Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:47 PM GMT

PDB ID	:	3S4S
Title	:	Crystal structure of CD4 mutant bound to HLA-DR1
Authors	:	Li, Y.
Deposited on	:	2011-05-20
Resolution	:	2.40 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:

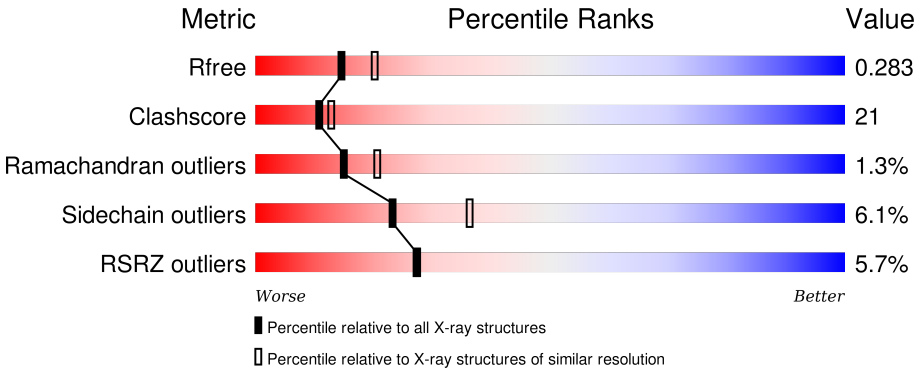
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	182	68% 29%
1	D	182	70% 27%
2	B	193	58% 35%
2	E	193	8% 58% 35%
3	C	13	62% 31% 8%

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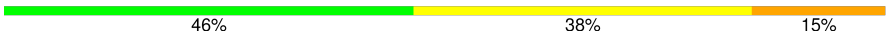
Mol	Chain	Length	Quality of chain
3	F	13	
4	G	191	
4	H	191	

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
5	GOL	E	961	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8924 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 HLA class II histocompatibility antigen, DR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1464	949	237	273	5			
1	D	180	Total	C	N	O	S	0	0	0
			1472	953	239	275	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	177	GLN	HIS	CONFLICT	UNP P01903
D	177	GLN	HIS	CONFLICT	UNP P01903

- Molecule 2 is a protein called HLA class II histocompatibility antigen, DRB1-1 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	186	Total	C	N	O	S	0	0	0
			1507	947	268	285	7			
2	E	185	Total	C	N	O	S	0	0	0
			1505	947	267	284	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	EXPRESSION TAG	UNP P04229
E	0	MET	-	EXPRESSION TAG	UNP P04229

- Molecule 3 is a protein called Hemagglutinin peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	13	Total	C	N	O	0	0	0
			105	69	18	18			
3	F	13	Total	C	N	O	0	0	0
			103	68	18	17			

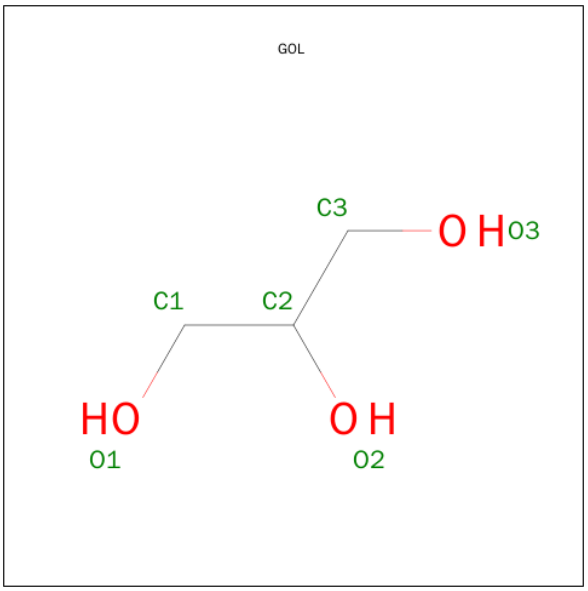
- Molecule 4 is a protein called T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	176	Total	C	N	O	S	0	0	0
			1354	852	236	262	4			
4	H	175	Total	C	N	O	S	0	0	0
			1328	833	233	258	4			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-3	ASP	-	EXPRESSION TAG	UNP P01730
G	-2	LEU	-	EXPRESSION TAG	UNP P01730
G	-1	GLY	-	EXPRESSION TAG	UNP P01730
G	0	SER	-	EXPRESSION TAG	UNP P01730
G	40	TYR	GLN	CONFLICT	UNP P01730
G	45	TRP	THR	CONFLICT	UNP P01730
G	179	ALA	-	EXPRESSION TAG	UNP P01730
G	180	ALA	-	EXPRESSION TAG	UNP P01730
G	181	ALA	-	EXPRESSION TAG	UNP P01730
G	182	HIS	-	EXPRESSION TAG	UNP P01730
G	183	HIS	-	EXPRESSION TAG	UNP P01730
G	184	HIS	-	EXPRESSION TAG	UNP P01730
G	185	HIS	-	EXPRESSION TAG	UNP P01730
G	186	HIS	-	EXPRESSION TAG	UNP P01730
G	187	HIS	-	EXPRESSION TAG	UNP P01730
H	-3	ASP	-	EXPRESSION TAG	UNP P01730
H	-2	LEU	-	EXPRESSION TAG	UNP P01730
H	-1	GLY	-	EXPRESSION TAG	UNP P01730
H	0	SER	-	EXPRESSION TAG	UNP P01730
H	40	TYR	GLN	CONFLICT	UNP P01730
H	45	TRP	THR	CONFLICT	UNP P01730
H	179	ALA	-	EXPRESSION TAG	UNP P01730
H	180	ALA	-	EXPRESSION TAG	UNP P01730
H	181	ALA	-	EXPRESSION TAG	UNP P01730
H	182	HIS	-	EXPRESSION TAG	UNP P01730
H	183	HIS	-	EXPRESSION TAG	UNP P01730
H	184	HIS	-	EXPRESSION TAG	UNP P01730
H	185	HIS	-	EXPRESSION TAG	UNP P01730
H	186	HIS	-	EXPRESSION TAG	UNP P01730
H	187	HIS	-	EXPRESSION TAG	UNP P01730

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

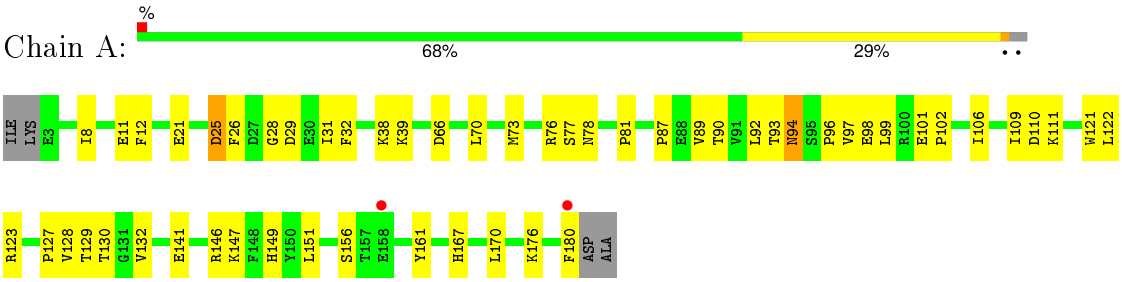
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	16	Total O 16 16	0	0
6	B	15	Total O 15 15	0	0
6	G	1	Total O 1 1	0	0
6	D	14	Total O 14 14	0	0
6	E	19	Total O 19 19	0	0
6	H	3	Total O 3 3	0	0

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.

