL:HG21	2.47	0.49
1:F:29:ILE:HG22	1:F:31:PRO:HD3	1.94	0.48
1:E:13:GLN:HG2	1:E:157:TYR:O	2.12	0.48
1:E:6:ILE:HD13	1:E:30:TYR:HB2	1.95	0.48
1:B:262:ASN:HD22	1:B:262:ASN:N	2.11	0.48
1:F:47:GLN:HG2	4:F:296:HOH:O	2.13	0.48
1:F:14:LEU:CD2	1:F:188:VAL:HG13	2.42	0.48
1:D:160:ASN:HD21	1:D:163:LYS:H	1.60	0.48
1:F:10:ALA:HA	1:F:15:GLY:HA3	1.95	0.48
1:E:95:GLY:HA2	4:E:304:HOH:O	2.13	0.48
1:C:14:LEU:CD2	1:C:188:VAL:HG13	2.43	0.48
1:D:161:PHE:CE1	1:D:165:MET:CE	2.96	0.48
1:C:18:LEU:HD21	1:C:58:ILE:HD13	1.96	0.48
1:E:32:PHE:HZ	1:E:52:ILE:HD11	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:104:ASP:HB3	1:E:254:PHE:CZ	2.48	0.48
1:F:109:GLY:HA3	1:F:249:PRO:HB3	1.96	0.48
1:C:102:SER:HB3	1:C:149:ARG:HG2	1.95	0.47
1:C:36:LEU:O	1:C:44:GLN:NE2	2.47	0.47
1:A:203:LEU:HD21	1:B:42:ILE:HG21	1.95	0.47
1:B:39:ILE:HD13	1:B:61:ALA:CB	2.43	0.47
1:A:204:TYR:O	1:B:85:ARG:HD2	2.14	0.47
1:D:121:PRO:HG2	1:D:132:TYR:CE1	2.50	0.47
1:F:104:ASP:C	1:F:106:VAL:H	2.18	0.47
1:F:103:THR:OG1	1:F:104:ASP:N	2.47	0.47
1:B:101:ILE:HG22	2:B:285[A]:NAP:H1D	1.97	0.47
1:C:168:LEU:HD22	1:C:172[A]:ARG:NH2	2.29	0.47
1:D:252:SER:OG	1:D:252:SER:O	2.31	0.47
1:C:149:ARG:HD2	1:C:208:HIS:CD2	2.50	0.47
1:B:173:GLU:N	1:B:173:GLU:OE1	2.48	0.47
1:D:109:GLY:HA3	1:D:249:PRO:CB	2.45	0.47
1:B:8:THR:O	1:B:60:CYS:HB2	2.14	0.47
1:E:154:TYR:CD2	1:E:162:VAL:HG21	2.50	0.47
1:E:8:THR:OG1	1:E:59:HIS:HA	2.15	0.47
1:F:190:ASP:OD1	1:F:276:ARG:NH2	2.47	0.47
1:A:39:ILE:HG22	2:A:285:NAP:H62A	1.80	0.47
1:C:160:ASN:ND2	1:C:160:ASN:C	2.64	0.46
1:D:113:GLU:OE2	1:D:113:GLU:N	2.36	0.46
1:B:274:LEU:O	1:B:277:PHE:HB3	2.15	0.46
1:A:174:GLU:HG2	1:A:233:ASN:HB2	1.97	0.46
1:D:147:ILE:HD12	1:D:206:THR:CG2	2.45	0.46
1:E:237:VAL:HG12	1:E:238:SER:N	2.31	0.46
1:A:181:GLN:HE21	1:A:239:THR:HG22	1.79	0.46
1:B:203:LEU:HD22	1:C:85:ARG:NH2	2.31	0.46
1:D:260:ARG:NH2	1:E:74:ASP:OD2	2.46	0.46
1:F:41:ASN:O	1:F:45:VAL:HG23	2.15	0.46
1:F:237:VAL:HG12	1:F:238:SER:N	2.31	0.46
1:A:215:CYS:SG	1:A:216:SER:N	2.87	0.46
1:D:152:TRP:CE2	1:D:183:GLY:HA3	2.51	0.46
1:B:22:LEU:HB2	1:B:29:ILE:HD11	1.98	0.46
1:D:42:ILE:HD12	1:F:203:LEU:HD23	1.97	0.45
1:A:191:LEU:HD12	1:A:209:VAL:HG11	1.98	0.45
1:F:94:VAL:HG12	1:F:94:VAL:O	2.15	0.45
1:E:53:ARG:HG2	1:E:53:ARG:HH11	1.80	0.45