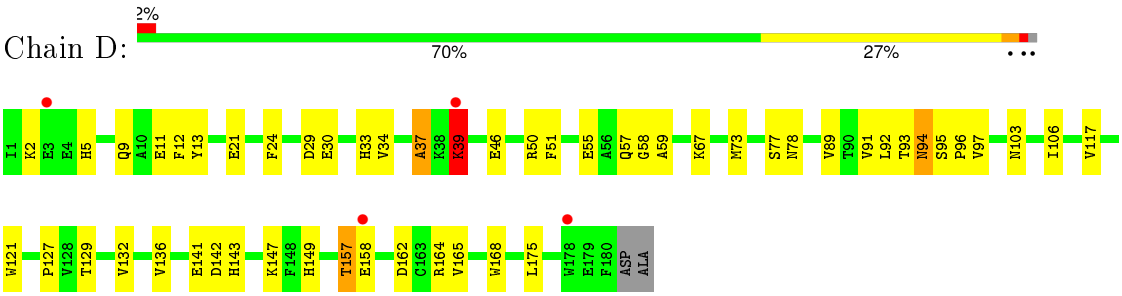
• Molecule 1: HLA class II histocompatibility antigen, DR alpha chain

Chain A:



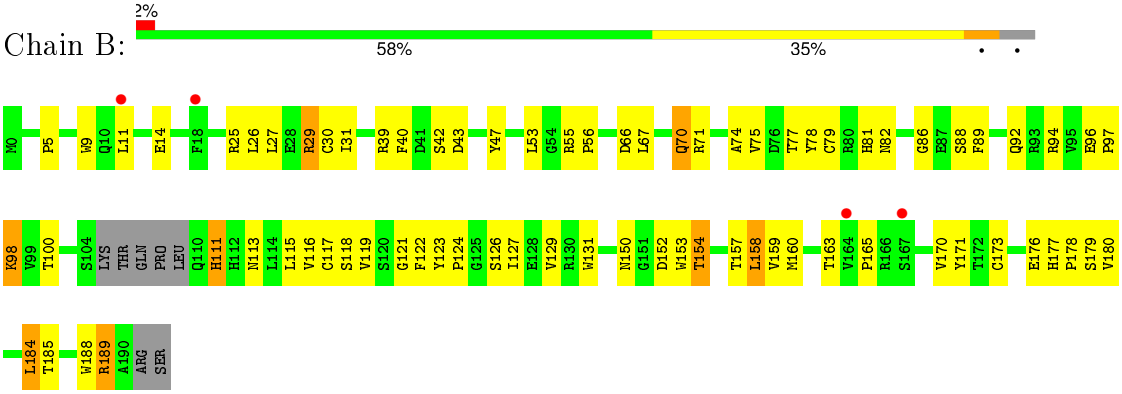
• Molecule 1: HLA class II histocompatibility antigen, DR alpha chain

Chain D:



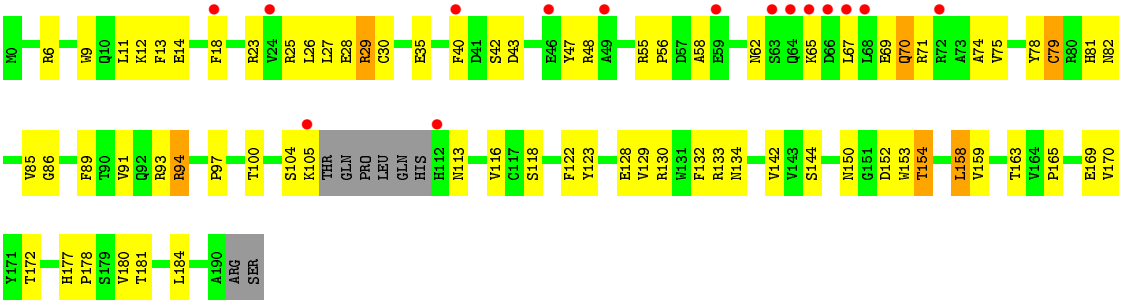
• Molecule 2: HLA class II histocompatibility antigen, DRB1-1 beta chain

Chain B:



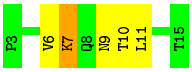
• Molecule 2: HLA class II histocompatibility antigen, DRB1-1 beta chain

Chain E:



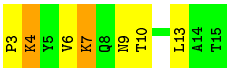
• Molecule 3: Hemagglutinin peptide

Chain C:



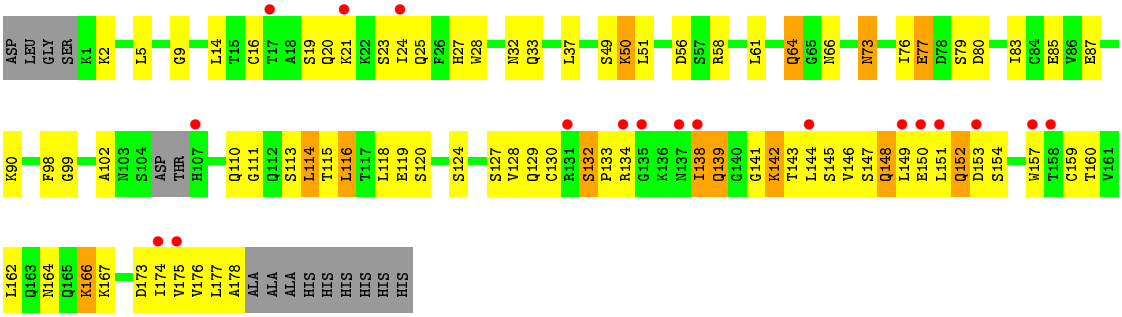
• Molecule 3: Hemagglutinin peptide

Chain F:



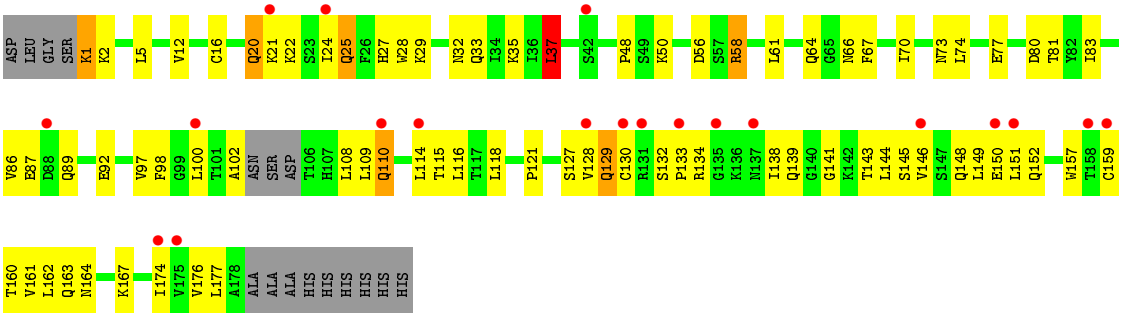
• Molecule 4: T-cell surface glycoprotein CD4