1:C:265:LEU:CD1	1:C:265:LEU:H	2.29	0.45
1:D:131:LYS:HA	1:D:131:LYS:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:VAL:O	1:A:93:LEU:HD13	2.16	0.45
1:F:168:LEU:HD13	1:F:172:ARG:HH21	1.81	0.45
1:E:33:ASP:OD2	1:E:35:LYS:NZ	2.49	0.45
1:E:27:TYR:OH	1:E:200:HIS:CE1	2.70	0.45
1:E:271:GLU:OE1	1:E:271:GLU:N	2.46	0.45
1:A:113:GLU:OE2	1:A:113:GLU:N	2.36	0.45
1:E:139:LYS:HG3	1:E:147:ILE:HD11	1.99	0.45
1:E:189:ALA:O	1:E:193:VAL:HG23	2.17	0.45
1:E:222:LYS:HB3	1:E:222:LYS:NZ	2.31	0.45
1:A:190:ASP:OD1	1:A:276:ARG:NH1	2.44	0.45
1:E:218:PHE:CZ	1:E:222:LYS:HD2	2.52	0.45
1:F:72:GLU:OE2	1:F:75:LEU:HD23	2.16	0.45
1:A:180:ASP:CG	1:A:239:THR:HG23	2.37	0.44
1:F:19:GLN:NE2	1:F:31:PRO:HG3	2.32	0.44
1:C:265:LEU:HD12	1:C:265:LEU:H	1.81	0.44
1:A:39:ILE:CD1	1:A:59:HIS:CE1	3.00	0.44
1:A:212:THR:HG22	1:A:213:GLY:N	2.31	0.44
1:E:57:ILE:HD12	1:E:91:SER:OG	2.18	0.44
1:E:73:ARG:NE	4:E:300:HOH:O	2.49	0.44
1:D:154:TYR:O	1:D:188:VAL:HG23	2.17	0.44
1:F:97:LYS:NZ	1:F:202:SER:HB3	2.32	0.44
1:C:207:TYR:OH	1:C:262:ASN:ND2	2.51	0.44
1:E:64:THR:O	1:E:64:THR:HG22	2.17	0.44
1:F:201:THR:HB	1:F:203:LEU:HG	1.99	0.44
1:B:203:LEU:HD23	1:C:42:ILE:HD12	1.99	0.44
1:C:13:GLN:NE2	1:C:159:ASN:O	2.50	0.44
1:C:32:PHE:HZ	1:C:52:ILE:HD11	1.83	0.44
1:F:42:ILE:HG22	4:F:318:HOH:O	2.17	0.44
1:B:191:LEU:HD23	1:B:191:LEU:O	2.18	0.43
1:B:103:THR:OG1	1:B:105:TYR:HD2	2.01	0.43
1:B:85:ARG:O	1:B:89:VAL:HG23	2.18	0.43
1:D:18:LEU:HD21	1:D:58:ILE:HG21	1.99	0.43
1:C:265:LEU:CD1	1:C:265:LEU:N	2.82	0.43
1:C:131:LYS:NZ	2:C:285:NAP:O3D	2.48	0.43
1:F:201:THR:O	1:F:202:SER:OG	2.23	0.43
1:E:168:LEU:HD22	1:E:172:ARG:NH2	2.33	0.43
1:F:220:PHE:O	1:F:224:ILE:HG13	2.18	0.43
1:C:59:HIS:CE1	1:C:87:VAL:HG21	2.54	0.43
1:B:14:LEU:CD1	1:B:188:VAL:HG13	2.48	0.43
1:D:39:ILE:HD13	1:D:61:ALA:CB	2.48	0.43
1:F:111:ARG:CG	1:F:111:ARG:NH1	2.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:18:LEU:HD21	1:E:58:ILE:HD13	2.00	0.43
1:C:206:THR:O	1:C:258:MET:HG3	2.19	0.43
1:C:121:PRO:HG2	1:C:132:TYR:CE1	2.54	0.43
1:D:175:ILE:HG22	1:D:176:SER:N	2.33	0.43
1:B:218:PHE:CE2	1:B:222:LYS:HE3	2.53	0.43
1:B:187:TYR:CE2	1:B:189:ALA:HB3	2.53	0.43
1:F:29:ILE:HD12	1:F:29:ILE:H	1.83	0.43
1:F:169:GLY:HA3	1:F:230:MET:CE	2.48	0.43