Chain G:



• Molecule 4: T-cell surface glycoprotein CD4

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	67.26Å 137.29Å 88.29Å 90.00° 106.64° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 46.98 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.40) 99.2 (46.98-2.39)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.53 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.251 , 0.286 0.250 , 0.283	Depositor DCC
R_{free} test set	3011 reflections (5.03%)	DCC
Wilson B-factor (Å^2)	37.7	Xtriage
Anisotropy	0.733	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 60314 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8924	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.56% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.46	0/1508	0.69	0/2056
1	D	0.44	0/1516	0.67	0/2066
2	B	0.42	0/1543	0.66	0/2092
2	E	0.41	0/1541	0.65	0/2091
3	C	0.43	0/106	0.69	0/141
3	F	0.38	0/104	0.62	0/138
4	G	0.35	0/1374	0.63	0/1854
4	H	0.33	0/1348	0.60	1/1816 (0.1%)
All	All	0.41	0/9040	0.65	1/12254 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	37	LEU	CA-CB-CG	5.07	126.97	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1464	0	1404	37	0
1	D	1472	0	1409	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1507	0	1431	65	0
2	E	1505	0	1432	66	0
3	C	105	0	119	12	0
3	F	103	0	114	14	0
4	G	1354	0	1360	84	0
4	H	1328	0	1317	83	0
5	B	6	0	8	2	0
5	D	6	0	8	1	0
5	E	6	0	8	1	0
6	A	16	0	0	1	0
6	B	15	0	0	0	0
6	D	14	0	0	0	0
6	E	19	0	0	0	0
6	G	1	0	0	0	0
6	H	3	0	0	0	0
All	All	8924	0	8610	369	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 21.