1:F:174:GLU:HG2	1:F:233:ASN:HB3	1.99	0.43
1:E:66:VAL:HG12	1:E:246:ALA:CB	2.49	0.43
1:D:109:GLY:HA3	1:D:249:PRO:HB3	2.01	0.43
1:E:8:THR:O	1:E:60:CYS:HB2	2.19	0.42
1:E:132:TYR:OH	1:E:136:GLN:NE2	2.51	0.42
1:B:39:ILE:HD13	1:B:61:ALA:HB3	2.00	0.42
1:A:218:PHE:CZ	1:A:222:LYS:HE2	2.53	0.42
1:D:134:GLY:O	1:D:138:VAL:HG23	2.19	0.42
1:A:203:LEU:HD23	1:B:42:ILE:HD12	2.01	0.42
1:B:207:TYR:CE1	1:B:258:MET:HB3	2.54	0.42
1:D:50:GLN:HA	1:D:50:GLN:NE2	2.35	0.42
1:D:182:ILE:CD1	1:D:182:ILE:N	2.82	0.42
1:D:61:ALA:O	1:D:62:ALA:HB2	2.19	0.42
1:A:18:LEU:CD2	1:A:58:ILE:HG21	2.50	0.42
1:F:56:ILE:HD13	1:F:199:ILE:HB	2.01	0.42
1:A:8:THR:OG1	1:A:59:HIS:HA	2.20	0.42
1:B:50:GLN:NE2	1:B:93:LEU:HD23	2.33	0.42
1:D:102:SER:HB3	1:D:149:ARG:HG2	2.01	0.42
1:A:193:VAL:O	1:A:197:LYS:HG3	2.20	0.42
1:E:54:PRO:O	1:E:96:ALA:HB2	2.19	0.42
1:C:111:ARG:HA	1:C:112:PRO:HD3	1.93	0.42
1:B:50:GLN:HE21	1:B:93:LEU:CD2	2.32	0.42
1:E:193:VAL:HG23	4:E:320:HOH:O	2.20	0.42
1:D:136:GLN:O	1:D:140:GLU:HG3	2.20	0.42
1:F:121:PRO:HG2	1:F:132:TYR:CE1	2.55	0.41
1:A:10:ALA:HA	1:A:15:GLY:HA3	2.02	0.41
1:A:54:PRO:O	1:A:96:ALA:HB2	2.20	0.41
1:D:101:ILE:N	1:D:101:ILE:CD1	2.83	0.41
1:E:13:GLN:OE1	1:E:160:ASN:HB3	2.21	0.41
1:C:131:LYS:NZ	2:C:285:NAP:O2D	2.49	0.41
1:D:170:LYS:O	1:D:170:LYS:HG3	2.20	0.41
1:A:121:PRO:HG2	1:A:132:TYR:CE1	2.56	0.41
1:F:33:ASP:OD1	1:F:34:LYS:N	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:94:VAL:O	1:E:94:VAL:HG13	2.20	0.41
1:E:36:LEU:O	1:E:44:GLN:NE2	2.54	0.41
1:B:228:ALA:O	1:B:229:ASN:C	2.58	0.41
1:C:103:THR:HG21	1:C:127:TYR:CE2	2.56	0.41
1:F:158:GLY:O	1:F:163:LYS:NZ	2.51	0.41
1:C:104:ASP:OD1	1:C:252:SER:HB3	2.20	0.41
1:A:187:TYR:CE2	1:A:189:ALA:HB3	2.55	0.41
1:F:4:ARG:HB2	1:F:54:PRO:HA	2.02	0.41
1:D:14:LEU:O	1:D:15:GLY:C	2.59	0.41
1:A:179:ALA:HB2	1:A:218:PHE:HB2	2.02	0.41
1:B:276:ARG:HA	1:B:279:ILE:HD12	2.03	0.41
1:A:6:ILE:CD1	1:A:54:PRO:HG3	2.49	0.41
1:E:78:VAL:O	1:E:82:ILE:HB	2.21	0.41
1:F:53:ARG:HG3	1:F:94:VAL:HG13	2.03	0.41
1:D:50:GLN:HE21	1:D:50:GLN:HA	1.86	0.41
1:B:171:GLU:O	1:B:172:ARG:HB2	2.21	0.41
1:B:6:ILE:HD12	1:B:54:PRO:HG3	2.02	0.41
1:A:72:GLU:OE2	1:A:75:LEU:HD23	2.20	0.41
2:B:285[B]:NAP:O3B	2:B:285[B]:NAP:O2A	2.35	0.40
1:B:103:THR:HG21	1:B:127:TYR:CE2	2.56	0.40
1:F:32:PHE:HZ	1:F:52:ILE:HD11	1.87	0.40
1:C:182:ILE:O	1:C:251:TYR:HA	2.21	0.40
1:D:15:GLY:O	1:D:19:GLN:HB2	2.21	0.40
1:D:23:ASN:HB3	4:D:317:HOH:O	2.21	0.40
1:B:162:VAL:HA	1:B:224:ILE:HD13	2.03	0.40
1:E:46:GLN:O	1:E:50:GLN:HG2	2.20	0.40
1:F:6:ILE:HD12	1:F:54:PRO:HG3	2.03	0.40
1:C:29:ILE:HG22	1:C:31:PRO:HD3	2.03	0.40
1:B:212:THR:HG22	1:B:213:GLY:N	2.36	0.40
1:A:39:ILE:HD11	1:A:59:HIS:CE1	2.55	0.40
1:A:5:VAL:HG23	1:A:5:VAL:O	2.21	0.40
1:A:270:TRP:CE2	1:A:271:GLU:HG3	2.56	0.40
1:D:6:ILE:HD12	1:D:54:PRO:HG3	2.03	0.40
1:D:199:ILE:HG13	1:D:200:HIS:CD2	2.57	0.40
1:B:207:TYR:CD1	1:B:258:MET:HB3	2.56	0.40
1:F:29:ILE:N	1:F:29:ILE:CD1	2.83	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	282/287 (98%)	265 (94%)	16 (6%)	1 (0%)	39	65
1	B	277/287 (96%)	266 (96%)	11 (4%)	0	100	100
1	C	282/287 (98%)	274 (97%)	8 (3%)	0	100	100
1	D	283/287 (99%)	266 (94%)	17 (6%)	0	100	100
1	E	275/287 (96%)	264 (96%)	11 (4%)	0	100	100
1	F	280/287 (98%)	266 (95%)	14 (5%)	0	100	100
All	All	1679/1722 (98%)	1601 (95%)	77 (5%)	1 (0%)	56	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	243	GLY

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	245/247 (99%)	245 (100%)	0	100	100
1	B	242/247 (98%)	241 (100%)	1 (0%)	93	98
1	C	245/247 (99%)	244 (100%)	1 (0%)	93	98
1	D	245/247 (99%)	242 (99%)	3 (1%)	78	92
1	E	243/247 (98%)	241 (99%)	2 (1%)	86	95
1	F	243/247 (98%)	238 (98%)	5 (2%)	61	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1463/1482 (99%)	1451 (99%)	12 (1%)	86	95

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	262	ASN
1	C	160	ASN
1	D	160	ASN
1	D	172	ARG
1	D	252	SER
1	E	53	ARG
1	E	113	GLU
1	F	11	ASN
1	F	111	ARG
1	F	160	ASN
1	F	197	LYS
1	F	265	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	47	GLN
1	A	59	HIS
1	A	68	GLN
1	A	181	GLN
1	A	255	GLN
1	A	262	ASN
1	B	13	GLN
1	B	47	GLN
1	B	50	GLN
1	B	92	GLN
1	B	181	GLN
1	B	211	ASN
1	B	229	ASN
1	B	266	GLN
1	C	47	GLN
1	C	92	GLN
1	C	108	GLN
1	C	160	ASN
1	C	255	GLN

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Mol	Chain	Res	Type
1	C	266	GLN
1	D	92	GLN
1	D	160	ASN
1	D	211	ASN
1	D	266	GLN
1	E	47	GLN
1	E	120	ASN
1	E	211	ASN
1	F	11	ASN
1	F	68	GLN
1	F	136	GLN
1	F	160	ASN
1	F	208	HIS
1	F	211	ASN
1	F	255	GLN