All (369) 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)
4:H:102:ALA:HB2	4:H:116:LEU:HD23	1.43	1.00
4:H:1:LYS:HG3	4:H:2:LYS:H	1.24	0.99
3:F:4:LYS:HE2	3:F:4:LYS:H	1.27	0.99
1:A:96:PRO:HG3	2:B:100:THR:HG21	1.43	0.98
4:G:50:LYS:H	4:G:50:LYS:HD2	1.28	0.97
2:B:150:ASN:HD22	2:B:154:THR:HG22	1.30	0.94
1:D:96:PRO:HG3	2:E:100:THR:HG21	1.49	0.91
2:E:150:ASN:HD22	2:E:154:THR:HG22	1.36	0.90
2:E:82:ASN:HD21	3:F:6:VAL:H	1.17	0.85
2:B:113:ASN:HD22	2:B:165:PRO:HG3	1.41	0.84
1:A:87:PRO:HD2	1:A:170:LEU:HD11	1.62	0.82
4:G:64:GLN:HE21	4:G:64:GLN:N	1.78	0.81
3:C:7:LYS:HE2	3:C:9:ASN:HD22	1.43	0.81
2:E:11:LEU:HD21	3:F:10:THR:HG23	1.61	0.81
4:G:144:LEU:HD23	4:G:145:SER:N	1.96	0.80
2:B:39:ARG:HH12	5:B:960:GOL:H11	1.45	0.78
2:B:82:ASN:HD21	3:C:6:VAL:H	1.31	0.78
4:H:102:ALA:HB2	4:H:116:LEU:CD2	2.12	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:PRO:HB3	2:B:122:PHE:HB3	1.66	0.77
4:H:116:LEU:HD12	4:H:144:LEU:HD22	1.65	0.77
2:B:180:VAL:HG11	2:B:184:LEU:HD11	1.68	0.76
4:G:50:LYS:CD	4:G:50:LYS:H	1.99	0.75
4:G:102:ALA:HB1	4:G:114:LEU:HD21	1.67	0.75
4:H:1:LYS:CG	4:H:2:LYS:H	1.99	0.74
2:B:67:LEU:HD11	3:C:11:LEU:HD11	1.69	0.74
4:H:102:ALA:CB	4:H:116:LEU:HD23	2.18	0.74
2:E:152:ASP:OD2	2:E:154:THR:HB	1.88	0.74
2:B:11:LEU:CD2	3:C:10:THR:HG23	2.18	0.73
4:G:152:GLN:HA	4:G:152:GLN:HE21	1.53	0.72
4:H:130:CYS:HA	4:H:159:CYS:HA	1.69	0.72
2:B:27:LEU:HG	2:B:29:ARG:HD3	1.74	0.70
4:H:163:GLN:HE21	4:H:164:ASN:ND2	1.88	0.70
4:H:58:ARG:HB3	4:H:58:ARG:HH21	1.54	0.70
4:G:14:LEU:N	4:G:14:LEU:HD22	2.06	0.70
4:H:118:LEU:HD22	4:H:128:VAL:HG21	1.74	0.69
2:E:11:LEU:CD2	3:F:10:THR:HG23	2.23	0.69
4:G:50:LYS:N	4:G:50:LYS:HD2	2.06	0.69
4:H:5:LEU:HD12	4:H:98:PHE:HE2	1.55	0.69
4:G:114:LEU:HD22	4:G:115:THR:N	2.08	0.68
1:A:8:ILE:HB	1:A:25:ASP:OD1	1.94	0.68
2:B:152:ASP:OD2	2:B:154:THR:HB	1.94	0.67
4:H:128:VAL:HG22	4:H:161:VAL:HG22	1.75	0.67
4:H:110:GLN:HG3	4:H:150:GLU:CA	2.24	0.67
4:H:114:LEU:HD12	4:H:146:VAL:HG23	1.76	0.66
2:B:98:LYS:N	2:B:98:LYS:HD2	2.10	0.66
4:H:1:LYS:HG3	4:H:2:LYS:N	2.06	0.66
2:B:113:ASN:HD22	2:B:165:PRO:CG	2.08	0.65
1:D:39:LYS:NZ	1:D:39:LYS:HB3	2.12	0.65
4:G:157:TRP:CD1	4:G:174:ILE:HD13	2.32	0.65
2:B:11:LEU:HD22	3:C:10:THR:HG23	1.79	0.64
4:H:132:SER:C	4:H:134:ARG:H	2.01	0.64
4:H:114:LEU:HB3	4:H:146:VAL:HB	1.81	0.63
1:D:147:LYS:HE3	1:D:149:HIS:HE1	1.60	0.63
4:G:142:LYS:HD2	4:G:142:LYS:H	1.63	0.63
2:B:31:ILE:HD12	2:B:31:ILE:N	2.13	0.62
3:C:7:LYS:HE2	3:C:9:ASN:ND2	2.14	0.62
4:G:174:ILE:N	4:G:174:ILE:HD12	2.14	0.62
4:H:20:GLN:H	4:H:20:GLN:NE2	1.96	0.62
3:F:4:LYS:HE2	3:F:4:LYS:N	2.09	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:9:TRP:CH2	2:E:30:CYS:HB3	2.34	0.62
2:E:13:PHE:CE2	2:E:28:GLU:HG3	2.35	0.62
3:F:7:LYS:O	3:F:7:LYS:HD2	1.99	0.62
4:G:115:THR:HG22	4:G:145:SER:CB	2.30	0.61
1:A:99:LEU:HD21	1:A:180:PHE:CE2	2.35	0.61
2:B:129:VAL:HB	2:B:159:VAL:HG21	1.83	0.61
4:H:129:GLN:HB2	4:H:139:GLN:HG2	1.82	0.61
4:G:142:LYS:HG2	4:G:143:THR:H	1.66	0.60
4:G:77:GLU:H	4:G:77:GLU:CD	2.05	0.60
2:E:65:LYS:O	2:E:69:GLU:HG3	2.01	0.60
1:D:157:THR:HG23	1:D:158:GLU:OE2	2.01	0.60
2:E:180:VAL:HG11	2:E:184:LEU:HD21	1.84	0.59
2:E:97:PRO:HB3	2:E:122:PHE:HB3	1.85	0.59
1:A:66:ASP:OD1	3:C:10:THR:HG21	2.02	0.59
1:D:94:ASN:HB3	1:D:106:ILE:HD11	1.85	0.59
1:D:94:ASN:HD22	1:D:94:ASN:N	2.00	0.59
4:H:5:LEU:HD12	4:H:98:PHE:CE2	2.37	0.59
1:D:11:GLU:HG3	2:E:11:LEU:HB2	1.85	0.58
2:E:104:SER:OG	2:E:105:LYS:N	2.35	0.58
2:B:74:ALA:O	2:B:78:TYR:HB3	2.03	0.58
4:H:32:ASN:O	4:H:33:GLN:HB2	2.03	0.58
2:B:150:ASN:ND2	2:B:154:THR:HG22	2.10	0.58
4:G:21:LYS:HB3	4:G:64:GLN:HA	1.85	0.58
2:B:100:THR:CG2	2:B:118:SER:HB3	2.34	0.58
4:G:115:THR:HG22	4:G:145:SER:HB3	1.86	0.58
1:A:94:ASN:HB3	1:A:106:ILE:HD11	1.86	0.58
2:B:94:ARG:HH21	2:B:94:ARG:HG2	1.68	0.58
4:G:157:TRP:HD1	4:G:174:ILE:HD13	1.68	0.57
4:H:50:LYS:HE3	4:H:50:LYS:HA	1.87	0.57
4:H:21:LYS:HB3	4:H:64:GLN:HA	1.86	0.57
2:E:40:PHE:HB2	2:E:47:TYR:CE1	2.40	0.57
4:G:151:LEU:HD21	4:G:178:ALA:HB2	1.86	0.57
4:G:61:LEU:HB3	4:G:66:ASN:HB2	1.85	0.57
1:A:167:HIS:HB3	1:A:170:LEU:CD1	2.35	0.57
4:H:5:LEU:N	4:H:5:LEU:HD22	2.19	0.56
4:H:114:LEU:HD11	4:H:116:LEU:HG	1.85	0.56
4:H:129:GLN:O	4:H:129:GLN:HG3	2.05	0.56
4:H:100:LEU:HD21	4:H:116:LEU:HB3	1.87	0.56
4:H:118:LEU:HD22	4:H:128:VAL:CG2	2.35	0.56
4:H:24:ILE:HG12	4:H:67:PHE:CZ	2.40	0.56
4:G:130:CYS:HA	4:G:159:CYS:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:100:THR:CG2	2:E:118:SER:HB3	2.35	0.56
1:D:13:TYR:CE2	1:D:67:LYS:HG3	2.40	0.56
4:G:111:GLY:O	4:G:148:GLN:HA	2.06	0.56
4:G:162:LEU:HD13	4:G:167:LYS:HE3	1.88	0.55
1:A:96:PRO:HG3	2:B:100:THR:CG2	2.27	0.55
4:H:27:HIS:NE2	4:H:29:LYS:HE3	2.20	0.55
1:A:109:ILE:HD12	1:A:109:ILE:N	2.22	0.55
4:H:109:LEU:HD12	4:H:109:LEU:N	2.21	0.55
4:G:162:LEU:HD13	4:G:167:LYS:CE	2.37	0.55
2:E:86:GLY:HA2	2:E:89:PHE:CE2	2.42	0.55
2:E:134:ASN:ND2	2:E:170:VAL:H	2.05	0.55
2:E:85:VAL:HG13	3:F:3:PRO:HB2	1.88	0.55
1:D:39:LYS:HZ2	1:D:39:LYS:HB3	1.68	0.54
1:D:30:GLU:OE1	1:D:33:HIS:HD2	1.90	0.54
1:A:93:THR:HG21	1:A:97:VAL:CG1	2.37	0.54
4:G:64:GLN:NE2	4:G:64:GLN:N	2.52	0.54
4:H:37:LEU:HD23	4:H:37:LEU:C	2.28	0.54
5:D:962:GOL:H11	2:E:152:ASP:HB3	1.90	0.54
4:G:133:PRO:HG2	4:G:153:ASP:O	2.07	0.54
2:B:127:ILE:HG13	2:B:177:HIS:HB2	1.89	0.54
4:H:24:ILE:HD11	4:H:86:VAL:CG2	2.37	0.54
1:A:121:TRP:O	1:A:127:PRO:HA	2.07	0.54
4:G:114:LEU:HD11	4:G:116:LEU:HD13	1.90	0.54
4:G:138:ILE:HD13	4:G:139:GLN:H	1.72	0.54
1:D:94:ASN:H	1:D:94:ASN:HD22	1.56	0.54