1	F	262	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

24 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	NAP	A	285	-	42,52,52	0.70	1 (2%)	54,80,80	1.71	7 (12%)
3	SO4	A	286	-	4,4,4	0.19	0	6,6,6	0.10	0
3	SO4	A	287	-	4,4,4	0.20	0	6,6,6	0.08	0
2	NAP	B	285[A]	-	42,52,52	0.68	1 (2%)	54,80,80	1.79	6 (11%)
2	NAP	B	285[B]	-	42,52,52	0.70	1 (2%)	54,80,80	1.67	4 (7%)
3	SO4	B	286	-	4,4,4	0.21	0	6,6,6	0.18	0
3	SO4	B	287	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	B	288	-	4,4,4	0.19	0	6,6,6	0.09	0
3	SO4	B	289	-	4,4,4	0.19	0	6,6,6	0.09	0
2	NAP	C	285	-	42,52,52	0.69	1 (2%)	54,80,80	1.65	5 (9%)
3	SO4	C	286	-	4,4,4	0.21	0	6,6,6	0.14	0
3	SO4	C	287	-	4,4,4	0.22	0	6,6,6	0.13	0
2	NAP	D	285	-	42,52,52	0.72	1 (2%)	54,80,80	1.78	6 (11%)
3	SO4	D	286	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	D	287	-	4,4,4	0.23	0	6,6,6	0.13	0
2	NAP	E	285	-	42,52,52	0.71	1 (2%)	54,80,80	1.85	7 (12%)
3	SO4	E	286	-	4,4,4	0.22	0	6,6,6	0.16	0
3	SO4	E	287	-	4,4,4	0.20	0	6,6,6	0.11	0
3	SO4	E	288	-	4,4,4	0.20	0	6,6,6	0.11	0
3	SO4	E	289	-	4,4,4	0.21	0	6,6,6	0.15	0
2	NAP	F	285	-	42,52,52	0.71	1 (2%)	54,80,80	1.76	4 (7%)
3	SO4	F	286	-	4,4,4	0.20	0	6,6,6	0.13	0
3	SO4	F	287	-	4,4,4	0.21	0	6,6,6	0.14	0
3	SO4	F	288	-	4,4,4	0.21	0	6,6,6	0.13	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	NAP	A	285	-	-	0/27/67/67	0/5/5/5
3	SO4	A	286	-	-	0/0/0/0	0/0/0/0
3	SO4	A	287	-	-	0/0/0/0	0/0/0/0
2	NAP	B	285[A]	-	-	0/27/67/67	0/5/5/5
2	NAP	B	285[B]	-	-	0/27/67/67	0/5/5/5
3	SO4	B	286	-	-	0/0/0/0	0/0/0/0
3	SO4	B	287	-	-	0/0/0/0	0/0/0/0
3	SO4	B	288	-	-	0/0/0/0	0/0/0/0
3	SO4	B	289	-	-	0/0/0/0	0/0/0/0
2	NAP	C	285	-	-	0/27/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	C	286	-	-	0/0/0/0	0/0/0/0
3	SO4	C	287	-	-	0/0/0/0	0/0/0/0
2	NAP	D	285	-	-	0/27/67/67	0/5/5/5
3	SO4	D	286	-	-	0/0/0/0	0/0/0/0
3	SO4	D	287	-	-	0/0/0/0	0/0/0/0
2	NAP	E	285	-	-	0/27/67/67	0/5/5/5
3	SO4	E	286	-	-	0/0/0/0	0/0/0/0
3	SO4	E	287	-	-	0/0/0/0	0/0/0/0
3	SO4	E	288	-	-	0/0/0/0	0/0/0/0
3	SO4	E	289	-	-	0/0/0/0	0/0/0/0
2	NAP	F	285	-	-	0/27/67/67	0/5/5/5
3	SO4	F	286	-	-	0/0/0/0	0/0/0/0
3	SO4	F	287	-	-	0/0/0/0	0/0/0/0
3	SO4	F	288	-	-	0/0/0/0	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	285	NAP	O4D-C1D	2.01	1.43	1.41