1:A:147:LYS:NZ	1:A:149:HIS:CE1	2.76	0.54
3:F:4:LYS:CE	3:F:4:LYS:H	2.12	0.53
4:G:64:GLN:H	4:G:64:GLN:NE2	2.06	0.53
4:G:173:ASP:C	4:G:174:ILE:HD12	2.29	0.53
4:H:141:GLY:C	4:H:143:THR:H	2.10	0.53
4:G:64:GLN:H	4:G:64:GLN:HE21	1.56	0.53
4:G:110:GLN:HE21	4:G:178:ALA:HA	1.73	0.53
2:E:134:ASN:HD21	2:E:169:GLU:HA	1.73	0.53
4:G:5:LEU:HD12	4:G:98:PHE:HE2	1.73	0.53
4:G:87:GLU:HG3	4:G:87:GLU:O	2.09	0.53
1:D:121:TRP:O	1:D:127:PRO:HA	2.09	0.53
4:H:160:THR:HG21	4:H:167:LYS:HD3	1.91	0.53
4:H:114:LEU:HD22	4:H:115:THR:N	2.24	0.53
3:F:7:LYS:NZ	3:F:9:ASN:OD1	2.39	0.52
4:H:129:GLN:CB	4:H:139:GLN:HG2	2.40	0.52
1:D:89:VAL:HG21	1:D:165:VAL:HG21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:VAL:O	1:A:176:LYS:HE3	2.08	0.52
4:G:162:LEU:HD12	4:G:166:LYS:O	2.09	0.52
2:E:163:THR:O	2:E:165:PRO:HD3	2.09	0.52
2:B:9:TRP:CH2	2:B:30:CYS:HB3	2.44	0.52
4:G:128:VAL:HG12	4:G:129:GLN:N	2.25	0.52
4:G:142:LYS:HG2	4:G:143:THR:N	2.24	0.52
2:E:94:ARG:HG3	2:E:94:ARG:NH1	2.24	0.52
2:B:40:PHE:HB2	2:B:47:TYR:CE1	2.45	0.52
2:B:88:SER:HA	2:B:92:GLN:NE2	2.25	0.52
2:E:142:VAL:O	4:H:48:PRO:HD3	2.10	0.51
4:G:16:CYS:HB2	4:G:28:TRP:CZ2	2.45	0.51
4:G:83:ILE:N	4:G:83:ILE:HD12	2.25	0.51
4:H:138:ILE:HD12	4:H:146:VAL:HG22	1.92	0.51
1:D:58:GLY:HA3	3:F:7:LYS:HE2	1.91	0.51
4:H:61:LEU:HB3	4:H:66:ASN:HB2	1.92	0.51
4:G:142:LYS:HD2	4:G:142:LYS:N	2.26	0.51
4:G:5:LEU:HD22	4:G:5:LEU:N	2.25	0.51
4:G:37:LEU:HD12	4:G:37:LEU:C	2.31	0.51
4:H:73:ASN:HD22	4:H:73:ASN:N	2.08	0.51
4:H:127:SER:HB3	4:H:162:LEU:HB3	1.91	0.51
4:H:114:LEU:HD22	4:H:115:THR:H	1.75	0.51
4:G:118:LEU:HD22	4:G:128:VAL:CG2	2.40	0.51
2:E:18:PHE:HB2	2:E:23:ARG:HB3	1.93	0.51
2:E:177:HIS:CD2	2:E:178:PRO:HD2	2.46	0.51
4:G:134:ARG:HD2	4:G:152:GLN:CB	2.41	0.50
4:G:138:ILE:HD13	4:G:139:GLN:N	2.25	0.50
4:H:12:VAL:HG12	4:H:74:LEU:HD11	1.94	0.50
4:G:138:ILE:CG2	4:G:144:LEU:HD21	2.41	0.50
4:G:32:ASN:O	4:G:33:GLN:HB2	2.11	0.50
2:B:116:VAL:HG22	2:B:160:MET:HG2	1.94	0.50
2:B:118:SER:HA	2:B:158:LEU:HD12	1.93	0.50
2:B:94:ARG:HG2	2:B:94:ARG:NH2	2.27	0.50
4:G:152:GLN:HA	4:G:152:GLN:NE2	2.23	0.50
4:G:110:GLN:HB2	4:G:177:LEU:O	2.11	0.49
1:D:92:LEU:N	1:D:92:LEU:HD23	2.27	0.49
4:H:58:ARG:NH2	4:H:58:ARG:HB3	2.26	0.49
1:D:143:HIS:HD2	2:E:12:LYS:NZ	2.10	0.49
4:H:1:LYS:NZ	4:H:1:LYS:HB3	2.27	0.49
2:B:14:GLU:OE1	2:B:29:ARG:NH1	2.45	0.49
2:B:115:LEU:HD11	2:B:188:TRP:CE3	2.47	0.49
2:E:13:PHE:CD2	2:E:28:GLU:HG3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:55:ARG:HB2	2:B:56:PRO:HD3	1.94	0.49
4:G:79:SER:O	4:G:80:ASP:HB2	2.13	0.49
4:H:114:LEU:HD12	4:H:146:VAL:CG2	2.42	0.49
2:E:28:GLU:HB3	2:E:40:PHE:HB3	1.95	0.49
4:G:99:GLY:O	4:G:118:LEU:HD12	2.12	0.49
2:B:115:LEU:HD21	2:B:188:TRP:CD2	2.48	0.49
2:B:173:CYS:O	2:B:185:THR:HA	2.13	0.49
2:E:93:ARG:O	2:E:94:ARG:NH1	2.46	0.49
1:D:9:GLN:HG3	1:D:24:PHE:CE1	2.47	0.49
4:G:175:VAL:HG13	4:G:175:VAL:O	2.12	0.48
2:E:26:LEU:HB3	2:E:42:SER:HB3	1.95	0.48
2:E:81:HIS:HD2	3:F:6:VAL:HG22	1.78	0.48
2:E:74:ALA:O	2:E:78:TYR:HB3	2.13	0.48
1:D:12:PHE:C	1:D:12:PHE:CD1	2.86	0.48
4:G:9:GLY:HA2	4:G:73:ASN:HD22	1.78	0.48
1:A:141:GLU:HG2	6:A:193:HOH:O	2.12	0.48
1:D:77:SER:O	1:D:78:ASN:HB2	2.13	0.48
2:B:100:THR:HG23	2:B:118:SER:HB3	1.95	0.48
3:F:6:VAL:O	3:F:6:VAL:HG23	2.14	0.48
2:E:116:VAL:HG13	2:E:158:LEU:HD21	1.96	0.48
1:A:77:SER:O	1:A:78:ASN:HB2	2.13	0.48
4:G:21:LYS:HD3	4:G:64:GLN:HB2	1.95	0.48
4:G:14:LEU:CD2	4:G:14:LEU:N	2.77	0.48
2:E:129:VAL:HB	2:E:159:VAL:HG21	1.96	0.48
4:H:110:GLN:HG3	4:H:150:GLU:N	2.29	0.48
2:E:128:GLU:OE1	2:E:130:ARG:NH1	2.42	0.48
4:H:114:LEU:O	4:H:145:SER:HA	2.14	0.47
3:C:7:LYS:HD3	3:C:7:LYS:C	2.35	0.47
2:E:40:PHE:HB2	2:E:47:TYR:CD1	2.49	0.47
2:B:67:LEU:HD21	3:C:11:LEU:HD13	1.96	0.47
4:G:174:ILE:N	4:G:174:ILE:CD1	2.76	0.47
4:G:114:LEU:HB2	4:G:149:LEU:HD11	1.95	0.47
1:D:147:LYS:HE3	1:D:149:HIS:CE1	2.47	0.47
4:H:151:LEU:H	4:H:176:VAL:HG11	1.79	0.47
2:E:25:ARG:HG2	2:E:25:ARG:HH11	1.78	0.47
2:E:94:ARG:HG3	2:E:94:ARG:HH11	1.79	0.47
2:B:70:GLN:HE22	2:B:71:ARG:HD2	1.79	0.47
2:B:177:HIS:CD2	2:B:178:PRO:HD2	2.49	0.47
1:D:11:GLU:HA	1:D:21:GLU:O	2.15	0.47
4:G:164:ASN:O	4:G:166:LYS:HE3	2.15	0.47
2:E:23:ARG:NH1	2:E:23:ARG:HG2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:116:VAL:CG1	2:E:158:LEU:HD21	2.44	0.47
4:G:49:SER:C	4:G:51:LEU:H	2.18	0.47
4:G:128:VAL:CG1	4:G:129:GLN:N	2.77	0.47
2:B:25:ARG:HD2	2:B:43:ASP:OD2	2.15	0.47
2:E:150:ASN:HD22	2:E:154:THR:CG2	2.17	0.46
4:G:76:ILE:HG13	4:G:119:GLU:HG2	1.97	0.46
4:H:87:GLU:O	4:H:87:GLU:HG3	2.15	0.46
4:H:16:CYS:HB2	4:H:28:TRP:CZ2	2.50	0.46
4:G:134:ARG:HD2	4:G:152:GLN:HB3	1.98	0.46
4:H:83:ILE:HG13	4:H:92:GLU:HG2	1.96	0.46
1:A:26:PHE:HB2	1:A:31:ILE:HD11	1.97	0.46
2:E:113:ASN:HD22	2:E:165:PRO:HG3	1.81	0.46
2:E:23:ARG:HG2	2:E:23:ARG:HH11	1.81	0.46
1:A:76:ARG:NH1	2:B:53:LEU:O	2.43	0.46
1:D:95:SER:HB2	1:D:96:PRO:HD2	1.98	0.46
2:E:100:THR:HG23	2:E:118:SER:HB3	1.98	0.46
4:H:97:VAL:O	4:H:121:PRO:HD3	2.15	0.46
4:H:132:SER:O	4:H:134:ARG:N	2.47	0.46
4:H:20:GLN:H	4:H:20:GLN:CD	2.18	0.46
1:A:70:LEU:HD13	2:B:9:TRP:HB2	1.97	0.46
2:B:117:CYS:HB2	2:B:131:TRP:CZ2	2.51	0.46
4:G:127:SER:HA	4:G:141:GLY:HA2	1.97	0.46
2:E:40:PHE:CZ	2:E:71:ARG:HB3	2.51	0.46
2:B:98:LYS:CD	2:B:98:LYS:N	2.77	0.46
2:E:152:ASP:O	2:E:153:TRP:HB2	2.15	0.45
4:G:139:GLN:HB2	4:G:139:GLN:HE21	1.57	0.45
1:A:73:MET:HG3	2:B:9:TRP:CZ3	2.51	0.45
4:H:5:LEU:N	4:H:5:LEU:CD2	2.79	0.45
1:D:34:VAL:HG21	1:D:59:ALA:CB	2.46	0.45
1:D:93:THR:HG21	1:D:97:VAL:CG1	2.47	0.45