2	B	285[B]	NAP	O4D-C1D	2.02	1.43	1.41
2	E	285	NAP	O4D-C1D	2.04	1.43	1.41
2	A	285	NAP	O4D-C1D	2.08	1.43	1.41
2	D	285	NAP	O4B-C1B	2.12	1.43	1.41
2	B	285[A]	NAP	O4D-C1D	2.13	1.43	1.41
2	F	285	NAP	O4D-C1D	2.25	1.44	1.41

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	285	NAP	N3A-C2A-N1A	-9.61	121.54	128.89
2	B	285[A]	NAP	N3A-C2A-N1A	-9.47	121.64	128.89
2	D	285	NAP	N3A-C2A-N1A	-9.47	121.64	128.89
2	B	285[B]	NAP	N3A-C2A-N1A	-9.25	121.81	128.89
2	A	285	NAP	N3A-C2A-N1A	-9.16	121.88	128.89
2	C	285	NAP	N3A-C2A-N1A	-9.01	122.00	128.89
2	F	285	NAP	N3A-C2A-N1A	-8.81	122.15	128.89
2	E	285	NAP	PN-O3-PA	-4.22	120.88	132.73
2	F	285	NAP	PN-O3-PA	-3.78	122.12	132.73
2	C	285	NAP	PN-O3-PA	-3.76	122.17	132.73
2	B	285[B]	NAP	PN-O3-PA	-3.55	122.76	132.73
2	A	285	NAP	PN-O3-PA	-3.43	123.09	132.73
2	B	285[A]	NAP	PN-O3-PA	-3.27	123.55	132.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	285[A]	NAP	C4B-O4B-C1B	-3.02	106.41	109.72
2	D	285	NAP	C4B-O4B-C1B	-2.69	106.76	109.72
2	D	285	NAP	PN-O3-PA	-2.56	125.54	132.73
2	E	285	NAP	C1B-N9A-C4A	-2.51	123.16	126.94
2	E	285	NAP	C4B-O4B-C1B	-2.43	107.05	109.72
2	C	285	NAP	C1B-N9A-C4A	-2.17	123.67	126.94
2	A	285	NAP	C4B-O4B-C1B	-2.05	107.46	109.72
2	A	285	NAP	C1B-N9A-C4A	-2.05	123.84	126.94
2	B	285[A]	NAP	C1B-N9A-C4A	-2.04	123.86	126.94
2	A	285	NAP	C3N-C7N-N7N	2.12	120.14	117.82
2	C	285	NAP	O4D-C1D-N1N	2.24	110.59	108.13
2	A	285	NAP	O4D-C1D-N1N	2.31	110.67	108.13
2	B	285[B]	NAP	O4B-C1B-N9A	2.33	112.97	108.10
2	D	285	NAP	C3N-C7N-N7N	2.36	120.41	117.82
2	E	285	NAP	C3N-C7N-N7N	2.40	120.44	117.82
2	B	285[A]	NAP	O4D-C1D-N1N	2.85	111.26	108.13
2	E	285	NAP	O4B-C1B-N9A	2.90	114.17	108.10
2	C	285	NAP	O4B-C1B-N9A	2.94	114.26	108.10
2	D	285	NAP	O4D-C1D-N1N	2.96	111.39	108.13
2	F	285	NAP	O4B-C1B-N9A	3.13	114.64	108.10
2	B	285[B]	NAP	O4D-C1D-N1N	3.40	111.86	108.13
2	A	285	NAP	O4B-C1B-N9A	3.40	115.22	108.10
2	E	285	NAP	O4D-C1D-N1N	3.54	112.02	108.13
2	B	285[A]	NAP	O4B-C1B-N9A	3.66	115.76	108.10
2	D	285	NAP	O4B-C1B-N9A	3.69	115.82	108.10
2	F	285	NAP	O4D-C1D-N1N	4.65	113.24	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	285	NAP	3	0
2	B	285[A]	NAP	2	0
2	B	285[B]	NAP	3	0
2	C	285	NAP	2	0
3	D	287	SO4	1	0