4:H:150:GLU:C	4:H:152:GLN:H	2.20	0.45
1:D:142:ASP:O	1:D:143:HIS:HB2	2.16	0.45
1:D:164:ARG:HG3	1:D:175:LEU:HD11	1.98	0.45
2:B:27:LEU:CG	2:B:29:ARG:HD3	2.45	0.45
1:A:38:LYS:O	1:A:39:LYS:C	2.55	0.45
1:D:5:HIS:HE1	2:E:91:VAL:HG13	1.81	0.45
4:H:160:THR:CG2	4:H:167:LYS:HD3	2.47	0.45
4:G:114:LEU:HD22	4:G:115:THR:H	1.79	0.45
2:E:14:GLU:OE1	2:E:29:ARG:HD3	2.17	0.45
2:B:123:TYR:CD1	2:B:124:PRO:HA	2.52	0.44
2:B:113:ASN:ND2	2:B:165:PRO:HG3	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:58:ARG:HD2	4:H:70:ILE:HD11	1.99	0.44
2:B:111:HIS:O	2:B:165:PRO:HD2	2.18	0.44
2:B:26:LEU:HB3	2:B:42:SER:HB3	1.99	0.44
1:A:81:PRO:HB3	2:B:5:PRO:HB2	1.99	0.44
2:B:82:ASN:HD21	3:C:6:VAL:HG12	1.83	0.44
4:H:12:VAL:CG1	4:H:74:LEU:HD11	2.47	0.44
1:A:12:PHE:C	1:A:12:PHE:CD1	2.90	0.44
4:H:22:LYS:NZ	4:H:22:LYS:HB2	2.33	0.44
2:E:40:PHE:C	2:E:40:PHE:CD1	2.90	0.44
2:B:74:ALA:HA	2:B:77:THR:OG1	2.17	0.44
1:A:29:ASP:HB3	2:B:153:TRP:CE2	2.52	0.44
2:B:97:PRO:CB	2:B:122:PHE:HB3	2.41	0.44
4:G:152:GLN:CA	4:G:152:GLN:HE21	2.20	0.44
1:D:91:VAL:HA	1:D:106:ILE:O	2.17	0.44
1:D:50:ARG:C	1:D:51:PHE:HD2	2.20	0.44
2:B:86:GLY:HA2	2:B:89:PHE:CE2	2.53	0.43
4:H:21:LYS:HG2	4:H:64:GLN:O	2.18	0.43
4:G:85:GLU:OE1	4:G:90:LYS:NZ	2.51	0.43
4:H:25:GLN:HE21	4:H:25:GLN:HA	1.83	0.43
1:A:147:LYS:HZ2	1:A:149:HIS:CE1	2.35	0.43
3:C:7:LYS:CD	3:C:7:LYS:C	2.87	0.43
2:E:93:ARG:HD3	2:E:123:TYR:CD1	2.53	0.43
1:D:168:TRP:CH2	2:E:6:ARG:CZ	3.01	0.43
2:B:180:VAL:HG21	2:B:184:LEU:HD13	1.99	0.43
2:B:170:VAL:HG22	2:B:189:ARG:HD3	2.00	0.43
4:H:108:LEU:C	4:H:109:LEU:HD12	2.39	0.43
4:H:114:LEU:C	4:H:114:LEU:HD13	2.39	0.43
4:H:132:SER:C	4:H:134:ARG:N	2.69	0.43
4:G:115:THR:HG22	4:G:145:SER:HB2	1.99	0.43
4:G:132:SER:HA	4:G:157:TRP:CD2	2.53	0.43
4:G:111:GLY:O	4:G:148:GLN:CG	2.67	0.43
4:G:146:VAL:HG13	4:G:146:VAL:O	2.19	0.43
4:G:113:SER:OG	4:G:147:SER:HA	2.19	0.43
1:A:110:ASP:OD2	1:A:146:ARG:HG2	2.19	0.42
1:D:55:GLU:OE2	1:D:57:GLN:HB2	2.19	0.42
4:H:29:LYS:HE2	4:H:35:LYS:HG2	2.00	0.42
1:D:92:LEU:H	1:D:92:LEU:HD23	1.85	0.42
4:H:25:GLN:HE21	4:H:25:GLN:CA	2.32	0.42
2:E:132:PHE:HB2	2:E:172:THR:HB	2.00	0.42
1:A:11:GLU:OE1	1:A:66:ASP:OD2	2.37	0.42
4:G:160:THR:CG2	4:G:167:LYS:HD2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:116:VAL:HG13	2:E:158:LEU:CD2	2.49	0.42
2:B:121:GLY:HA2	2:B:154:THR:HG23	2.01	0.42
4:G:142:LYS:NZ	4:G:142:LYS:HB3	2.35	0.42
2:B:81:HIS:HD2	3:C:6:VAL:HG12	1.85	0.42
4:G:175:VAL:HG22	4:G:175:VAL:O	2.18	0.42
1:D:129:THR:O	1:D:132:VAL:HG22	2.19	0.42
2:B:66:ASP:OD2	2:B:66:ASP:N	2.51	0.42
1:A:28:GLY:O	1:A:146:ARG:NH2	2.51	0.42
2:E:55:ARG:HB2	2:E:56:PRO:HD3	2.01	0.42
4:H:102:ALA:HB1	4:H:115:THR:O	2.20	0.42
2:B:66:ASP:CG	2:B:67:LEU:H	2.23	0.42
4:H:80:ASP:CG	4:H:81:THR:N	2.72	0.42
1:A:101:GLU:HA	1:A:102:PRO:HD3	1.89	0.42
2:E:18:PHE:N	2:E:18:PHE:CD1	2.88	0.42
2:B:163:THR:HG21	2:B:171:TYR:CE1	2.55	0.42
2:E:48:ARG:HG3	2:E:48:ARG:HH21	1.85	0.42
4:G:23:SER:O	4:G:24:ILE:HG23	2.19	0.42
4:H:176:VAL:O	4:H:177:LEU:HD23	2.20	0.41
1:D:29:ASP:HB3	2:E:153:TRP:CE2	2.54	0.41
1:A:147:LYS:HZ3	1:A:149:HIS:CE1	2.38	0.41
1:D:93:THR:HB	1:D:103:ASN:OD1	2.20	0.41
2:E:75:VAL:O	2:E:79:CYS:HB2	2.21	0.41
4:G:114:LEU:CB	4:G:149:LEU:HD11	2.50	0.41
4:G:150:GLU:O	4:G:153:ASP:HB2	2.21	0.41
4:H:157:TRP:CD1	4:H:174:ILE:HG12	2.55	0.41
1:A:123:ARG:HG3	1:A:161:TYR:CE2	2.55	0.41
2:E:58:ALA:O	2:E:62:ASN:ND2	2.54	0.41
4:G:132:SER:HA	4:G:157:TRP:CE3	2.56	0.41
2:E:70:GLN:NE2	2:E:70:GLN:C	2.74	0.41
4:H:114:LEU:CD1	4:H:116:LEU:HG	2.50	0.41
4:G:133:PRO:HD3	4:G:157:TRP:CE2	2.55	0.41
4:G:111:GLY:O	4:G:148:GLN:HG3	2.21	0.41
2:E:93:ARG:HH11	2:E:93:ARG:HG3	1.85	0.41
2:B:119:VAL:HB	2:B:157:THR:HG22	2.02	0.41
4:G:154:SER:OG	4:G:176:VAL:HB	2.20	0.41
4:H:1:LYS:CG	4:H:2:LYS:N	2.70	0.41
1:D:37:ALA:C	1:D:39:LYS:H	2.24	0.41
1:D:51:PHE:O	3:F:3:PRO:HD2	2.21	0.41
4:H:141:GLY:C	4:H:143:THR:N	2.73	0.41
1:D:5:HIS:CE1	2:E:91:VAL:HG13	2.56	0.41
1:A:98:GLU:HA	1:A:98:GLU:OE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:VAL:HG12	1:A:129:THR:N	2.35	0.41
1:D:73:MET:HG2	3:F:13:LEU:CD1	2.50	0.41
2:B:39:ARG:HH22	5:B:960:GOL:H12	1.85	0.41
2:E:113:ASN:HD22	2:E:165:PRO:CG	2.34	0.41
2:B:96:GLU:HA	2:B:179:SER:OG	2.20	0.41
2:E:67:LEU:C	2:E:67:LEU:HD23	2.42	0.41
4:H:77:GLU:OE1	4:H:77:GLU:N	2.48	0.41
4:G:120:SER:HB3	4:G:124:SER:OG	2.21	0.41
2:B:26:LEU:HD12	2:B:27:LEU:H	1.86	0.41
4:H:20:GLN:N	4:H:20:GLN:NE2	2.67	0.41
2:E:27:LEU:HG	2:E:29:ARG:HD2	2.03	0.41
1:A:98:GLU:O	1:A:101:GLU:HB3	2.21	0.41
1:A:11:GLU:HA	1:A:21:GLU:O	2.21	0.40
4:H:110:GLN:HG3	4:H:150:GLU:H	1.86	0.40
1:A:147:LYS:NZ	1:A:149:HIS:HE1	2.18	0.40
1:A:132:VAL:HG12	1:A:151:LEU:HD13	2.03	0.40
4:G:19:SER:N	4:G:87:GLU:OE1	2.45	0.40
4:H:73:ASN:N	4:H:73:ASN:ND2	2.68	0.40
4:H:87:GLU:OE1	4:H:89:GLN:NE2	2.55	0.40
4:H:80:ASP:CG	4:H:81:THR:H	2.23	0.40
2:E:144:SER:OG	5:E:961:GOL:H11	2.21	0.40
1:A:32:PHE:C	1:A:32:PHE:CD1	2.95	0.40
4:H:138:ILE:CD1	4:H:146:VAL:HG22	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	176/182 (97%)	166 (94%)	10 (6%)	0	100 100
1	D	178/182 (98%)	166 (93%)	7 (4%)	5 (3%)	6 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	182/193 (94%)	168 (92%)	12 (7%)	2 (1%)	17 25
2	E	181/193 (94%)	164 (91%)	16 (9%)	1 (1%)	30 43
3	C	11/13 (85%)	11 (100%)	0	0	100 100
3	F	11/13 (85%)	11 (100%)	0	0	100 100
4	G	172/191 (90%)	153 (89%)	17 (10%)	2 (1%)	16 23
4	H	171/191 (90%)	148 (86%)	19 (11%)	4 (2%)	8 8
All	All	1082/1158 (93%)	987 (91%)	81 (8%)	14 (1%)	15 21

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	2	LYS
4	H	148	GLN
4	H	149	LEU
4	G	148	GLN
2	B	79	CYS
2	B	111	HIS
1	D	39	LYS
4	H	110	GLN
4	G	132	SER
1	D	46	GLU
2	E	79	CYS
1	D	37	ALA
1	D	136	VAL
4	H	133	PRO

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	163/166 (98%)	155 (95%)	8 (5%)	31 48
1	D	163/166 (98%)	157 (96%)	6 (4%)	41 62
2	B	164/174 (94%)	154 (94%)	10 (6%)	23 36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	E	164/174 (94%)	155 (94%)	9 (6%)	27 42
3	C	12/12 (100%)	11 (92%)	1 (8%)	14 21
3	F	11/12 (92%)	9 (82%)	2 (18%)	2 2
4	G	152/170 (89%)	135 (89%)	17 (11%)	7 10
4	H	147/170 (86%)	140 (95%)	7 (5%)	31 49
All	All	976/1044 (94%)	916 (94%)	60 (6%)	23 36

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ASP
1	A	90	THR
1	A	92	LEU
1	A	94	ASN
1	A	111	LYS
1	A	122	LEU
1	A	130	THR
1	A	156	SER
2	B	29	ARG
2	B	70	GLN
2	B	75	VAL
2	B	98	LYS
2	B	126	SER
2	B	154	THR
2	B	158	LEU
2	B	176	GLU
2	B	184	LEU
2	B	189	ARG
3	C	7	LYS
4	G	2	LYS
4	G	20	GLN
4	G	25	GLN
4	G	27	HIS
4	G	50	LYS
4	G	56	ASP
4	G	58	ARG
4	G	64	GLN
4	G	73	ASN
4	G	77	GLU
4	G	114	LEU