2	F	285	NAP	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, 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	281/287 (97%)	0.12	8 (2%) 56 55	36, 63, 89, 109	0
1	B	280/287 (97%)	-0.15	0 100 100	31, 49, 67, 75	0
1	C	281/287 (97%)	-0.26	1 (0%) 93 94	37, 53, 71, 85	0
1	D	283/287 (98%)	0.05	8 (2%) 56 55	38, 59, 83, 98	0
1	E	278/287 (96%)	-0.07	2 (0%) 89 89	39, 57, 80, 95	0
1	F	281/287 (97%)	-0.08	3 (1%) 82 82	36, 51, 69, 89	0
All	All	1684/1722 (97%)	-0.06	22 (1%) 79 79	31, 55, 80, 109	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	282	LYS	4.6
1	A	245	ALA	4.3
1	F	1	MET	3.5
1	E	242	PHE	3.2
1	D	244	ALA	3.0
1	D	172	ARG	2.9
1	D	25	GLU	2.9
1	A	240	GLU	2.8
1	F	101	ILE	2.7
1	A	244	ALA	2.5
1	D	73	ARG	2.4
1	A	278	PHE	2.4
1	D	101	ILE	2.3
1	F	25	GLU	2.2
1	A	36	LEU	2.2
1	A	241	GLU	2.1
1	D	168	LEU	2.1
1	E	159	ASN	2.1
1	D	243	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	151	SER	2.1
1	A	242	PHE	2.0
1	D	148	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	SO4	B	288	5/5	0.85	0.23	2.01	73,73,75,75	5
3	SO4	D	287	5/5	0.86	0.24	1.24	67,69,70,71	5
3	SO4	F	287	5/5	0.82	0.29	1.09	78,79,79,80	5
2	NAP	B	285[A]	48/48	0.94	0.21	0.43	23,36,53,56	48
2	NAP	B	285[B]	48/48	0.94	0.21	0.39	65,68,82,83	48
2	NAP	D	285	48/48	0.93	0.17	-0.36	49,54,68,70	0
3	SO4	E	289	5/5	0.89	0.17	-0.62	73,74,75,75	5
2	NAP	E	285	48/48	0.95	0.14	-0.79	46,55,70,72	0
2	NAP	C	285	48/48	0.96	0.13	-0.83	42,49,61,63	0
2	NAP	A	285	48/48	0.95	0.15	-0.92	48,59,76,77	0
2	NAP	F	285	48/48	0.96	0.13	-1.03	47,51,66,68	0
3	SO4	C	287	5/5	0.91	0.18	-	67,69,69,70	5
3	SO4	E	288	5/5	0.83	0.44	-	89,89,90,90	5
3	SO4	C	286	5/5	0.95	0.22	-	52,54,55,56	5
3	SO4	A	287	5/5	0.82	0.40	-	100,100,100,100	5
3	SO4	B	286	5/5	0.95	0.16	-	69,71,72,74	0
3	SO4	B	287	5/5	0.95	0.15	-	69,71,72,72	5
3	SO4	E	286	5/5	0.89	0.18	-	73,73,75,75	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	SO4	F	288	5/5	0.52	0.34	-	104,104,105,105	5
3	SO4	D	286	5/5	0.87	0.20	-	78,79,79,80	5
3	SO4	A	286	5/5	0.89	0.24	-	80,80,80,81	5
3	SO4	E	287	5/5	0.77	0.42	-	90,90,91,91	5
3	SO4	F	286	5/5	0.69	0.29	-	77,78,79,79	5
3	SO4	B	289	5/5	0.76	0.47	-	95,95,95,95	5

6.5 Other polymers [i](#)

There are no such residues in this entry.