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Mol	Chain	Res	Type
4	G	116	LEU
4	G	138	ILE
4	G	139	GLN
4	G	142	LYS
4	G	152	GLN
4	G	166	LYS
1	D	39	LYS
1	D	94	ASN
1	D	117	VAL
1	D	141	GLU
1	D	157	THR
1	D	162	ASP
2	E	29	ARG
2	E	35	GLU
2	E	43	ASP
2	E	70	GLN
2	E	94	ARG
2	E	133	ARG
2	E	154	THR
2	E	158	LEU
2	E	181	THR
3	F	4	LYS
3	F	7	LYS
4	H	1	LYS
4	H	20	GLN
4	H	25	GLN
4	H	37	LEU
4	H	56	ASP
4	H	58	ARG
4	H	129	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	78	ASN
1	A	94	ASN
1	A	143	HIS
1	A	149	HIS
1	A	177	GLN
2	B	70	GLN
2	B	82	ASN

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Mol	Chain	Res	Type
2	B	92	GLN
2	B	113	ASN
2	B	150	ASN
3	C	8	GLN
3	C	9	ASN
4	G	25	GLN
4	G	52	ASN
4	G	64	GLN
4	G	66	ASN
4	G	73	ASN
4	G	89	GLN
4	G	110	GLN
4	G	112	GLN
4	G	129	GLN
4	G	139	GLN
4	G	148	GLN
4	G	152	GLN
4	G	165	GLN
1	D	5	HIS
1	D	33	HIS
1	D	94	ASN
1	D	143	HIS
1	D	149	HIS
2	E	62	ASN
2	E	70	GLN
2	E	82	ASN
2	E	113	ASN
2	E	134	ASN
2	E	149	GLN
2	E	150	ASN
2	E	156	GLN
4	H	20	GLN
4	H	25	GLN
4	H	33	GLN
4	H	52	ASN
4	H	73	ASN
4	H	89	GLN
4	H	110	GLN
4	H	164	ASN

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

3 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	$\#\|Z\| > 2$
5	GOL	B	960	-	5,5,5	0.17	0	5,5,5	0.19	0
5	GOL	D	962	-	5,5,5	0.25	0	5,5,5	0.28	0
5	GOL	E	961	-	5,5,5	0.43	0	5,5,5	0.24	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
5	GOL	B	960	-	-	0/4/4/4	0/0/0/0
5	GOL	D	962	-	-	0/4/4/4	0/0/0/0
5	GOL	E	961	-	-	0/4/4/4	0/0/0/0

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.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	960	GOL	2	0
5	D	962	GOL	1	0
5	E	961	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	178/182 (97%)	0.33	2 (1%) 82 82	19, 32, 54, 62	0
1	D	180/182 (98%)	0.41	4 (2%) 65 64	24, 37, 63, 74	0
2	B	186/193 (96%)	0.29	4 (2%) 65 64	21, 38, 59, 70	0
2	E	185/193 (95%)	0.54	15 (8%) 15 14	24, 42, 71, 79	0
3	C	13/13 (100%)	0.29	0 100 100	37, 42, 48, 50	0
3	F	13/13 (100%)	0.41	0 100 100	48, 55, 62, 63	0
4	G	176/191 (92%)	0.75	18 (10%) 9 8	30, 57, 81, 88	0
4	H	175/191 (91%)	0.79	20 (11%) 7 7	30, 61, 81, 85	0
All	All	1106/1158 (95%)	0.51	63 (5%) 27 27	19, 43, 75, 88	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	150	GLU	7.4
4	G	150	GLU	4.1
4	G	138	ILE	3.8
2	E	18	PHE	3.8
4	G	137	ASN	3.8
4	H	137	ASN	3.7
4	H	88	ASP	3.7
4	H	130	CYS	3.6
4	G	157	TRP	3.5
2	E	112	HIS	3.5
2	E	63	SER	3.3
1	D	3	GLU	3.3
4	H	110	GLN	3.2
4	H	128	VAL	3.2
4	G	174	ILE	3.1
4	G	158	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	39	LYS	3.1
2	B	18	PHE	2.9
4	G	21	LYS	2.9
4	G	149	LEU	2.9
2	E	49	ALA	2.8
2	E	72	ARG	2.7
4	G	131	ARG	2.7
4	G	175	VAL	2.7
2	B	167	SER	2.7
2	E	66	ASP	2.7
2	E	67	LEU	2.7
4	G	153	ASP	2.6
4	H	174	ILE	2.6
4	H	24	ILE	2.6
4	G	135	GLY	2.5
4	H	21	LYS	2.5
1	A	180	PHE	2.5
4	G	107	HIS	2.5
2	E	68	LEU	2.4
4	H	151	LEU	2.4
4	H	133	PRO	2.4
4	H	175	VAL	2.4
4	G	144	LEU	2.3
4	G	151	LEU	2.3
4	H	114	LEU	2.3
2	E	46	GLU	2.3
2	E	59	GLU	2.2
2	E	65	LYS	2.2
4	G	134	ARG	2.2
4	H	146	VAL	2.2
2	B	11	LEU	2.2
4	G	24	ILE	2.2
2	B	164	VAL	2.2
1	D	178	TRP	2.2
1	A	158	GLU	2.1
2	E	64	GLN	2.1
2	E	40	PHE	2.1
4	G	17	THR	2.1
4	H	158	THR	2.1
1	D	158	GLU	2.1
4	H	100	LEU	2.1
4	H	135	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
4	H	131	ARG	2.0
2	E	24	VAL	2.0
4	H	42	SER	2.0
4	H	159	CYS	2.0
2	E	105	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	GOL	E	961	6/6	0.80	0.25	5.44	51,52,55,56	0
5	GOL	D	962	6/6	0.90	0.22	1.66	41,44,46,47	0
5	GOL	B	960	6/6	0.87	0.20	-	63,63,64,66	0

6.5 Other polymers (i)

There are no such residues in this entry.